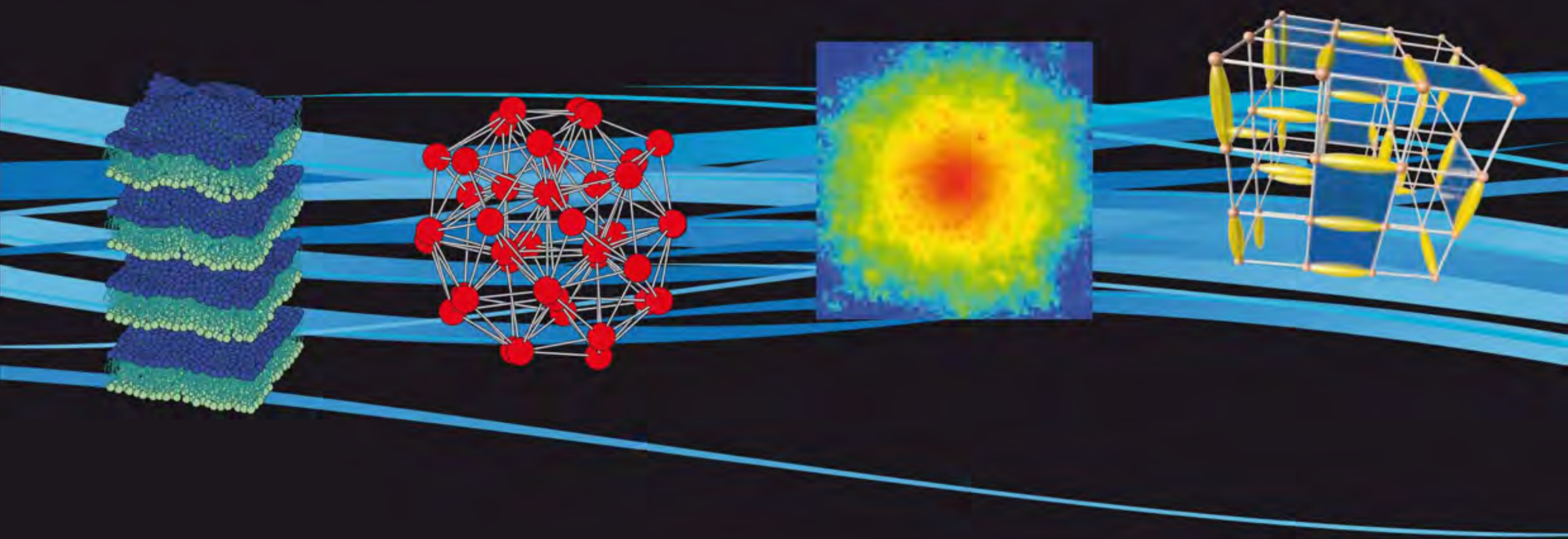
Université
de Toulouse

Laboratoire de Physique Théorique



UMR 5152 CNRS & Université Toulouse III

Scientific Report

Bilan Scientifique

2005-2009

Contents

General presentation of the LPT (summary in English)

This chapter introduces the LABORATOIRE DE PHYSIQUE THÉORIQUE (LPT) **and summarizes the following chapters concerning the** LPT **staff, the financial resources of the** LPT**, our computing infrastructure, our contributions to the diffusion of scientific knowledge, and of course, our research activity and scientific production.**

A brief history of the LPT

In 1991, Jean BELLISSARD moved to Toulouse (from the CPT in Marseille) along with a few freshly recruited CNRS scientists to found a small **Groupe de Physique Théorique (GPT)** with the support of the **CNRS** and the **Université Paul Sabatier (UPS; Université de Toulouse III)**. This group was hosted by the LABORATOIRE DE PHYSIQUE QUANTIQUE [1] (now LCPQ). Roughly at the same time, the INSTITUT DE RECHERCHE SUR LES SYSTÈMES ATOMIQUES ET MOLÉCULAIRES COMPLEXES (IRSAMC) [2] was created, regrouping three laboratories including LCPQ. IRSAMC was soon recognized by the CNRS and UPS as the FÉDÉRATION DE RECHERCHE DE PHYSIQUE ET CHIMIE FONDAMENTALES (FR 2568), although the institute kept its IRSAMC name for all practical purposes.

Meanwhile, the GPT eventually grew and obtained undeniable scientific recognition and visibility to be finally recognized in 2003 [3] as an **Unité Mixte de Recherche of CNRS and UPS (UMR 5152)**. Didier POILBLANC was the first director of the LPT between 2003 and 2006, and was succeeded by Clément SIRE for the 2007-2010 period (they were both members of the GPT from its inception).

Since 2003, the LPT is one of the four laboratories constituting the Fédération IRSAMC (FR 2568), along with the LABORATOIRE COLLISIONS AGRÉGATS RÉACTIVITÉ – LCAR (UMR 5589; experimental atomic and cluster physics), the LABORATOIRE DE CHIMIE ET PHYSIQUE QUANTIQUES – LCPQ (UMR 5626; theoretical chemistry), and the LABORATOIRE DE PHYSIQUE ET CHIMIE DES NANO-OBJETS – LPCNO (UMR 5215; nanophysics and nanochemistry).

---

1. The LPT will always be grateful to this laboratory – headed at the time by the late Jean-Pierre DAUDEY and by Jean-Paul MALRIEU – for its warm hospitality.
2. Throughout this report, all text in light colors is clickable and links to web sites, *pdf* documents (articles, preprints...), references, tables, figures, chapters, and sections.
3. For personal reasons, J. BELLISSARD left Toulouse for Georgia Tech in 2002, before the creation of the LPT. It is however clear that the LPT is extremely grateful for his dedication to the original GPT, directly at the origin of the LPT.

NAME & First name	Position	Comments	CNRS
ALET Fabien	CR2 - 10/2005	—	06
CAPPONI Sylvain	PR2 - 10/2000	HDR; PEDR; ANR; Promoted 10/2008	06
CHAVANIS Pierre-Henri	CR1 - 10/1998	Promoted 10/2001	02
BRAUN Daniel	PR2 - 10/2004	HDR; PEDR; CNRS	02
DEAN David	PR1 - 10/1998	HDR; PEDR; IUF 2007; CNRS; Promoted 10/2006	02/05
DESTAINVILLE Nicolas	MCF - 10/1998	HDR; PEDR; CNRS	02/05
FRAHM Klaus	PR2 - 10/1997	HDR; CNRS; Promoted 02/2000	02
GEORGEOT Bertrand	CR1 - 10/1996	Promoted 10/2000; HDR expected in 2009-2010	02
GIRAUD Olivier	CR2 - 10/2005	—	02
MAMBRINI Matthieu	CR1 - 10/2002	Promoted 10/2006	06
MANGHI Manoel	MCF - 02/2005	HDR expected in 2009-2010; CNRS	05/02
PALMERI John	CR1 - 09/2006	HDR; Promoted 10/1997	05
POILBLANC Didier	DR1 - 07/1992	HDR; Promoted 10/2006	06
PUJOL Pierre	PR2 - 10/2006	HDR; PEDR	06/02
SÈVE-DINH Mai	MCF - 10/2003	HDR expected in 12/2009	05/04
SHEPELYANSKY Dima	DR1 - 10/1992	HDR; Promoted 10/2004	02
SIRE Clément	DR2 - 10/1991	HDR; Promoted 10/2005	02
SURAUD Éric	PREX - 10/1992	HDR; PEDR; IUF 1994; CNRS; Promoted 10/2007	04/05
FLECKINGER Robert	PR Émérite	HDR; Retired in 12/2006	02
BELKACEM Mohamed	MCF 10/2000	HDR; Portfolio Manager, *Abu Dhabi Investment Authority*, UAE (*Disponibilité* since 10/2005)	04
SØRENSEN Erik	PR2 - 12/1996	HDR; PR at *McMaster University*, Canada (*Disponibilité* since 12/2001)	06
SCALDAFERRO Sylvia	AI - 01/1993	Secretary and Administration of LPT	—
LE MAGOAROU Sandrine	AI - 10/2006	Computer technician (IRSAMC; 50% at LPT)	—

Table 1 : *Permanent staff of the LPT as on June 2009. The second column indicates the position currently held and the hiring date at the LPT. The third column provides additional information: HDR, PEDR, IUF, Délégation CNRS, ANR teaching dispensation, and date of promotion to the current position. The last column shows the CNRS Section(s) of affiliation. See Chapter 1 for more details.*

LPT groups

Since 2003, the LPT is structured into four groups covering a wide spectrum of modern physics, excluding particle and nuclear physics:

❍ FFC: Fermions Fortement Corrélés ; *Strongly Correlated Fermions*
(Head: Didier Poilblanc)
Key words: quantum magnetism, frustrated magnetism, unconventional superconductivity, low-dimensionality materials, quantum phase transitions, cold atoms, numerical simulations.

❍ Quantware: Information et Chaos Quantiques ; *Quantum Information and Chaos*
(Head: Dima Shepelyansky)
Key words: quantum computers, quantum algorithms, quantum coherence, role of disorder and impurities, classical and quantum chaos, mesoscopic physics, cold atoms, astrophysics.

❍ PhyStat: Physique Statistique des Systèmes Complexes ; *Statistical Physics of Complex Systems*
(Head: David Dean)

Key words: soft condensed matter and biophysics, out-of-equilibrium physics, disordered systems, long-range interacting systems, stochastic processes and their applications, astrophysics.

❍ AGRÉGATS: SYSTÈMES DE FERMIONS FINIS – AGRÉGATS ; *Finite Fermionic Systems – Clusters*
(Head: Éric SURAUD)
Key words: laser-matter interaction, clusters in external fields, physics of embedded or deposited clusters, clusters of biophysical interest, numerical simulations and methodology.

LPT personnel

The permanent research staff (see Tab. 1) is balanced between 9 CNRS researchers and 9 university employees (+1 retired Emeritus Professor, and 2 on leave of absence). As on January 1st 2010, the mean – and median – age of the 18 active scientists working at the LPT will be 42.

The LPT has one CNRS secretary/administrator who manages the budget of the LPT and IRSAMC (see Chapter 2). Moreover, the Fédération IRSAMC recruited a CNRS computer technician in 2006, who is located in the LPT, and works at least 50 % of her time for the LPT (see Chapter 3).

In October 2009, 5 postdocs and 9 PhD students were also working at the LPT. In addition, many foreign scientists have visited the LPT for periods of more than one month, mainly thanks to CNRS *guest scientist* (∼6-9 months/year) and UPS *invited professor* (∼3 months/year) programs.

The organization diagram of the LPT is presented in the Tab. 1.2 of the next chapter.

Scientific production

The diversity of subjects treated at the LPT translates into an equally large variety of scientific journals and conferences where LPT scientists publish or present their work. The scientific production of the LPT during the last four years is listed in Chapter 9 and consists of:

❍ **Articles published in refereed journals** (ACL; page 68): **278**
FFC: 66 – QUANTWARE: 59 – PHYSTAT: 121 – AGRÉGATS: 32

❍ **Articles without reference (preprints)** (SRP; page 80): **21**
FFC: 4 – QUANTWARE: 5 – PHYSTAT: 4 – AGRÉGATS: 8

❍ **Invited talks in international and national conferences** (INV; page 81): **115**
FFC: 26 – QUANTWARE: 31 – PHYSTAT: 32 – AGRÉGATS: 26

❍ **Oral communications with a conference proceeding (international conferences)** (ACTI; page 87): **27**
FFC: 15 – QUANTWARE: 1 – PHYSTAT: 9 – AGRÉGATS: 2

❍ **Oral communications not leading to a conference proceeding** (COM; page 90): **32**
FFC: 8 – QUANTWARE: 3 – PHYSTAT: 11 – AGRÉGATS: 10

❍ **Posters in conferences** (AFF; page 91): **34**
FFC: 11 – QUANTWARE: 11 – PHYSTAT: 9 – AGRÉGATS: 3

❍ **Books or book chapters** (OS; page 93): **11**
FFC: 5 – QUANTWARE: 3 – PHYSTAT: 1 – AGRÉGATS: 2

❍ **Vulgarization publications** (OV; page 94): **11**
FFC: 1 – QUANTWARE: 2 – PHYSTAT: 7 – AGRÉGATS: 1

❍ **Books as Editor** (DO; page 95): **4**
FFC: 1 – QUANTWARE: 1 – PHYSTAT: 1 – AGRÉGATS: 1

❍ **Commercial and Open Source softwares** (COD; page 95): **3**
FFC: 1 – QUANTWARE: 1 – PHYSTAT: 1 – AGRÉGATS: 0

❍ **Habilitation thesis to supervise researches** (HDR; page 96): **2**
FFC: 1 – QUANTWARE: 0 – PHYSTAT: 1 – AGRÉGATS: 0

❍ **PhD thesis completed or in progess** (TH; page 96): **23**
FFC: 7 – Quantware: 3 – PhyStat: 8 – Agrégats: 5

The **18 active LPT scientists are all "publiant/publishing"** according to the criteria of the *AERES*.

Main objectives of the 2007-2010 LPT project and previous Evaluation committee recommendations

Multidisciplinarity

In its previous scientific report, the LPT clearly expressed the will to strengthen its biophysics/soft condensed matter component. With the arrival of M. Manghi (02/2005) and of J. Palmeri (09/2006), the recognition in 2008 by Section 05 of CNRS of this activity developed by the PhyStat and Agrégats groups (paving the way to possible future recruitment in this Section), and the development of a second independent collaboration with experimentalists at Institut de Pharmacologie et de Biologie Structurale, we consider that this objective has been to a great extent fulfilled. Section 7.1 and Chapter 8 of the present scientific report clearly illustrate the dynamism of LPT researchers in this field.

The preceding report emphasized the project to develop applications of quantum information in the framework of condensed matter physics, a goal which has been partly achieved and is still in full development (see Chapters 5 and 6). In this regard, the FFC and Quantware groups have initiated promising discussions with the new Cold Atoms team at LCAR.

It was noted by the preceding Evaluation Committee (organized by CNRS) that, although at the leading edge in the field of numerical simulations in condensed matter physics, the FFC group would benefit from the recruitment of physicists less involved in numerical simulations (field theorist/phenomenologist). The hiring of P. Pujol in 2006 (PR2 UPS) and the hiring of R. Ramazashvili (CR1 CNRS; Section 06) in October 2009 were clearly intended to address this matter.

Multidisciplinarity has been a vital and inspiring motor of the scientific activity of the LPT since 1991. With the recognition of the LPT by Section 05 of CNRS, LPT's scientific activity is now evaluated by four different CNRS Sections of the Comité National de la Recherche Scientifique (see Tab. 1):

- ❍ **Section 02:** Théories physiques – Méthodes, modèles et applications (main Section)
- ❍ **Section 04:** Atomes et molécules – Optique et lasers – Plasmas chauds
- ❍ **Section 05:** Matière condensée – Organisation et dynamique
- ❍ **Section 06:** Matière condensée – Structures et propriétés électroniques

Local, national, and international collaborations

In accordance with the preceding scientific project and Evaluation Committee recommendations, the LPT has strengthened and developed many collaborations with theoretical and experimental laboratories. Since 2005, LPT researchers have ongoing collaborations (*i.e.* share publications) with six laboratories on the UPS campus and with more than 200 scientists (excluding LPT postdocs and PhD) from more than 130 institutions in 21 countries (see the introduction of Chapter 9).

Postdocs

The preceding report noted that the LPT suffered from the lack of qualified non-permanent staff (*i.e.* postdocs) compared to its main international competitors. Thanks to the foundation of the ANR in 2005 and the high success rate of LPT researchers in obtaining grants (7 ANR, 2 EU contracts, and 2 UPS grants... See Chapter 2), this weakness has been clearly addressed: 10 postdocs have been working at the LPT between 01/01/2007 and 01/10/2009.

Computer technician

The last LPT report and the Evaluation Committee expressed their worries concerning the lack of computer technician at the LPT, a problem addressed in 2006 by the recruitment of S. Le

Magoarou at IRSAMC, who is located in the LPT's premises, and works for at least 50 % of her time for the LPT (see Chapter 3). In addition, the maintenance of LPT's computer cluster has been outsourced to its provider (*ALINEOS*).

Finances

During the period 2007-2009, the funding of the LPT directly managed by the laboratory came essentially from the **CNRS**, the **Ministère de l'Enseignement supérieur et de la Recherche (MESR) & Université Paul Sabatier (UPS)**, seven contracts with the **Agence Nationale de la Recherche (ANR)**, and two contracts with the **European Union (EU)**. In addition, the LPT occasionally receives other funding from CNRS, MESR & UPS, or the **région Midi-Pyrénées**, but which are directly managed by these institutions. Including these different sources of funding, the total budget of the LPT was just below **half a million €** during each year of the period 2007-2009 (see Chapter 2). It is clear that LPT researchers have fully adapted themselves to the recent evolution in the French research funding system, and in particular, the creation of the ANR in 2005, which generated a strong influx of postdoctoral researchers working at the LPT.

Management of the LPT

Thanks to its moderate size, the mode of management of the LPT involves its **entire permanent staff**. LPT members meet every Tuesday for the *lunch meeting* (at 13h00; typically for 15-25 minutes), just before the LPT seminar (14h00) and are informed of important issues (deadlines, local and national news concerning the LPT, finances...). Most information is also transmitted by email by the head of the LPT or the secretary. In addition, this *lunch meeting* serves principally to discuss important issues regarding the scientific policy of the LPT.

The LPT and IRSAMC seminars

The LPT seminar, which follows the *lunch meeting* (an efficient way of making sure that everybody attend the seminar!), ensures that all LPT permanent and not permanent staff remain aware of the problems of interest for their colleagues in other fields. This "general culture" is essential in theoretical physics, where physical mechanisms or methods from one domain soon or later prove useful in other fields.

The IRSAMC has its own seminar, and invite speakers from any domain represented or not at the institute, with the strict instruction that the talk should be understandable by non specialists.

Computing infrastructure

As a theoretical laboratory, the LPT is a heavy consumer of computing resources. In 2007-2008, and thanks to a specific CNRS grant and other funding resources, the LPT has equipped itself with a powerful computer cluster of more than 300 effective processors in addition to a network of around 75 up-to-date servers, terminals, and laptops (see Chapter 3). LPT scientists also have access to local (CALMIP) and national (IDRIS) computing facilities. In March 2009, the LPT and IRSAMC were recognized by the CNRS as a *Centre Automatisé de Traitement de l'Information (CATI; IT Center)*.

Teachings and diffusion of knowledge

UPS employees, but also 5 out of 9 CNRS researchers at the LPT ensure many responsibilities and teaching duties at all levels of the Licence-Master-Doctorat (LMD) structure of the university teaching system, in physics, biophysics, chemistry, mathematics, and computer sciences (see Chapter 4), at UPS, and other universities/engineering schools.

During the last four years (as on October 2009), 16 PhD theses have been completed and 7 are in progress, and 10 postdocs have been working at the LPT (see Chapters 4 and 9). It is certainly a positive sign that **18 out of 19 former non-permanent researchers at the LPT** mentioned in this report (PhD in Tab. 4.1 and postdocs) **have already found a permanent academic job (13) or a CDI job** (Contrat à Durée Indéterminée; contract of undetermined duration) **in the private sector (5)**.

Finally, LPT scientists are also involved in conference organization and scientific popularization (articles, conferences, high-school visits...). The LPT participates every year in *La Fête de la Science*, through a series of conferences and laboratory visits organized by the Fédération IRSAMC and the CNRS.

Involvement in the local and national administration of research and education

LPT scientists are also deeply involved in the **local and national organization and administration of research and education** (see Section 4.2), at the CNRS (as DSA; at *Comité National de la recherche Scientifique – Sections 02 & 06* and USAR), CNU, UPS (at many levels), CEA, ANR, and work as expert referees for AERES, ANR, EU (ICT-FET Programs), NSF & DOE (USA), DFG (Germany), ISF (Israel), NWO (Netherlands), Academy of Finland...

The next three chapters describe the organization of the LPT, its financial resources, and computer infrastructure. Chapter 4 addresses the participation of LPT scientists in the diffusion of scientific knowledge. In Chapters 5-8, the four LPT groups present their scientific activity since the beginning of the present *contrat quadriennal* (01/01/2007). This report is concluded by a detailed list of the LPT's scientific production over the last four years. The LPT 2011-2014 *Project* is presented in a separate document, including its self-evaluation, along with statistical data concerning the laboratory, and short individual reports for each LPT researcher (in French).

Despite the large spectrum of research themes addressed at the LPT, our scientists are unified by common interests, methods and language, their dynamism and enthusiasm, not to mention a rich shared human experience since the creation of the GPT in 1991, and the recognition of the LPT in 2003. We sincerely hope that you will enjoy reading this introduction to the recent scientific achievements of the Laboratoire de Physique Théorique.

Toulouse, 30th June 2009

Clément Sire
Head of the LPT

Présentation générale du LPT (résumé en français)

Ce chapitre présente le Laboratoire de Physique Théorique (LPT) **et résume les chapitres suivants concernant le personnel du** LPT**, ses ressources financières, ses infrastructures informatiques, ses contributions à l'enseignement et à la diffusion de l'information scientifique, et bien sûr, les activités de recherche développées au** LPT **et la production scientifique qui en découle.**

Un bref historique du LPT

En 1991, Jean Bellissard (en provenance du CPT de Marseille) et une poignée de jeunes chercheurs du CNRS créent le **Groupe de Physique Théorique (GPT)** avec le soutien du **CNRS** et de l'**Université Paul Sabatier (UPS ; Université de Toulouse III)**, un groupe alors hébergé par le Laboratoire de Physique Quantique [4] (aujourd'hui LCPQ). À la même époque, trois laboratoires du site toulousain, dont le LCPQ, forment l'Institut de Recherche sur les Systèmes Atomiques et Moléculaires Complexes (IRSAMC) [5]. L'IRSAMC est rapidement reconnu par le CNRS et l'UPS en tant que Fédération de Recherche de Physique et Chimie Fondamentales (FR 2568), même si l'institut continue à utiliser l'appellation IRSAMC, à toute fin utile.

En 2003 [6], alors que le GPT a atteint une taille critique et a obtenu une reconnaissance et une visibilité scientifiques indéniables, il obtient le statut d'**Unité Mixte de Recherche du CNRS et de l'UPS (UMR 5152)**, sous son nom actuel. Didier Poilblanc est le premier directeur du LPT entre 2003 et 2006, et Clément Sire lui succède pour la période 2007-2010 (ils étaient tous les deux membres du GPT à sa création).

Depuis 2003, le LPT est l'un des quatre laboratoires constituant la Fédération IRSAMC (FR 2568), avec le Laboratoire Collisions Agrégats Réactivité – LCAR (UMR 5589 ; physique atomique et des agrégats), le Laboratoire de Chimie et Physique Quantiques – LCPQ (UMR 5626 ; chimie théorique), et le Laboratoire de Physique et Chimie des Nano-Objets – LPCNO (UMR 5215 ; nanophysique et nanochimie).

---

4. LPT restera à jamais reconnaissant envers ce laboratoire – dirigé à l'époque par le regretté Jean-Pierre Daudey et par Jean-Paul Malrieu – pour leur accueil chaleureux.

5. Dans ce rapport, le texte en couleur claire peut être "cliqué" et renvoie à des sites Web, des documents *pdf* (articles, prépublications...), et à des références, tableaux, figures, chapitres, et sections.

6. Pour raisons personnelles, J. Bellissard a quitté Toulouse en 2002, pour un poste de full professor à Georgia Tech, avant la création du LPT. Il est cependant clair que le LPT reste extrêmement reconnaissant de son implication déterminante au GPT, directement à l'origine du LPT.

Les quatre équipes du LPT

NOM & Prénom	Poste	Commentaires	CNRS
ALET Fabien	CR2 - 10/2005	—	06
CAPPONI Sylvain	PR2 - 10/2000	HDR ; PEDR ; ANR ; Promu en 10/2008	06
CHAVANIS Pierre-Henri	CR1 - 10/1998	Promu en 10/2001	02
BRAUN Daniel	PR2 - 10/2004	HDR ; PEDR ; CNRS	02
DEAN David	PR1 - 10/1998	HDR ; PEDR ; IUF 2007 ; CNRS ; Promu en 10/2006	02/05
DESTAINVILLE Nicolas	MCF - 10/1998	HDR ; PEDR ; CNRS	02/05
FRAHM Klaus	PR2 - 10/1997	HDR ; CNRS ; Promu en 02/2000	02
GEORGEOT Bertrand	CR1 - 10/1996	Promu en 10/2000 ; HDR prévue en 2009-2010	02
GIRAUD Olivier	CR2 - 10/2005	—	02
MAMBRINI Matthieu	CR1 - 10/2002	Promu en 10/2006	06
MANGHI Manoel	MCF - 02/2005	HDR prévue en 2009-2010 ; CNRS	05/02
PALMERI John	CR1 - 09/2006	HDR ; Promu en 10/1997	05
POILBLANC Didier	DR1 - 07/1992	HDR ; Promu en 10/2006	06
PUJOL Pierre	PR2 - 10/2006	HDR ; PEDR	06/02
SÈVE-DINH Mai	MCF - 10/2003	HDR prévue en 12/2010	05/04
SHEPELYANSKY Dima	DR1 - 10/1992	HDR ; Promu en 10/2004	02
SIRE Clément	DR2 - 10/1991	HDR ; Promu en 10/2005	02
SURAUD Éric	PREX - 10/1992	HDR ; PEDR ; IUF 1994 ; CNRS ; Promu en 10/2007	04/05
FLECKINGER Robert	PR Émérite	HDR ; à la retraite depuis 12/2006	02
BELKACEM Mohamed	MCF 10/2000	HDR ; Portfolio Manager, *Abu Dhabi Investment Authority*, UAE (*Disponibilité* depuis 10/2005)	04
SØRENSEN Erik	PR2 - 12/1996	HDR ; PR à *McMaster University*, Canada (*Disponibilité* depuis 12/2001)	06
SCALDAFERRO Sylvia	AI - 01/1993	Secrétaire/gestionnaire du LPT	—
LE MAGOAROU Sandrine	AI - 10/2006	Technicienne informatique (IRSAMC ; 50% au LPT)	—

Tableau 2 : *Personnel permanent du LPT en juin 2009. La seconde colonne indique le poste actuel et la date de recrutement au LPT. La troisième colonne précise : HDR, PEDR, IUF, Délégation CNRS, décharge de service financée par l'ANR, et la date de la dernière promotion. La dernière colonne indique la ou les Section(s) CNRS d'affiliation. Voir le Chapitre 1 pour plus de détails.*

Depuis 2003, le LPT est structuré en quatre équipes, dont l'activité couvre un large champ de la physique moderne, à l'exclusion de la physique nucléaire et des particules :

❍ FFC : Fermions Fortement Corrélés ; *Strongly Correlated Fermions*
(Directeur : Didier Poilblanc)
Mots clés : magnétisme quantique, frustration magnétique, supraconductivité non conventionnelle, matériaux de basse dimensionnalité, transitions de phases quantiques, atomes froids, simulations numériques.

❍ Quantware : Information et Chaos Quantiques ; *Quantum Information and Chaos*
(Directeur : Dima Shepelyansky)
Mots clés : ordinateur quantique, algorithmes quantiques, cohérence quantique, rôle du désordre et des impuretés, chaos classique et quantique, physique mésoscopique, atomes froids, astrophysique.

❍ PhyStat : Physique Statistique des Systèmes Complexes ; *Statistical Physics of Complex Systems*
(Directeur : David Dean)

Mots clés : physique de la matière molle et biophysique, systèmes fortement hors d'équilibre, systèmes désordonnés, systèmes interagissant à longue portée, processus stochastiques et leurs applications, astrophysique.

❍ Agrégats : Systèmes de Fermions Finis – Agrégats ; *Finite Fermionic Systems* (Directeur : Éric Suraud)
Mots clés : interaction laser-matière, agrégats en champs externes, physique des agrégats en matrice ou déposés, agrégats d'intérêt biologique, simulations numériques et méthodologie.

Personnel du LPT

Le personnel permanent du LPT (voir Tab. 2) s'équilibre entre 9 chercheurs CNRS et 9 enseignants-chercheurs (EC) à l'UPS (+1 Professeur Émérite à la retraite, et 2 EC en *disponibilité*). Au 1er janvier 2010, l'âge moyen – et médian – des 18 membres actifs du LPT est de 42 ans.

La gestionnaire du LPT (AI CNRS) suit et gère le budget du laboratoire et de la Fédération IRSAMC (voir le Chapitre 2) et assure les tâches de secrétariat. De plus, la Fédération IRSAMC a recruté en 2006 une technicienne en informatique (AI CNRS), qui travaille dans les locaux du LPT, et qui consacre au moins 50 % de son temps pour le LPT (voir le Chapitre 3).

En octobre 2009, 5 postdocs et 9 thésards travaillent aussi au LPT. En outre, de nombreux scientifiques visitent le LPT pour des périodes de plus d'un mois, grâce notamment aux postes de *chercheur invité* CNRS (∼ 6-9 mois/an) et de *professeur invité* UPS (∼ 3 mois/an).

L'organigramme du LPT est présenté en Tab. 1.2 du prochain chapitre.

Production scientifique

La diversité des sujets abordés au LPT se traduit par une large variété de journaux scientifiques et de conférences où les physiciens du LPT publient ou exposent leurs travaux. Les **18 chercheurs actifs du LPT sont tous "publiant"** selon les critères de l'*AERES*. La production scientifique du LPT au cours de quatre dernières années est présentée en détail au Chapitre 9, et consiste en :

❍ **Articles publiés dans des revues avec comité de lecture** (ACL ; page 68) : **278**
FFC : 66 – Quantware : 59 – PhyStat : 121 – Agrégats : 32

❍ **Articles sans référence de publication (prépublications)** (SRP ; page 80) : **21**
FFC : 4 – Quantware : 5 – PhyStat : 4 – Agrégats : 8

❍ **Conférences nationales et internationales en tant qu'invité** (INV ; page 81) : **115**
FFC : 26 – Quantware : 31 – PhyStat : 32 – Agrégats : 26

❍ **Communications orales avec acte dans un congrès international** (ACTI ; page 87) : **27**
FFC : 15 – Quantware : 1 – PhyStat : 9 – Agrégats : 2

❍ **Communications orales sans acte dans un congrès** (COM ; page 90) : **32**
FFC : 8 – Quantware : 3 – PhyStat : 11 – Agrégats : 10

❍ **Communications par affiche dans un congrès** (AFF ; page 91) : **34**
FFC : 11 – Quantware : 11 – PhyStat : 9 – Agrégats : 3

❍ **Ouvrages ou chapitres d'ouvrages scientifiques** (OS ; page 93) : **11**
FFC : 5 – Quantware : 3 – PhyStat : 1 – Agrégats : 2

❍ **Ouvrages ou chapitres d'ouvrages de vulgarisation** (OV ; page 94) : **11**
FFC : 1 – Quantware : 2 – PhyStat : 7 – Agrégats : 1

❍ **Direction d'ouvrages** (DO ; page 95) : **4**
FFC : 1 – Quantware : 1 – PhyStat : 1 – Agrégats : 1

❍ **Codes commerciaux ou en licence Open Source** (COD ; page 95) : **3**
FFC : 1 – Quantware : 1 – PhyStat : 1 – Agrégats : 0

❍ **Habilitations à diriger des recherches** (HDR ; page 96) : **2**
FFC : 1 – Quantware : 0 – PhyStat : 1 – Agrégats : 0

❍ **Thèses soutenues ou en cours** (TH ; page 96) : **23**
FFC : 7 – Quantware : 3 – PhyStat : 8 – Agrégats : 5

Objectifs principaux du projet 2007-2010 du LPT et recommandations du précédent Comité d'Évaluation

Pluridisciplinarité

Dans son précédent rapport scientifique, le LPT avait clairement exprimé sa volonté de développer sa composante physique de la matière molle/biophysique (MMBP). Avec l'arrivée de M. Manghi (02/2005) et de J. Palmeri (09/2006), la reconnaissance en 2008 de cette activité MMBP au sein des équipes PhyStat et Agrégats par la Section 05 du CNRS (permettant d'espérer des recrutements futurs dans cette Section), et l'émergence d'une seconde collaboration indépendante avec l'Institut de Pharmacologie et de Biologie Structurale, le LPT considère que cet objectif est pratiquement rempli. La Section 7.1 et le Chapitre 8 du présent rapport scientifique témoignent du dynamisme des chercheurs du LPT dans ce domaine.

Le rapport précédent exprimait le projet de développer des applications transversales entre physique de la matière condensée et information quantique, un objectif qui est en cours de développement actuellement et qui a déjà porté ses premiers fruits (voir les Chapitres 5 et 6). À cet égard, les équipes FFC et Quantware ont entamé des discussions prometteuses avec le nouveau groupe Atomes Froids du LCAR.

Lors de la précédente évaluation du LPT organisée par le CNRS, il fut noté que, bien qu'à la pointe des simulations numériques en physique de la matière condensée, l'équipe FFC bénéficierait certainement de l'apport d'un théoricien non numéricien, un constat partagé par le LPT. Le recrutement de P. Pujol en 2006 (PR2 UPS) et l'arrivée de R. Ramazashvili (CR1 CNRS ; Section 06) en octobre 2009 répondent ouvertement à cette recommandation.

La **pluridisciplinarité** est un moteur essentiel de l'activité scientifique du LPT depuis sa création. Avec la reconnaissance du LPT par la Section 05 du CNRS, cette activité est maintenant évaluée par quatre Sections différentes du Comité National de la Recherche Scientifique (voir Tab. 2) :

❍ **Section 02 :** Théories physiques – Méthodes, modèles et applications (Section principale)

❍ **Section 04 :** Atomes et molécules – Optique et lasers – Plasmas chauds

❍ **Section 05 :** Matière condensée – Organisation et dynamique

❍ **Section 06 :** Matière condensée – Structures et propriétés électroniques

Collaborations locales, nationales, et internationales

Conformément au précédent rapport scientifique du LPT et aux recommandations du précédent Comité d'Évaluation, le LPT s'est attaché à solidifier et à développer de nombreuses collaborations scientifiques avec des laboratoires théoriques et expérimentaux. Depuis 2005, les chercheurs du LPT ont des collaborations (*i.e.* conduisant à des publications) actives avec six laboratoires sur le campus de l'UPS et avec plus de 200 scientifiques (en excluant postdocs et thésards du LPT) provenant de 130 institutions dans 21 pays (voir l'introduction du Chapitre 9).

Postdocs

Le précédent rapport scientifique notait que le LPT souffrait du faible nombre de chercheurs non permanents (postdocs) qu'il hébergeait, en comparaison avec ses principaux compétiteurs internationaux. Grâce à la création de l'ANR et aux succès des chercheurs du LPT obtenus dans le cadre de divers appels d'offres (7 contrats ANR, 2 contrats européens, 2 Appels d'offres bisannuel du Conseil Scientifique de l'UPS... Voir le Chapitre 2), cette faiblesse a été amplement corrigée : 10 postdocs travaillent ou ont travaillé au LPT pendant la période allant du 01/01/2007 au 01/10/2009.

Technicien informatique

Le précédent rapport scientifique du LPT et les conclusions du rapport d'évaluation exprimaient leur inquiétude vis-à-vis du manque de technicien informatique au LPT. Avec le recrutement de S. Le Magoarou à l'IRSAMC, qui travaille au moins à 50 % de son temps pour le LPT, et avec l'externalisation de la maintenance de la grappe de calcul du LPT dans des conditions très avantageuses, la situation dans ce domaine s'est très clairement améliorée (voir le Chapitre 3).

Finances

Durant la période 2007-2009, les ressources financières directement gérées par le LPT émanaient principalement du **CNRS**, du **Ministère de l'Enseignement supérieur et de la Recherche (MESR) & Université Paul Sabatier (UPS)**, de sept contrats avec l'**Agence Nationale de la Recherche (ANR)**, et de deux **Contrats européens**. En outre, le LPT a reçu d'autres financements ponctuels du CNRS, du MESR & UPS, ou de la **région Midi-Pyrénées**, qui sont gérés par ces institutions, bien que bénéficiant directement au LPT. En incluant ces différentes sources de crédits, les ressources du LPT se sont établies juste en dessous de **500 000 € HT** au cours de chacune des années de la période 2007-2009 (Voir le Chapitre 2). Il est ainsi clair que les chercheurs du LPT se sont parfaitement adaptés aux évolutions récentes du système national de financement de la recherche, et en particulier, à la création de l'ANR en 2005, qui a engendré un influx important de postdocs venant travailler au LPT.

Management du LPT

La taille modeste du LPT permet un management du laboratoire qui implique **l'ensemble de ses permanents**. Les membres du LPT se réunissent tous les mardis pour le *lunch meeting* (à 13h ; d'une durée typique de 15-25 minutes), juste avant le séminaire du LPT (14h). Ils sont informés des sujets d'actualité importants (appels d'offres, échéances, informations administratives générales, finances,...), dont la plupart sont aussi transmis par courrier électronique par la gestionnaire ou le directeur du LPT. Bien sûr, ce *lunch meeting* sert avant tout à discuter les décisions importantes à prendre concernant la politique scientifique du LPT.

Les séminaires du LPT et de l'IRSAMC

Le séminaire hebdomadaire du LPT, qui suit le *lunch meeting* (un moyen efficace de s'assurer que tout le monde y participe !), permet à l'ensemble des personnels permanents et non permanents du LPT de rester informé des sujets scientifiques d'importance pour leurs collègues travaillant dans d'autres domaines. Cette *culture générale* est essentielle en physique théorique, où de nombreux mécanismes physiques et méthodes d'un domaine sont amenés tôt ou tard à s'appliquer dans d'autres domaines.

Par ailleurs, l'IRSAMC organise son propre séminaire général, et invite donc des intervenants dans des domaines représentés ou non à l'institut, avec comme consigne majeure de s'adresser à un public de non spécialistes. Les trois autres laboratoires de l'IRSAMC organisent bien sûr leurs propres séminaires, qui sont relayés dans l'institut, notamment sur le site Web du LPT.

Infrastructure informatique

De part la nature de son activité théorique, le LPT est un consommateur intensif de ressources de calcul numérique. En 2007-2008, le LPT s'est équipé d'une puissante grappe de calcul de plus de 300 processeurs effectifs, qui s'ajoute à un réseau d'environ 75 serveurs, terminaux, et ordinateurs portables (voir le Chapitre 3). Les physiciens du LPT ont aussi accès à des ressources de calcul mutualisées, tant au niveau local (CALMIP) que national (IDRIS). En mars 2009, le LPT et l'IRSAMC ont été reconnus par le CNRS en tant que *Centre Automatisé de Traitement de l'Information (CATI)*.

Enseignement et diffusion de l'information scientifique

Les enseignants-chercheurs à l'UPS, mais aussi 5 des 9 chercheurs CNRS du LPT assurent de nombreuses responsabilités et tâches d'enseignement à tous les niveaux du cycle Licence-Master-Doctorat (LMD), en physique, biophysique, chimie, mathématique, et informatique, à l'UPS et dans d'autres universités et écoles d'ingénieurs (voir le Chapitre 4).

Durant les quatre dernières années (octobre 2009), 16 thèses de doctorat dirigées par des membres du LPT ont été décernées, et 7 thèses sont actuellement en cours. Par ailleurs, 10 postdocs ont travaillé au LPT depuis le début du *contrat quadriennal* (voir les Chapitres 4 et 9). Le LPT se réjouit du fait que **18 des 19 anciens chercheurs non permanents du LPT** mentionnés dans le présent rapport (thésards en Tab. 4.1 et postdocs) **ont déjà trouvé un poste permanent dans le secteur académique (13) ou un poste en CDI** (Contrat à Durée Indéterminée) **dans le secteur privé (5)**.

Finalement, les physiciens du LPT sont aussi impliqués dans l'organisation de conférences et dans de multiples opérations de vulgarisation scientifique (articles, conférences publiques et en établissements scolaires, visites du laboratoire,...). Chaque année, les membres du LPT participent activement à *La Fête de la Science* organisée à l'IRSAMC (conférences et visites des quatre laboratoires), ainsi qu'aux événements organisés par le CNRS.

Implication dans l'administration locale et nationale de l'éducation supérieure et de la recherche

Les chercheurs du LPT sont aussi particulièrement impliqués dans **l'organisation locale et nationale et l'administration de la recherche et du système d'éducation supérieure** (voir Section 4.2), au CNRS (en tant que DSA ; au *Comité National de la recherche Scientifique – Sections 02 & 06*, et à l'USAR), au CNU, à l'UPS (à de nombreux niveaux), au CEA, à l'ANR, et sont sollicités en tant qu'experts auprès de l'AERES, l'ANR, l'Union Européenne (Programmes ICT-FE), la NSF & DOE (USA), la DFG (Allemagne), l'ISF (Israël), la NWO (Pays-Bas), l'Académie de Finlande...

Les trois prochains chapitre détaillent respectivement l'organisation du LPT, ses ressources financières, et ses moyens informatiques. Le Chapitre 4 présente les enseignements et la participation des membres du LPT à la diffusion de l'information scientifique. Dans les Chapitres 5-8, les quatre équipes du LPT présentent les points principaux de leur activité scientifique depuis le début du présent *Plan quadriennal* (01/01/2007). La liste complète de la production scientifique des physiciens du LPT est finalement présentée dans le Chapitre 9. Le *Projet* 2011-2014 du LPT, incluant son auto-analyse, fait l'objet d'un document séparé, de même que les données statistiques requises par l'AERES concernant le laboratoire, et les fiches individuelles d'activité des enseignants-chercheurs UPS et chercheurs CNRS du LPT.

Malgré le large spectre de domaines de recherche couvert au LPT, les physiciens de ce laboratoire sont unis par leurs intérêts scientifiques, des méthodes et un langage communs, par leur dynamisme et leur enthousiasme, et par une riche aventure humaine commune depuis la création du GPT en 1991, et celle du LPT en 2003. Nous espérons sincèrement que vous prendrez plaisir à lire cette introduction aux récentes contributions scientifiques réalisées au Laboratoire de Physique Théorique.

Toulouse, le 30 juin 2009

Clément Sire
Directeur du LPT

1

Organization of the LPT

This chapter focuses on the structure and organization of the LPT and the laboratory's permanent researchers and technicians. In addition, we provide a list of indicators (number of foreign LPT scientists, age pyramid, career evolution, HDR, PEDR, IUF fellowships, Délégations CNRS, ANR financed teaching dispensation...) illustrating the dynamism of LPT researchers. We then present some generalities about the management of the LPT, training program, and hygiene and security.

1.1 The four LPT groups

The LPT is organized into four groups covering a wide spectrum of modern physics, excluding particle and nuclear physics:

- FFC: Fermions Fortement Corrélés; *Strongly Correlated Fermions* (Head: Didier Poilblanc)
- Quantware: Information et Chaos Quantiques; *Quantum Information and Chaos* (Head: Dima Shepelyansky)
- PhyStat: Physique Statistique des Systèmes Complexes; *Statistical Physics of Complex Systems* (Head: David Dean)
- Agrégats: Systèmes de Fermions Finis – Agrégats; *Finite Fermionic Systems – Clusters* (Head: Éric Suraud)

1.2 Permanent staff of the LPT

Permanent research staff

As of October 2009, the LPT is comprised of 9 **CNRS** researchers [1] and 9 active enseignants-chercheurs [2] (EC) employed by **Ministère de l'Enseignement supérieur et de la Recherche (MESR) & Université Paul Sabatier (UPS)**. In addition, one retired EC (in 10/2006) is Professeur Émérite (Emeritus Professor with an office at the LPT) and two EC are "en disponibilité" (on leave of absence), and left the LPT before the period considered in this report.

The LPT has presently 6 foreign scientists in its permanent staff (+2 on leave of absence). 3 former PhD students at the LPT were recruited by the LPT since 1991, all after spending postdoctoral periods abroad: 2 CR in Section 06 of CNRS in 2002 and 2005, 1 MCF in 2000 (now PR2 at the UPS).

1. CNRS employees do not have mandatory teaching duties.
2. EC have 192 hours/year ("équivalent TD") of mandatory teaching duties at the UPS, except when they obtain teaching dispensations (IUF fellowships, Délégation CNRS, ANR grants including dispensation, EC hired since less than two years).

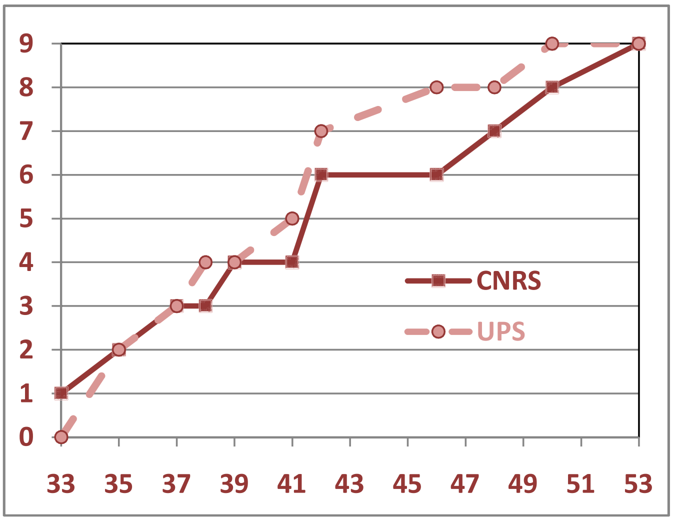


Figure 1.1 : Number of CNRS researchers and UPS EC having less than a given age (01/01/2010).

As of October 2009, 5 postdocs and 10 PhD students were also working at the LPT (see Chapter 4.1).

Among the CNRS researchers, 3 are Directeur de Recherche (2 DR1, 1 DR2: DR 1st/2nd *classe*; senior scientists) and 6 are Chargé de Recherche (4 CR1, 2 CR2; junior scientists), while 6 EC are Professeur (1 PREX, 1 PR1, 4 PR2: *classe exceptionnelle*, 1st/2nd *classe* full professors) and 3 are Maître de Conférences (MCF; assistant professors).

As on January 1st 2010, the **mean – and median – age** of the 18 LPT active scientists will be **just under 42** (around 47 at the CNRS and French scientific universities, in 2007; see Fig. 1.1).

11 out of the 18 active LPT scientists (7 EC and 4 CNRS) have the **Habilitation à Diriger des Recherches (HDR; habilitation to supervise doctoral research)** or equivalent, and 6 EC out of 9 currently benefit of the **Primes d'Encadrement Doctoral et de Recherche (PEDR; salary bonus for supervising PhD's and for outstanding research activities)**. About 30 % of EC in physics (20 % in chemistry) are currently awarded the PEDR at the UPS (close to the national average).

Moreover, one EC is a 2007-2011 junior fellow[3] of the Institut Universitaire de France (IUF), and another one was a senior fellow of the IUF during the 1994-1998 period. IUF junior fellowships provide a 15 k€ (VAT included)/year grant and teaching dispensation.

Finally, during the last four years, 5 EC were awarded one or more 6 months period of **Délégation au CNRS (sabbatical period as a CNRS employee)**, which includes a full teaching dispensation, and 1 EC benefits from a teaching dispensation from an ANR contract.

Tab. 1.1 lists the permanent staff of the LPT, describes their current position and hiring date at the LPT, the date of their last promotion to their current position, and other relevant information (HDR, PEDR, IUF, Délégation CNRS, ANR teaching dispensation). The LPT being **evaluated by Sections 02, 04, 05, and 06 of the CNRS**, we also list the CNRS Section(s) to which CNRS researchers belong and EC are affiliated (see the *Multidisciplinarity* subsection in the introductory chapter and the subsection *Recent evolution of the LPT permanent staff* below). The entire LPT

3. In 2007, among the 7 new IUF fellows working in the three universities in Toulouse, 4 were members of the Fédération IRSAMC (1 in each IRSAMC laboratory).

staff is associated with the 29th Section of the Conseil National des Universités (CNU).

Permanent administrative staff

Sylvia MIRALLES-SCALDAFERRO is *Assistante Ingénieur* (AI CNRS) at the LPT, in charge of secretarial and general administration. In particular, she manages the LPT budget (see Chapter 2), as well as the budget of the Fédération IRSAMC (160 k€/year in 2007-2010). The financial management of the LPT was barely affected by the somewhat chaotic introduction of the new version of the CNRS financial software *X-LAB* (coupled with the introduction of *BFC*) in 01/2007. Thanks to S. MIRALLES-SCALDAFERRO, we hope that we will also go unscathed during the introduction in 01/2009 of the UPS-MESR new financial software *SIFAC*.

Sandrine LE MAGOAROU is a computer technician (AI CNRS) at the Fédération IRSAMC, but is based at the LPT, and works at least 50 % of her time for the LPT (see Chapter 3). She is *Chargé de la Sécurité des Systèmes d'Informations* (CSSI; CNRS & UPS) and *Autorité d'Enregistrement (AE)* CNRS-Plus et CNRS-Standard for both LPT and LCPQ (control of access to CNRS IT applications).

NAME & First name	Position	Comments	CNRS
ALET Fabien	CR2 - 10/2005	—	06
CAPPONI Sylvain	PR2 - 10/2000	HDR; PEDR; ANR; Promoted 10/2008	06
CHAVANIS Pierre-Henri	CR1 - 10/1998	Promoted 10/2001	02
BRAUN Daniel	PR2 - 10/2004	HDR; PEDR; CNRS	02
DEAN David	PR1 - 10/1998	HDR; PEDR; IUF 2007; CNRS; Promoted 10/2006	02/05
DESTAINVILLE Nicolas	MCF - 10/1998	HDR; PEDR; CNRS	02/05
FRAHM Klaus	PR2 - 10/1997	HDR; CNRS; Promoted 02/2000	02
GEORGEOT Bertrand	CR1 - 10/1996	Promoted 10/2000; HDR expected in 2009-2010	02
GIRAUD Olivier	CR2 - 10/2005	—	02
MAMBRINI Matthieu	CR1 - 10/2002	Promoted 10/2006	06
MANGHI Manoel	MCF - 02/2005	HDR expected in 2009-2010; CNRS	05/02
PALMERI John	CR1 - 09/2006	HDR; Promoted 10/1997	05
POILBLANC Didier	DR1 - 07/1992	HDR; Promoted 10/2006	06
PUJOL Pierre	PR2 - 10/2006	HDR; PEDR	06/02
SÈVE-DINH Mai	MCF - 10/2003	HDR expected in 12/2009	05/04
SHEPELYANSKY Dima	DR1 - 10/1992	HDR; Promoted 10/2004	02
SIRE Clément	DR2 - 10/1991	HDR; Promoted 10/2005	02
SURAUD Éric	PREX - 10/1992	HDR; PEDR; IUF 1994; CNRS; Promoted 10/2007	04/05
FLECKINGER Robert	PR Émérite	HDR; Retired in 12/2006	02
BELKACEM Mohamed	MCF 10/2000	HDR; Portfolio Manager, *Abu Dhabi Investment Authority*, UAE (*Disponibilité* since 10/2005)	04
SØRENSEN Erik	PR2 - 12/1996	HDR; PR at *McMaster University*, Canada (*Disponibilité* since 12/2001)	06
SCALDAFERRO Sylvia	AI - 01/1993	Secretary and Administration of LPT	—
LE MAGOAROU Sandrine	AI - 10/2006	Computer technician (IRSAMC ; 50% at LPT)	—

Table 1.1 : *Permanent staff of the LPT as on June 2009. The second column indicates the position currently held and the hiring date at the LPT. The third column provides additional information: HDR, PEDR, IUF, Délégation CNRS, ANR teaching dispensation, and date of promotion to the current position. The last column shows the CNRS Section(s) of affiliation.*

Organization diagram of the LPT

The affiliation of CNRS researchers and EC with the four LPT groups is described in the organization diagram of Tab. 1.2. The different administrative tasks assumed by LPT members are also listed below.

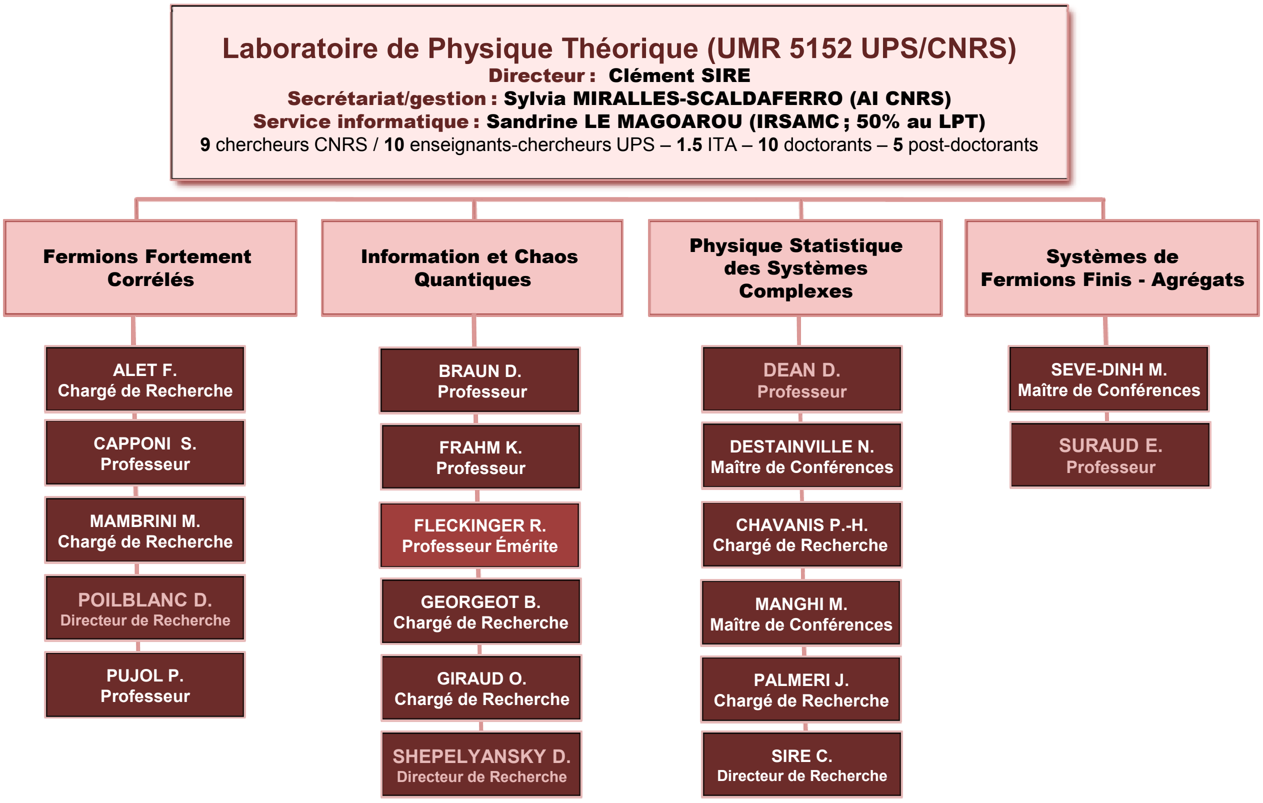


Table 1.2 : Organization diagram of the LPT. Group leader names are in light red (see also Tab. 1.1).

- **Head of the LPT:** C. Sire (LPT representative at the *Bureau de l'IRSAMC*)
- **Secretary and administration:** S. Miralles-Scaldaferro
- **Training program:** S. Miralles-Scaldaferro
- **Computer technician, AE (CNRS), and CSSI (CNRS & UPS):** S. Le Magoarou
- **Webmaster:** F. Alet
- **Communication:** S. Miralles-Scaldaferro and C. Sire
- **LPT seminar:** P. Pujol; **IRSAMC seminar:** B. Georgeot
- **Hygiene and security:** B. Georgeot

Recent evolution of the LPT permanent staff

The LPT was awarded two CNRS CR2 positions (Olivier Giraud in Section 02; Fabien Alet in Section 06) both starting in October 2005, and two UPS PR2 positions, one in 10/2006 (P. Pujol; previously MCF at the ENS Lyon), and one in 2008, which was used to promote a MCF at the LPT (S. Capponi; first internal promotion since the very first one in 2000). In addition, Revaz Ramazashvili was selected by Section 06 in the CR1 competition, and will start working at the LPT in October 2009.

In September 2006, John Palmeri joined the LPT from Institut Européen des Membranes (IEM-UMR 5635, Montpellier). In September 2008, J. Palmeri moved from the CNRS Section 15 to Section 05, better adapted to his research activity. Furthermore, the LPT obtained its evaluation by Section 05 (in addition to Sections 02, 04, and 06) with regard to the *soft condensed matter physics/biophysics* activity of the PhyStat group and part of the activity of the Agrégat group (in particular, a former PhD student in this group was hired in Section 05).

For personal reasons, Olivier Giraud is expected to join Laboratoire de Physique Théorique et Modèles Statistiques (UMR 8626 Orsay) in early 2010. LPT wishes him good luck in his new laboratory, and is confident that his collaborations with LPT scientists will not be affected by his departure.

1.3 Management of the LPT

Although a laboratory of reasonable size in the French theoretical physics community, the LPT remains rather small compared to many physics CNRS *Unités Mixtes de Recherche*. The mode of management of the LPT is adapted to its size, and thus involves its **entire permanent staff**. LPT members meet every Tuesday for the lunch meeting (at 13h00; typically for 15-25 minutes), just before the LPT seminar (14h00) and are informed of important issues (deadlines, local and national news concerning the LPT, finances...). Most information is also transmitted by email by the head of the LPT or the secretary. In addition, this lunch meeting serves principally to discuss important issues regarding the scientific policy of the LPT. All LPT members can, and do, express their points of view on all issues. Although the head of the LPT obviously makes the final decisions (with ultimately the interest of the LPT in mind), these are fully justified and explained to the LPT members, and taken in full consideration of view expressed by the LPT members.

1.4 LPT and Fédération IRSAMC

The director of the IRSAMC (P. Labastie – LCAR), the directors of its four laboratories (constituting the *Bureau de l'IRSAMC*), and the *Conseil de l'IRSAMC* manage the institute, and in particular its MESR budget of about 160 k€. Despite some recent discussions, there is no current plan to regroup the four laboratories into one big *Unité Mixte de Recherche*[4] (see the LPT *Project*). However, IRSAMC already mutualizes several services: the pool of computer technicians, computer network, mail and web servers, computer room (in 2009-2010), IRSAMC library... Moreover, the secretaries of the LPT and the LCPQ are able to share the administrative duties of the two laboratories so that in the absence of one, the other can assume her colleague's responsibilities. In addition, from 2007 on, the IRSAMC has managed internally its PhD fellowships obtained from MESR through the *École doctorale Sciences de la Matière*, and submits a ranked list, according to its scientific priorities, of its demands for MCF/PR positions to the *UFR Physique-Chimie-Automatique* (starting in 2009). Hence, IRSAMC is clearly destined to become the privileged contact body with the UPS for matters common to our four laboratories. The positive and even friendly atmosphere within the IRSAMC (and in particular between the five directors), illustrated by the yearly organization of *Les Journées de l'IRSAMC* and *La Fête de la Science*, certainly facilitates this pooling of resources.

4. In 2009, the Fédération IRSAMC is comprised of around 100 permanent CNRS and UPS researchers, 25 CNRS and UPS technicians, and 55 PhD students and postdocs.

1.5 Training programs

The administrative and research staff of the LPT have attended several training programs, most of them organized by the CNRS *Délégation Midi-Pyrénées* (CNRS-DR14) or the UPS.

Administrative staff

S. Scaldaferro-Miralles has attended the following training programs since 2005:

- *Techniques de mémorisation* (3 days; *IRFA Conseil*, CNRS-DR14, 2006)
- *Préparation aux concours internes* (5 days; *IRFA Conseil*, CNRS-DR14, 2007)
- *Dossier annuel d'activité* (0.5 day; *IRFA Conseil*, CNRS-DR14, 2008)
- *Mieux comprendre la décentralisation* (1 day; UPS, 2008)
- *Perfectionnement* Powerpoint (1 day; *JMC Solutions*, 2008)
- *Formation SIFAC* (6 days; UPS, 2009)
- *Les achats au CNRS* (1 day; CNRS-DR14, 2009)
- *Améliorer l'accueil en anglais des scientifiques étrangers* (18 hours; *Cépière formation*, CNRS-DR14, 2009)

S. Le Magoarou has attended the following training programs since her arrival at the LPT:

- *Aide à l'acquisition d'informations sur machines piratées* (1 day, CNRS-DR14, 2007)
- *Helpdesk, gestion de parc – OCS inventory* (0.5 day, Journées *Capitoul*, 2007)
- *Métrologie, supervision* (0.5 day, Journées *Capitoul*, 2008)
- *Kit Spip développeur* (3 days, *IFORM*, CNRS-DR14, 2008)
- *Kit Spip administrateur* (2 days, *IFORM*, CNRS-DR14, 2008)
- *HTML/XHTML/CSS* (3 days, *IFORM*, CNRS-DR14, 2008)
- *Charte graphique du CNRS* (1 day, *IFORM*, CNRS-DR14, 2008)
- *Linux : administration serveurs* (5 days, *IFORM*, CICT, CNRS-DR14, 2008)

Research staff

- F. Alet and O. Giraud have participated in the *Journées des Entrants ENCRE*, La Rochelle (5-8 November 2007).
- S. Capponi has participated in the training program *Langage C++* (5 days, CNRS-DR14, 10/2007)
- C. Sire has participated in 6 CNRS training programs during the period 2006-2009 (at CNRS headquarter and *Délégation Midi-Pyrénées*), concerning various aspects (management, organization, finances, legal matters...) of the function of laboratory head, for a total period of around 15 days.
- C. Sire has been selected, along with 15 other CNRS employees, to participate in the CNRS training program *Cadres à Haut Potentiel (High-Potential Managers)*; three weeks in France and abroad between June and December 2009.
- M. Capello and A. Ralko (LPT postdocs) have participated in the *Formation 2008 "Outplacement" pour les Contractuels* organized by CNRS-DR14, a training program designed to facilitate the insertion of postdocs in the job market. U. F. Ndongmouo Taffoti will follow the 2009-2010 session.
- M. Capello (LPT postdoc) has participated in the training program *Français – Langue étrangère* (10×3 hours, *Alliance Française – Toulouse*, CNRS-DR14, 03/2007).

1.6 Hygiene and security

Working in a theoretical physics laboratory, the members of the LPT are only mildly exposed to risks directly related to their scientific activity (computer and network security is addressed in Section 3.4). Still, this section summarizes various precautions taken in order to improve the safety of people working at the LPT. Bertrand Georgeot is in charge of *hygiene and security* at the LPT, and receives the periodic CNRS information letter on this matter.

Concerning safety at work, the LPT's electricity supply network has been modernized in 2007 and developed in 2008 (on LPT and IRSAMC own MESR financial resources), in particular to accommodate the new computer cluster and the additional air conditioning need for the LPT computer room.

A first-aid closet is located in the secretarial office and is regularly updated. Together with the other laboratories of the Fédération IRSAMC, we have ensured that at least one person in each laboratory has received first-aid training. The names of these persons are posted on each floor of the IRSAMC building. The occasional sanitary warnings from the UPS and CNRS, (*e.g.* bird or swine flu), are dutifully relayed to the members of the LPT.

Concerning hygiene, a persistent problem is the lack of regular/proper cleaning of the offices, which seems to be getting worse every year, especially since the UPS has outsourced some cleaning operations.

2

Finances

This chapter details the financial resources of the LPT during the period 2007-2009 and the corresponding expenses of the laboratory. The researchers at LPT have fully adapted themselves to the recent evolution of the French research funding system, and in particular, the creation of the AGENCE NATIONALE DE LA RECHERCHE (ANR). Annual CNRS and MESR funding, which dominated the budget of most French laboratories just a few years ago, now represents less than 15 % of the LPT's total financial resources.

2.1 Budget of the LPT

During the period 2007-2009, LPT funding directly managed by the laboratory came essentially from the **CNRS**, the **Ministère de l'Enseignement supérieur et de la Recherche (MESR) & Université Paul Sabatier (UPS)**, seven contracts with the **Agence Nationale de la Recherche (ANR)**, and two contracts with the **European Union (EU)**. In addition, the LPT occasionally receives other funding from the CNRS, the MESR & UPS, or the **Midi-Pyrénées region**, which are managed by these institutions, but from which the LPT fully benefits. These different sources of funding are explicitly described in the next two sections. Tab. 2.1 details the total LPT budget in 2007, 2008, and 2009 (preliminary figures), including the resources not directly managed by the LPT. The expenses of the LPT in 2007 and 2008 are described in Tab. 2.2 and Tab. 2.3.

Remarks:

❍ All amounts are given in k€ HT (thousands of € Hors Taxe, *i.e.* excluding the VAT of 19.6 %). MESR funding is initially attributed to the LPT including VAT (Toutes Taxes Comprises; TTC).

❍ The term "Missions" includes travel expenses (tickets, hotels, taxi...), conference registration costs,... In 2007, E. SURAUD was Co-Scientific Director (Directeur scientifique adjoint; DSA) of the INSTITUT NATIONAL DE PHYSIQUE NUCLÉAIRE ET DE PHYSIQUE DES PARTICULES (IN2P3) and hence received a specific budget from the IN2P3 covering in particular his large travel expenses.

❍ The field "Salaries" essentially refers to the salaries of ANR and EU postdocs.

❍ The field "Other expenses" mostly refers to the LPT contribution to the university on-line and paper library, network costs, phone bills, copier and paper costs, postal costs, furniture, office supply, electrical work, air conditioning of the LPT computer room, paint work...

❍ Most of the LPT computer cluster was financed in 2007, 2/3 on a CNRS *Crédit mi-lourd* and 1/3 by the LPT's CNRS/IN2P3/MESR annual funding and contracts.

❍ CNRS and MESR annual funding allocations were entirely spent at the end of each year in 2007 and 2008 ("reliquats"/balance lower than 50 € on each account). A fraction of the PPF and

Origin	2007	2008	2009
CNRS			
Crédits annuels CNRS	25	23	23
Dotation mi-lourd	100	—	—
Dotation IN2P3	40	—	—
Other CNRS funding	3	30	—
TOTAL CNRS	168	53	23
MESR & Université Paul Sabatier			
Crédits annuels MESR	38	38	38
PPF FFC	14	14	14
Chaire IUF junior	12	12	12
AO 2007 du CS de l'UPS	4	—	—
IRSAMC funding of LPT	3	12	21
TOTAL MESR & UPS	71	76	85
ANR & European contracts			
EU contract EuroSQIP	39	11	—
ANR INFOSYSQQ	45	15	—
ANR NPMSFFC	51	122	41
ANR MICONANO	13	13	4
ANR MIRRAMO	32	32	48
ANR SIMONANOMEM	—	35	47
EU contract NANOBORON	—	3	4
ANR NANOTERRA	—	—	27
ANR Q-BONDS	—	—	42
TOTAL CONTRACTS	180	231	213
TOTAL MANAGED BY LPT	**419**	**360**	**321**
Other funding not managed by LPT (estimates)			
Chercheurs invités CNRS	30	15	30
Postdoc CNRS	—	11	45
PhD CNRS	—	—	10
Professeurs invités UPS	12	18	18
AO 2007 du CS de l'UPS	30	30	30
AO 2009 du CS de l'UPS	—	—	42
Chaire P. de Fermat (Région)	—	60	—
TOTAL NOT MANAGED BY LPT	**72**	**134**	**175**
TOTAL RESOURCES	**491**	**494**	**496**

Table 2.1 : *Budget of the LPT in 2007, 2008, and 2009 (preliminary figures), in k€ HT.*

Expenses 2007	CNRS	Contracts	MESR	TOTAL
Missions LPT	37	25	7	69
Missions guests	9	9	2	20
Computers	113	9	26	148
Salaries	—	137	5	142
Other expenses	9	—	22	31
TOTAL	**168**	**180**	**62**	**410**

Table 2.2 : *Expenses of the LPT in 2007 (resources directly managed by the LPT), in k€ HT.*

Expenses 2008	CNRS	Contracts	MESR	TOTAL
Missions LPT	6	25	16	47
Missions guests	6	23	3	32
Computers	12	12	30	54
Salaries	—	171	—	171
Other expenses	29	—	26	55
TOTAL	**53**	**231**	**75**	**359**

Table 2.3 : *Expenses of the LPT in 2008 (resources directly managed by the LPT), in k€ HT.*

IUF funds was carried forward from 2007 to 2008. A large part of the NPMSFFC ANR contract funds from 2006-2007 was carried forward to 2008 and extended to 2009.

Overall, and despite the exceptional funds allocated by the CNRS in 2007 (*Crédit mi-lourd* and *Dotation IN2P3*), the **total annual resources of the LPT** (managed or not by the laboratory) have remained stable during the period 2007-2009 at just below **500 k€ HT**.

2.2 Active ANR end EU contracts

EuroSQIP – European Superconducting Quantum Information Processor	
LPT coordinator: **D. SHEPELYANSKY**	Coordinator: G WENDIN (Chalmers Un., Sweden)
Program: *European Contract 2005*	LPT group : QUANTWARE
Starting date: **01/11/2005**	Ending date : **31/10/2009**
	Amount attributed to the LPT (including salaries) : 150 k€
INFOSYSQQ – Intrication, décoherence et algorithmes quantiques	
LPT coordinator: **B. GEORGEOT**	Coordinator: B. GEORGEOT
Program: *ANR Jeunes-Chercheurs 2005*	LPT group : QUANTWARE
Starting date: **30/11/2005**	Ending date : **29/11/2008**
	Amount attributed to the LPT (including salaries) : 150 k€
NPMSFFC – Nouvelles Phases de la Matière dans les Systèmes de Fermions Fortement Corrélés	
LPT coordinator: **D. POILBLANC**	Coordinator: D. POILBLANC
Program: *ANR Blanc 2005*	LPT group : FFC
Starting date: **30/11/2005**	Ending date : **29/11/2009**
	Amount attributed to the LPT (including salaries) : 170 k€
MICONANO – Transport dans des structures nanoscopiques contrôlé par micro-onde	
LPT coordinator: **D. SHEPELYANSKY**	Coordinator: J.-C. PORTAL (LNCMI, Grenoble & Toulouse)
Program: *ANR NANO 2005*	LPT group : QUANTWARE
Starting date: **01/12/2005**	Ending date : **30/04/2009**
	Amount attributed to the LPT (including salaries) : 42 k€
MIRRAMO – Mécanismes élémentaires d'IRRAdiation de MOlécules biologiques	
LPT coordinator: **E. SURAUD**	Coordinator: M. FARIZON (IPNL, Lyon)
Program: *ANR Blanc 2006*	LPT group : AGRÉGATS
Starting date: **06/11/2006**	Ending date : **05/11/2009**
	Amount attributed to the LPT (including salaries) : 91 k€
SIMONANOMEM – Simulation and modeling of the transport across polymeric nanoporous membranes	
LPT coordinator: **J. PALMERI**	Coordinator: J. PALMERI
Program: *ANR NANO 2007*	LPT group : PHYSTAT
Starting date: **05/02/2008**	Ending date : **04/02/2011**
	Amount attributed to the LPT (including salaries) : 116 k€
NANOBORON – Study of membranes processes for the treatment of residual waters from the ceramic industry	
LPT coordinator: **J. PALMERI**	Coordinator: A. DERATANI (IEM, Un. Montpellier-CNRS)
Program: *European Contract Euréka 2008*	LPT group : PHYSTAT
Starting date: **20/02/2008**	Ending date : **19/02/2010**
	Amount attributed to the LPT (including salaries) : 10 k€
NANOTERRA – Nanodétecteurs de radiation microondes et terahertz basés sur l'effet ratchet	
LPT coordinator: **D. SHEPELYANSKY**	Coordinator: J.-C. PORTAL (LNCMI, Grenoble & Toulouse)
Program: *ANR NANO 2008*	LPT group : QUANTWARE
Starting date: **01/01/2009**	Ending date : **31/12/2011**
	Amount attributed to the LPT (including salaries) : 110 k€
Q-BONDS – Corrélations quantiques et intrication dans les états liens de valence	
LPT coordinator: **F. ALET**	Coordinator: F. ALET
Program: *ANR Jeunes-Chercheurs 2008*	LPT group : FFC
Starting date: **01/01/2009**	Ending date : **31/12/2011**
	Amount attributed to the LPT (including salaries) : 200 k€

Table 2.4 : *Active ANR et European contracts during the period 2007-2009.*

2.3 Other financial resources

This section details the recurrent LPT funding for the period 2007-2010 (Tab. 2.5), the occasional funding (excluding ANR and EU contracts) managed by the LPT (Tab. 2.6), and the estimated equivalent of punctual funding received by the LPT but managed by the corresponding funding institutions (Tab. 2.7; excluding PhD fellowships from the MESR or directly obtained by the PhD student from other sources: DGA, École Polytechnique, AS ENS, AUF...).

Annual CNRS funding	
Coordinator: **LPT**	
Source: *CNRS*	LPT group: LPT
Periode: **2007-2010**	Remark: **25 k€ in 2007, 23 k€ in 2008 and 2009**
	Annual amount for LPT: ∼23 k€/year
Annual MESR funding	
Coordinator: **LPT**	
Source: *MESR*	LPT group: LPT
Periode: **2007-2010**	Remark: **UPS charges deducted (library, phone...)**
	Annual amount for LPT: ∼38 k€/year
PPF Fermions Fortement Corrélés	
Coordinator: **D. POILBLANC**	
Source: *MESR & CNRS*	LPT group: FFC
Periode: **2007-2010**	Remark: –
	Annual amount for LPT: 14 k€/year
Funding from the annual MESR funding of IRSAMC	
Coordinator: **LPT**	
Source: *Fédération IRSAMC*	LPT group: LPT
Periode: **2007-2010**	Remark: **36 k€ in 2007-2009**
	Annual amount for LPT: ∼12 k€/year
Chaire junior de l'Institut Universitaire de France	
Coordinator: **D. DEAN**	
Source: *IUF 2007*	LPT group: PhyStat
Periode: **2007-2011**	Remark: **12 k€/year + teaching dispensation**
	Annual amount for LPT: 12 k€/year

Table 2.5 : *Reccurent resources managed by the LPT.*

Dotation mi-lourd CNRS	
Coordinator: **LPT**	
Source: *CNRS 2007*	LPT group: LPT
Period: **2007**	
	Amount for the LPT: 100 k€

Dotation IN2P3	
Coordinator: **E. SURAUD**	
Source: *CNRS-IN2P3 2007*	LPT group: Agrégats *and LPT*
Period: **2007**	
	Amount for the LPT: 40 k€

CNRS-CONICET Program	
Coordinator: **P. PUJOL**	
Source: *CNRS 2007*	LPT group: FFC
Period: **2007**	
	Amount for the LPT: 3 k€

Partenariat Hubert Curien franco-allemand	
Coordinator: **S. CAPPONI**	
Source: *PROCOPE 2007*	LPT group: FFC
Period: **2007-2008**	
	Amount for the LPT: 5 k€

Appel d'offres bisannuel du Conseil Scientifique de l'UPS	
Coordinator: **N. DESTAINVILLE**	
Source: *Université Paul Sabatier 2007*	LPT group: PhyStat
Period: **2008**	
	Amount for the LPT: 4 k€

Interface physique, biologie et chimie : soutien à la prise de risque	
Coordinator: **N. DESTAINVILLE**	
Source: *CNRS 2008*	LPT group: PhyStat
Period: **2008**	
	Amount for the LPT: 30 k€

CENEC – Étude de la faisabilité de filtrer des effluents de l'industrie de traitements de surface	
Coordinator: **J. PALMERI**	
Source: *CEA 2008*	LPT group: PhyStat
Period: **2008**	
	Amount for the LPT: 6 k€

Table 2.6 : *Ponctual resources managed by the LPT.*

CNRS guest scientists program	
Coordinator: **LPT**	
Source: *CNRS 2007*	LPT group: LPT
Period: **2007-2010**	Nature of funding: **~6 months/year at the CR1 level**
	Estimated equivalent amount for LPT: ~25 k€/an
Université Paul Sabatier guest professors program	
Coordinator: **LPT**	
Source: *Université Paul Sabatier 2007*	LPT group: LPT
Period: **2007-2010**	Nature of funding: **~3 months/year at the PR1 level**
	Estimated equivalent amount for LPT: ~16 k€/year
Appel d'offres bisannuel du Conseil Scientifique de l'UPS	
Coordinator: **N. DESTAINVILLE**	
Source: *Université Paul Sabatier 2007*	LPT group: PhyStat
Period: **2008-2010**	Nature of funding: **1 PhD fellowship (codirection LPT-IPBS)**
	Estimated equivalent amount for LPT: 90 k€
Postdoc CNRS	
Coordinator: **LPT**	
Source: *CNRS 2008*	LPT group: PhyStat
Period: **2009-2010**	Nature of funding: **24 months postdoctoral position**
	Estimated equivalent amount for LPT: ~95 k€
Chaire d'excellence Pierre de Fermat (filled by Frédéric Mila)	
Coordinator: **D. POILBLANC**	
Source: *Région Midi-Pyrénées 2008*	LPT group: FFC
Period: **2008**	Nature of funding: **salary, computers, and other expenses**
	Estimated equivalent amount for LPT: ~60 k€
Appel d'offres bisannuel du Conseil Scientifique de l'UPS	
Coordinator: **D. POILBLANC**	
Source: *Université Paul Sabatier 2009*	LPT group: FFC
Period: **2009-2011**	Nature of funding: **1 PhD (LNCMI) + 12 months postdoc (LPT)**
	Estimated equivalent amount for LPT: ~40 k€
PhD fellowship CNRS	
Coordinator: **LPT**	
Source: *CNRS 2009*	LPT group: FFC
Period: **2009-2012**	Nature of funding: **36 months PhD fellowship**
	Estimated equivalent amount for LPT: ~90 k€

Table 2.7 : Funding attributed to the LPT, but directly managed by the corresponding funding institution.

3 Computer systems

As a theoretical laboratory, the LPT is a heavy consumer of computing resources. This chapter presents the computer infrastructure of LPT (network, terminals, computer cluster...), and the people maintaining it. In March 2009, the LPT and the Fédération IRSAMC were recognized by the CNRS as a *Centre Automatisé de Traitement de l'Information (CATI; IT Center)*.

3.1 Computers at the LPT

Network

The LPT shares a local network with the Fédération IRSAMC and the web and mail servers are also managed at the IRSAMC level. The network is only accessible from outside LPT's network through one unique secure server. Inside the LPT, laptops can be connected on any Ethernet socket once the MAC number of the computer has been duly registered (for security reasons). In addition, the Université Paul Sabatier provides free Wi-Fi access to any registered user (researchers, postdocs, and students) working at the LPT.

Terminals

The LPT manages around 60 recent *PC-Fedora Linux* and *Mac-OS X* terminals and servers. During the last two years, most of the terminals have been upgraded to the current standard. In addition, LPT permanent staff have personal access to 15 or so laptop computers (*PC-Linux*, *PC-Windows XP/Vista*, or *Mac-OS X*, depending on user's choice). A dozen external network drives are installed to save non essential numerical data or for other personal backups and are managed by their users.

Cluster

Two-thirds of the LPT permanent staff perform heavy numerical simulations in the framework of their scientific activity. Although the LPT has always had a network of workstations (starting with *HP* workstations in 1992), and a small Mirinet cluster since 2005, the LPT has long felt the need for a powerful computer cluster. With the help of a specific CNRS *Crédit milourd* of 100 k€ HT obtained in 2007, and with an additional investment of around 60 k€ HT from its own resources in 2007-2009, the LPT has now equipped itself with a computer cluster of significant computing power:

- 37 *Intel* biprocessors quad-core 2.6 or 3.0 GHz, with 8 Go RAM and 250 Go disk (296 effective processors).
- 4 *Intel* biprocessors dual-core 3.0 GHz, with 24 to 32 Go RAM and 250 Go disk.
- 8 *AMD* Opteron 2.6 GHz with 4 Go RAM and fast Mirinet connection for parallel computing (installed in 2005).
- 1 frontal server *Intel* biprocessor quad-core 3.0 GHz, with 8 Go RAM and 4×1.5 To disks.
- The cluster is electrically protected by a series of *UPS* surge suppressors.
- The full hardware and software maintenance is ensured by the company *ALINEOS* from whom the cluster was bought.

In 2009-2010, the IRSAMC will regroup all its computer clusters and main servers in a unique computer room (∼ 80 k€ investment).

3.2 Human resources devoted to LPT computer systems

The LPT does not have any computer technician of its own. However, Sandrine Le Magoarou (AI CNRS), from the mutualized pool of IRSAMC technicians, works at least 50 % for the LPT and is located on the LPT floor. She is involved in most maintenance operations (terminals, IRSAMC web and mail server), and orders and repairs of computer hardware (excluding the cluster). She also orders and installs most software on the LPT servers and terminals.

F. Alet is the official webmaster of the LPT, in coordination with S. Le Magoarou who supervises the development of the new IRSAMC web site which is currently under construction.

F. Alet, S. Capponi, M. Mambrini survey the good functioning of the cluster and are the local LPT contacts for *ALINEOS*. K. Frahm and these three researchers also provide valuable assistance to LPT computer users.

3.3 Web site and communication

LPT web site follows the CNRS *charte graphique* since 2006. In March 2009, F. Alet (LPT webmaster) upgraded the LPT web site to the latest version of the more secure CNRS *Spip* package. The web site is now bilingual (French/English), although many scientific articles can only be found in English.

After logging on to the secure Intranet, each user/group maintains its own personal web page and LPT publication list, and can publish scientific news, job offers (postdocs, PhD, ATER), or any other document.

The administrative section (Intranet) contains useful information and documents regarding guest scientist invitations, missions, CNRS credit cards... This section and the public and fully bilingual practical information section are maintained by S. Scaldaferro-Miralles. P. Pujol is currently in charge of maintaining the seminar section, succeeding D. Shepelyansky in 2008.

3.4 Network and computer security

Network and computer security is a constant concern at the LPT. Although most of the network security (network surveillance, anti-spam...) is ensured by the *Centre Interuniversitaire de Calcul de Toulouse (CICT)*, the LPT and in particular S. Le Magoarou (CSSI) and her colleagues from the IRSAMC computer technician pool are extremely vigilant on security matters:

❍ A unique way of accessing the LPT network from outside (this server has a collection of "sniffers" for detecting hostile attacks).

❍ S. Le Magoarou receives security alerts from CICT (bugs, security holes, patches...) and swiftly applies their recommendations.

❍ The 8 mounted user home disks and the servers are backed up every week.

❍ Operating systems are regularly updated/upgraded.

❍ The good functioning of sensitive services (DHCP, Mail, NIS, Web) is monitored.

❍ Systematic installation of antivirus and antispywares on *Windows* laptops.

❍ DHCP at the LPT only works for registered computers and laptops (through their MAC address).

❍ Every new person working at the LPT signs a formal *Charte informatique IRSAMC*, and old accounts are archived except if the user comes back regularly at the LPT.

❍ S. Le Magoarou has followed several CNRS training courses on computer security (See Section 1.5). She is also *Autorité d'Enregistrement (AE)* CNRS-Plus et CNRS-Standard for the LPT and LCPQ (control of the access to CNRS IT applications).

3.5 External computing resources

The powerful LPT cluster does not always fully meet the needs of our researchers heavily involved in numerical simulations. LPT scientists have thus free access to the local computing facility *Calcul en Midi-Pyrénées* (CALMIP) which has a 1.5 Teraflops computing power, and to the national CNRS facility *Institut du Développement et des Ressources en Informatique Scientifique* (IDRIS) which is currently the 9th most powerful computing center in the world.

4

Teaching and diffusion of scientific knowledge

The LPT's UPS enseignants-chercheurs and CNRS researchers devote a large part of their activity to teaching a variety of subject matters in physics, but also in biophysics, mathematics, chemistry, and computer sciences, at all university levels. Moreover, 10 PhD students and 5 postdocs have typically been working at the LPT each year since 2007. These students and postdocs have shown a very high success rate in finding permanent jobs in the academic sector or stable jobs in the private sector. LPT scientists participate in a large variety of activities and events in order to promote the diffusion of scientific knowledge (conference organization, editorial committees, popular conferences, laboratory visits...), and are also deeply involved in the local and national organization and administration of research and education.

4.1 PhD and postdoc supervision

PhD thesis completed or in progress

This section lists the PhD theses completed [1] under the supervision of LPT permanent scientists during the period 06/2005-06/2009 (10), during the period 07/2009-10/2009 (4 at LPT + 2 PhD theses co-supervised by LPT scientists), or in progress after 10/2009 (7). 5 + 2 PhD theses will hence be defended in 2009 and 3 students from the École Polytechnique, the Université du Maine, and the Indian Institute of Technology in Madras (India) will start their PhD at LPT in October 2009, financed by three different funding sources (AMX, MESR/UPS, CNRS).

Tab. 4.1 summarizes the current status of LPT PhD students having completed their PhD between 2002 and 2008. We also list the 10 postdocs who have worked at LPT since 2005, indicating the source of financing of their salary. For the 4 postdocs having completed their contract before 01/01/2009, we also mention their current employment.

It is certainly an encouraging sign that **18 out of 19 [2] former non-permanent LPT researchers** mentioned in this report (15 PhD students in Tab. 4.1 and 4 postdocs) **have already found a permanent academic job (9 in France; 4 abroad) or a stable CDI [3] job in the private sector (4 in France; 1 abroad)**.

1. Note that many PhD theses were completed in 2004-2005, explaining the dip in theses completed in 2006, and the large number of PhD theses expected to be completed at the end of 2009 (see Tab. 4.1 and the list of LPT PhD's).
2. The LPT was shocked and deeply sadden by the death of Fabien Mégi, a former PhD student at LPT, in May 2008.
3. CDI: Contrat à Durée Indéterminée; contract of undetermined duration.

Fermions Fortement Corrélés

[TH-1] G. Roux, *Échelles de spins dopées sous champ magnétique (Doped spin ladders in strong magnetic field)*, PhD thesis, Université Paul Sabatier (01/09/2004-12/07/2007); supervisors: D. Poilblanc and S. Capponi.

[TH-2] A. Abendschein, *Modèles effectifs pour des systèmes magnétiques sous champ (Effective models for spin systems in magnetic field)*, PhD thesis, Université Paul Sabatier (01/10/2005-23/10/2008); supervisor: S. Capponi.

[TH-3] M. Moliner, *Effects of lattice distortions on low dimensional strongly correlated systems (Effets des distortions du réseau sur les systèmes fortement corrélés de basse dimensionnalité)*, PhD thesis, Université de Strasbourg and Université Paul Sabatier (01/09/2004-03/02/2009); supervisors: D. Cabra and P. Pujol.

[TH-4] F. Trousselet, *Modèles contraints classiques et quantiques à deux dimensions (Constrained classical and quantum models in 2D*, PhD thesis, Université Paul Sabatier (01/10/2005-26/06/2009); supervisors: D. Poilblanc and P. Pujol.

[TH-5] D. Charrier, *Modèles effectifs pour les systèmes magnétiques frutsrés (Effective models for frustrated magnetic systems)*, PhD thesis, Université Paul Sabatier (01/09/2005-18/09/2009); supervisors: P. Pujol and C. Chamon.

[TH-6] D. Schwandt, *Théorie RVB des phases magnétiques exotiques (RVB theory of exotic magnetic phases)*, PhD thesis, Université Paul Sabatier (01/10/2008-∼10/2011); supervisor: F. Alet and M. Mambrini.

[TH-7] Y. Iqbal, *Liquides de spins de Dirac dans des antiferro-aimants quantiques frustrés (Dirac spin liquids in quantum frustrated antiferromagnets)*, PhD thesis, Université Paul Sabatier (01/10/2009-∼10/2012); supervisor: D. Poilblanc.

Information et Chaos Quantiques

[TH-8] L. Arnaud, *Étude de l'interférence et de la décohérence en informatique quantique (Study of interference and decoherence in quantum information)*, PhD thesis, Université Paul Sabatier (01/12/2006-15/10/2009); supervisor: D. Braun.

[TH-9] B. Roubert, *Analyse semiclassique en informatique quantique (Semiclassical analysis in quantum information)*, PhD thesis, Université Paul Sabatier (01/10/2007-∼30/09/2010); supervisor: D. Braun.

[TH-10] M. Pasek, *Application des méthodes du chaos quantique aux oscillations d'étoiles en rotation rapide (Applications of quantum chaos semiclassical methods to the oscillations of rapidly spinning stars)*, PhD thesis, Université Paul Sabatier (01/10/2009-∼30/09/2012); supervisors: B. Georgeot and F. Lignières (LATT-OMP).

Physique Statistique des Systèmes Complexes

[TH-11] V. Desoutter, *Étude de deux systèmes dynamiques dominés par des phénomènes entropiques (Study of two dynamical systems dominated by entropic phenomena)*, PhD thesis, Université Paul Sabatier (01/10/2001-4/10/2005); supervisor: N. Destainville.

[TH-12] M. Metaiche, *Optimization of reverse osmosis desalination systems, operating parameters and numerical simulations (Optimisation des systèmes de désalination, paramètres opératoires, et simulations numériques)*, PhD thesis (co-direction), École Nationale Polytechnique d'Alger (Algeria) and University de Montpellier II, France (01/10/2004-15/12/2007); supervisors: A. Kettab and J. Palmeri.

[TH-13] J. Sopik, *Dynamique de marcheurs aléatoires en interaction (Dynamics of interacting random walkers*, PhD thesis, Université Paul Sabatier (01/10/2003-26/06/2007); supervisor: C. Sire.

[TH-14] J. Dweik, *Molecular modeling of membrane transport (Modélisation moléculaire du transport membranaire)*, PhD thesis, University de Montpellier II (01/09/2005-19/12/2008); supervisor: J. Palmeri.

[TH-15] L. Horvath, *Molecular dynamics studies of water, ions, and macromolecules in nanopores (Étude de dynamique moléculaire de l'eau, des ions, et des macromolécules dans des nanopores)*, PhD thesis (co-direction), Université Paul Sabatier and University Babes-Bolyai (Cluj-Napoca, Romania) (01/10/2006-∼ 10/2009); supervisors: J. Palmeri and T. Beu.

[TH-16] C. Touya, *Diffusion dans des potentiels aléatoires non gaussiens (Diffusion in non-Gaussian random potentials)*, PhD thesis, Université Paul Sabatier (01/10/2006-∼ 30/09/2009); supervisor: D. S Dean.

[TH-17] T. Portet, *Étude de l'électroperméablisation de vésicules artificiels (Study of the electropermeabilisation of artificial vesicles)*, PhD thesis, Université Paul Sabatier (01/10/2007-∼ 10/2010); supervisors: D. S Dean and M.-P. Rols (IPBS).

[TH-18] V. Demery, *Modèles physiques pour l'électroperméabilisation des membranes (Physical models of membrane electropermeabilization)*, PhD thesis, Université Paul Sabatier (01/10/2009-∼ 30/09/2012); supervisor: D. S Dean.

Systèmes de Fermions Finis – Agrégats

[TH-19] F. Mégi, *Étude théorique d'agrégats soumis à des champs lasers intenses (Theoretical study of clusters in intense laser fields)*, PhD thesis, Université Paul Sabatier (01/09/2001-13/06/2005); supervisor: M. Belkacem and É. Suraud.

[TH-20] G. Bousquet, *Modélisation numérique d'agrégats de sodium en matrice d'argon (Numerical modeling of sodium clusters in argon matrices)*, PhD thesis, Université Paul Sabatier (01/10/2004-14/02/2008); supervisor: É. Suraud.

[TH-21] J. Messud, *Correction d'auto-interaction dépendant du temps (Time-dependent self-interaction correction)*, PhD thesis, Université Paul Sabatier (01/09/2007-∼ 09/2009); supervisor: É. Suraud.

[TH-22] Z. P. Wang, *Time-dependent description of irradiation of organic molecules (Dynamique de l'irradiation de molécules organiques)*, PhD thesis, Beijing Normal University and Université Paul Sabatier (01/09/2006-∼ 09/2009); Z. P. Wang spent one year in Toulouse for her PhD from 10/2007 to 10/2008; supervisors: F. S. Zhang and É. Suraud.

[TH-23] S. Vidal, *Méthodes hiérarchiques pour la dynamique des agrégats et molécules en contact avec un environnement (Hierarchical methods for the dynamics of clusters and molecules in contact with an environment)*, PhD thesis, Université Paul Sabatier (01/09/2008-∼ 09/2011); supervisor: P. M. Dinh.

L. Arnaud received the prize of the best talk given at the Journées de l'École doctorale *Sciences de la Matière* (UPS doctoral school of physic, chemistry, and material sciences), presenting a summary of his ongoing PhD thesis (1000 € to fund his research/travel expenses; May 2009).

NAME & First name	PhD	Current situation (06/2009)
ABENDSCHEIN Andreas	10/2008	Engineer (CDI) at *Sew-Eurodrive* (Karlsruhe, Germany)
BOUSQUET Gaspard	02/2008	Unemployed (Toulouse)
ROUX Guillaume	07/2007	MCF Section CNU 29 at LPTMS, U. Paris-Sud (Orsay)
SOPIK Jullien	06/2007	Engineer (CDI) at *Sogeti* (Toulouse)
DESOUTTER Vianney	10/2005	Physics teacher CAPES (Prépa Agrégation)
MÉGI Fabien	06/2005	Deceased
LÉVI Benjamin	11/2004	Engineer (CDI) at *Areva* (Paris)
POMERANKSI Andrei	10/2004	Permanent researcher at Budker Institute (Novosibirsk, Russia)
LAFLORENCIE Nicolas	07/2004	CR2 Section 06 CNRS at LPS, U. Paris-Sud (Orsay)
MING MA Leang	03/2004	Engineer (CDI) at *Sogeti* (Toulouse); MBA at ECT
MAGNOUX David	07/2003	Physics teacher Agrégé (Lycée A. Chamson, Le Vigan)
LEFÈVRE Alexandre	07/2003	CR2 CNRS at IPHT, CEA (Saclay)
CHERRIER Raphaël	07/2003	MCF Section CNU 29 at ENSAM (Bordeaux)
CALDARA Gaétan	12/2002	Physics teacher Agrégé; Prépa PC (Lycée A. Briand, Évreux)
ALET Fabien	06/2002	CR2 Section 06 CNRS at LPT, U. Paul Sabatier (Toulouse)
GIGLIO Éric	01/2002	CR1 Section 05 CNRS at CIMAP (Caen)

Table 4.1 : *current status of LPT PhD students having completed their PhD between 2002 and 2008. CDI (Contrat à Durée Indéterminée) refers to a contract of undetermined duration.*

Postdocs

Fermions Fortement Corrélés

[PD-1] A. Ralko, financed by *ANR NPMSFFC* (10/2006-10/2008). Supervisor: D. Poilblanc. MCF at Institut Néel (Grenoble).

[PD-2] M. Capello, financed by *ANR NPMSFFC* and *CNRS* (10/2006-10/2008): Supervisor: D. Poilblanc. Engineer (CDI) at *ATOS Origin* (subcontractor of CNES, Toulouse).

[PD-3] F. Albuquerque, financed by *ANR Q-BONDS* (06/2009-06/2011). Supervisor: F. Alet.

[PD-4] J. Almeida, financed by *Conseil Scientifique de l'UPS* (10/2009-10/2010). Supervisor: D. Poilblanc.

Information et Chaos Quantiques

[PD-5] I. García-Mata, financed by *EU contract EuroSQIP* (04/2006-04/2008) and *ANR INFOSYSQQ* (04/2008-10/2008). Supervisors: D. Shepelyansky and B. Georgeot. Permanent CONICET researcher at TANDAR Lab – CNEA (Argentina).

[PD-6] J. Martin, financed by *ANR INFOSYSQQ* (10/2006-10/2008). Supervisor: B. Georgeot. FNRS researcher at IPNAS, Université de Liège (Belgium).

[PD-7] L. Ermann, financed by *ANR NANOTERRA* (09/2009-09/2011). Supervisor: D. Shepelyansky.

Physique Statistique des Systèmes Complexes

[PD-8] S. Buyukdagli, financed by *ANR SIMONANOMEM* (12/2008-12/2010). Supervisor: J. Palmeri.

[PD-9] L. Delfini, financed by *CNRS Postdoctoral Program* (10/2008-10/2010). Supervisor: P. H. Chavanis.

Systèmes de Fermions Finis – Agrégats

[PD-10] U. F. Ndongmouo Taffoti, financed by *ANR MIRRAMO* (07/2007-07/2009). Supervisor: E. Suraud.

4.2 Teaching and administrative responsibilities

Within the Licence-Master-Doctorat (LMD) structure of the university teaching system, UPS enseignants-chercheurs (EC), but also 5 out of 9 CNRS researchers at the LPT ensure various teaching duties[4] (CM, TD, TP), in physics, biophysics, mathematics, chemistry, and computer sciences (scientific lectures given at summer schools and conferences are listed in Section 9.3).

Teaching dispensed at the Université Paul Sabatier

The main courses taught by EC and CNRS researchers at the Université Paul Sabatier are listed below (in the physics degree course except when specified):

L1 level:

- CM in electrical physics
- CM in mechanics
- CM on nuclear risks (all degree courses)
- CM in electromagnetism
- TD in biophysics at UPS Medical School (PCEM1)
- TD in general physic (all degree courses)
- TD in thermodynamics (biology degree course)

L2 level:

- CM in statistical physics
- TD and TP in computer sciences (physics and chemistry degree courses)
- TD in analytical methods in physics
- TP in general physics
- TD in mathematics

L3 level:

- CM and TD in statistical physics
- CM and TD in mathematics
- CM in quantum mechanics
- CM in nuclear physics
- CM in relativity theory
- CM in mechanics of continuous media
- CM on symmetries in physics
- CM in analytical mechanics
- TD and TP in computer sciences
- TP in general physics

4. Cours Magistraux: lectures; Travaux Dirigés: exercise solving classes related to lectures; Travaux Pratiques: practical and lab work.

M1 level:

- ❍ CM and TD in irreversible processes
- ❍ CM, TD, numerical TP in non-linear physics
- ❍ CM in numerical methods
- ❍ TD in statistical physics

M2 level:

- ❍ CM in condensed matter physics
- ❍ CM in cluster physics
- ❍ CM in out of equilibrium physics
- ❍ CM in statistical physics
- ❍ CM in numerical methods
- ❍ TD in scientific English

Teaching dispensed at other universities and schools

❍ CM in chemistry of solids (M1) at École Nationale Supérieure de Chimie de Montpellier & Université de Montpellier II

❍ CM in material sciences (M2) at Université de Montpellier II

❍ CM in cluster physics (M2) at Université de Bordeaux

❍ CM in advanced quantum mechanics (M2) at ENS Lyon

❍ TD in mathematics (∼L3-M1) at École Nationale Supérieure de l'Aéronautique et de l'Espace (ENSAE Toulouse – Sup'Aéro)

❍ Several CM (∼M1) for the *Préparation à l'Agrégation de Physique* and *Préparation à l'Agrégation de Physique Appliquée* at UPS

❍ Colles (oral exercises; ∼L1-L2) at Lycée Pierre de Fermat and Lycée Bellevue (Toulouse)

Responsibilities in physics degree courses

❍ K. Frahm: responsible for organizing the *L3 – Physique Fondamentale* at UPS since 2007. This also involves writing the "dossier d'habilitation".

❍ D. S. Dean: co-responsible (with M. A. Bouchène, LCAR) for organizing the *M2 – Physique de la Matière* at UPS since 2005. This also involves writing the "dossier d'habilitation".

❍ D. Braun: coordinator of the "module" *Physique quantique et outils pour la physique I* (L3; ∼10 teachers) and of the "Unités d'Enseignement" *Mécanique et ses applications en astrophysique* (L2; 5 teachers), *Outils mathématiques pour la physique* (L3; 5 teachers), and *Mécanique quantique* (M2).

❍ N. Destainville: coordinator of the "module" *Physique statistique et outils pour la physique II* (L3; ∼10 teachers). Responsible for organizing the future Master (M1-M2) *Physique et chimie pour le vivant et la santé* leading to 2 M2: *Physique du vivant* and *Chimie et santé*. This also involves writing the first "dossier d'habilitation".

❍ K. Frahm: coordinator of the "module" *Physique non-linéaire et méthodes numériques* (M1; ∼8 teachers) since 2000.

❍ M. Manghi: coordinator of the "module" *Physique classique* (L3; ∼8 teachers); creation and responsibility of the L3 option *Symmetries in physics* (now under the responsibility of S. Capponi).

❍ M. Sève-Dinh: coordinator of the "module" *Méthodes analytiques pour la physique et modélisation* (L2; ∼7 teachers) and *Outils de la physique statistique* (L3).

❍ S. Capponi: Président d'un jury du baccalauréat (2008).

Administrative responsibilities

LPT scientists are also deeply involved in the **local and national organization and administration of research and education**. We list below a non exhaustive list of the main responsibilities assumed during the past four years by LPT members (see their attached personal activity report):

- Directeur Scientifique Adjoint (DSA) IN2P3-CNRS
- Comité National de la Recherche Scientifique (CNRS Sections 02 & 06)
- Conseil National des Universités (29ième section)
- Conseil Scientifique de l'UPS
- Direction Stratégique de la Recherche de l'UPS
- Direction de la Fédération IRSAMC; Bureau et Conseil de la Fédération IRSAMC
- Conseil Scientifique de l'UFR Physique-Chimie-Automatique de l'UPS
- Conseil du Département de Physique de l'UPS
- Conseil de l'École Doctorale *Science de la Matière* de l'UPS
- Collège Scientifique de Physique & Sciences de l'Univers de l'UPS
- Several researcher/technician recruiting committees at UPS, CNRS, and other universities
- Coordination Scientifique de la CSD4 – Physique au sein de l'USAR, unité support de l'ANR du CNRS
- Comité Scientifique Disciplinaire des programmes *Blanc* et *Jeunes Chercheuses et Jeunes Chercheurs* pour la physique (CSD4 – Physique)
- AERES, CNRS, and CEA evaluation committees
- Expert referees for ANR, EU (ICT-FET Programs), NSF & DOE (USA), DFG (Germany), ISF (Israel), NWO (Netherlands), Academy of Finland...

4.3 Diffusion of scientific information

Conference organization

We list below the conferences organized or co-organized by LPT members since 2005. Invited scientific lectures given in summer schools and conferences are listed in Section 9.3 of LPT's scientific production.

[ORG-1] S. Capponi, member of the local organization committee of the *10ièmes Journées de la Matière Condensée de la SFP (JMC10)*, Toulouse, France (28 August-1 September 2006).

[ORG-2] S. Capponi, member of the national organization committee of the *11ièmes Journées de la Matière Condensée de la SFP (JMC11)*, Strasbourg, France (25-29 August 2008).

[ORG-3] D. Poilblanc, *European Science Foundation (ESF) Exploratory Workshop "Effective models for low-dimensional strongly correlated systems"*; Organizers: G. G. Batrouni and D. Poilblanc; Peyresq, France (12-16 September 2005).

[ORG-4] P. Pujol, *Novel theoretical aspects of frustrated spin systems*; Organizers: P. Pujol, D. C. Cabra, and F. Mila; CECAM, Lyon, France (9-11 March 2006).

[ORG-5] P. Pujol, *School on "Modern theories of correlated electron systems"*; School directors: D. C. Cabra, A. Honecker, and P. Pujol; Les Houches, France (11-29 May 2009).

[ORG-6] F. Alet and M. Mambrini, local corganizers of the *Colloque thématique du GdR NEEM*, Aspet, France (October 2009).

[ORG-7] D. Shepelyansky, *Quantum Computers, Algorithms and Chaos*, E. Fermi Summer School; School Directors: G. Casati, D. L. Shepelyansky, and P. Zoller; Scientific secretary: G. Benenti; Varenna, Como Lake, Italy (5-15 July, 2005).

[ORG-8] D. Shepelyansky, *Quantum Information, Computation and Complexity*, Program at the Institut Henri Poincaré; Organizers: Ph. Grangier, M. Santha, and D. L. Shepelyansky; IHP, Paris, France (4 January-7 April, 2006).

[ORG-9] B. Georgeot, national and local co-organizer of the *Colloque thématique du GdR 2285 : "Aspects théoriques de l'information quantique"*, Aspet, France (6-8 June 2008).

[ORG-10] N. Destainville, *Membranes biologiques : relations entre propriétés physiques et fonctions*, colloquium (80 registered participants) organized at the *10ièmes Journées de la Matière Condensée de la SFP (JMC10)*; Organizer: N. Destainville; Toulouse, France (28 August-1 September 2006).

[ORG-11] N. Destainville, co-organizer of the *Journées plénières du GDR CellTiss (Physique de la cellule au tissu)*, Sète, France (12-14 November 2008).

[ORG-12] P. H. Chavanis, *12th Marcel Grossmann Meeting. Parallel session: Self-Gravitating Systems*; Organizer: P. H. Chavanis; UNESCO, Paris, France (12-18 July 2009).

[ORG-13] C. Sire, co-organizer of the LPT-Institut de Mathématiques de Toulouse Colloquium, Toulouse, France (12 june 2009).

[ORG-14] C. Sire, co-organizer of the colloquium Mathématiques, Informatique, Physique, Biologie Intégrative : un Pas vers la Biologie des Systèmes, Toulouse, France (18 june 2009).

Conference advisory committees

❍ D. Dean, member of *Comité de Programmation Scientifique de l'Institut Henri Poincaré*.

❍ D. Poilblanc, member of the Advisory Committee, *The European Conference, Physics of Magnetism 2008* (Poznan, Poland, 24-27 June 2008).

❍ D. Poilblanc, member of Advisory Committee, *School on "Modern theories of correlated electron systems"*, École de Physique (Les Houches, France, 11-29 May 2009).

❍ D. Poilblanc, Scientific Advisor, *KITP Program on Computational Approaches to Quantum Many-body Systems*, University of California Santa Barbara (USA, 4 October-3 December 2010).

Commercial and Open Source software

Hosting many scientists with a strong expertise in numerical simulation, LPT groups have developed one commercial and several Open Source softwares used by the engineering and physics community, which are listed below.

Fermions Fortement Corrélés

[COD-1] F. Alet, *The ALPS project (Algorithms and Libraries for Physics Simulations)*. The ALPS Project is an open source effort aiming at providing high-end simulation codes for strongly correlated quantum mechanical systems as well as C++ libraries for simplifying the development of such code. F. Alet is actively involved in the libraries and applications development.

Information et Chaos Quantiques

[COD-2] K. M. Frahm and D. L. Shepelyansky (Eds.), *Quantware Software Library*. Quantum Numerical Recipes is an Open Source library which contains several software packages enabling simulations of *quantum computer* evolution on *classical computers*.

Physique Statistique des Systèmes Complexes

[COD-3] J. Palmeri, P. David, and X. Lefebvre, *NanoFlux*, Commercial software developed by the Laboratoire de Physique Théorique (LPT-UMR 5152, Toulouse) and the Institut Européen des Membranes (IEM-UMR 5635, Montpellier) under the NanoFlux Project. *NanoFlux Software* is an advanced tool for the prediction and scaling-up of nanofiltration membrane processes (research and development and industrial filtration and separation applications). Three licences were recently sold to Université de Nantes, CEA, and Aker Kvaerner Chemetics (Vancouver, Canada).

Refereeing for international journals

LPT scientists are referees for the following international journals, in a wide range of domains illustrating LPT's **multidisciplinarity**:

Physical Review Letters[5], *Physical Review A; B; C; D; E*, *Nature*, *Nature Physics*, *Europhysics Letters*, *European Physical Journal B; D; E*, *Journal of Physics A; B; C; G*, *European Journal of Physics*, *Journal of Statistical Physics*, *Journal of Statistical Mechanics*, *Physica A; B; C; D*, *Journal of Mathematical Physics*, *International Journal of Theoretical Physics*, *New Journal of Physics*, *Proceedings of the Royal Society*, *Soft Matter*, *Physical Chemistry Chemical Physics*, *Journal of Physical Chemistry*, *Journal of Chemical Physics*, *Langmuir*, *Bulletin of Mathematical Biology*, *Chemical Physics*, *Journal of Membrane Science*, *Chemical Engineering Science*, *Computational Materials Science*, *Physics Letters A; B*, *Nuclear Physics A; B*, *Journal of Magnetism and Magnetic Materials*, *Solid State Communications*, *Acta Crystallographica A*, *Quantum Information Processing*, *International Journal of Quantum Information*, *Inverse Problems*, *Nonlinearity*, *Journal of Computational Physics*, *Theoretical Computer Science*, *Theoretical Informatics and Applications (RAIRO)*, *Discrete Mathematics*, *Astronomy & Astrophysics*, *Monthly Notices of the Royal Astronomical Society*.

Other responsibilities

❍ S. Capponi is a member of *bureau de la division "Matière condensée" de la Société Française de Physique* since 2006.

❍ D. Dean is a member of the *Comité de Lecture* of the Prix *Le Monde* de la recherche – Sciences Exactes (2008).

❍ B. Georgeot was a member of the jury of the *Prix Fermat de Mathématiques*, attributed every two year to a mathematician of less than 45, working on subjects related to the works of Pierre de Fermat (2005).

❍ B. Georgeot is co-organizer of the IRSAMC seminar since 2000.

❍ M. Manghi is co-organizer with B. Chatel (LCAR) of *Les Journées de l'IRSAMC*, where the entire Fédération IRSAMC gathers near Toulouse for 3 days (2008 and 2009).

❍ P. Pujol is the organizer of the LPT seminar, succeeding D. Shepelyansky (2005-2008).

4.4 Communication and vulgarization

Scientific communication

Editorial work

❍ C. Sire was coeditor of *Images de la Physique* between 2002 and 2007.

❍ É. Suraud is the current editor-in-chief of *Annales de Physique* (Paris).

❍ É. Suraud is a member of the editorial committee of *Le Temps des Savoirs* (IUF, Éditions *Odile Jacob*, Paris).

5. D. Shepelyansky has been honored as *Outstanding Referee of the American Physical Society* (since 2008), along with 25 other physicists from France.

Images de la Physique

LPT researchers contributed to two recent articles (and one in 2004) in *Images de la Physique*, a yearly magazine edited by CNRS exposing recent trends in physics for non specialists.

❍ L. Salomé, P.-F. Lenne, and N. Destainville, *Membranes biologiques : vers un modèle physique*, Images de la Physique 2006, p. 74 (CNRS, 2006).

❍ C. Proust and D. Poilblanc, *Des champs magnétiques intenses pour sonder les supraconducteurs*, Images de la Physique 2009, 6 pages (in press, CNRS, 2009).

Magazine scientifique de l'UPS

Since 2004, Université Paul Sabatier publishes every four months the *Magazine scientifique de l'UPS*.

❍ N. Destainville, *Systèmes complexes, physique et biologique*, Magazine scientifique de l'UPS **4**, 9 (2005).

❍ P. H. Chavanis and C. Sire, *Mettre de l'ordre dans le chaos*, Magazine scientifique de l'UPS **4**, 11 (2005).

❍ N. Destainville, M. Manghi, and J. Palmeri, *Quand les physiciens se penchent sur l'ADN*, Magazine scientifique de l'UPS **11**, 12 (2007).

Scientific news

❍ J. Palmeri, M. Manghi, and N. Destainville's work of Refs. [ACL-192, ACL-236] was featured on the scientific news section of CNRS *Institut de Physique* web site.

❍ C. Sire's work of Ref. [ACL-197] has received important media coverage (Scientific American, PhysOrg.com, and many others).

Other communication activities

❍ B. Chirikov and D. L. Shepelyansky, *Chirikov standard map*, Scholarpedia **3(3)**, 3550 (2008). *Scholarpedia* is a peer-reviewed open-access encyclopedia written by scholars from all around the world.

❍ D. L. Shepelyansky, *Boris Valerianovich Chirikov*, Scholarpedia **3(10)**, 6628 (2008). Biography of the late Boris Chirikov on *Scholarpedia*. See also the section devoted to Boris Chirikov on the Quantware group web site.

❍ C. Sire represented CNRS at the *Salon InfoSup 2009*, an educational show for high-school students, Parc des expositions, Toulouse (21-24 January 2009).

❍ C. Sire was consulted on several occasions about the scientific aspects of poker following his work of Ref. [ACL-197] (*The New Scientist*, *BBC Focus Magazine*, Magazine *Live Poker*, Magazine *Toulouse Mag*, and a consulting agency working for the Israeli government on the chance *vs* skill and legal aspects of online poker).

Popularization of science

LPT scientists are involved in various scientific popularization activities (articles, conferences, high-school visits...). In particular, the LPT participates every year in *La Fête de la Science* through a series of conferences and laboratory visits organized by the Fédération IRSAMC and conferences in high-schools organized by the CNRS (C. Sire & É. Suraud).

❍ M. Dinh, J. Navarro, É. Suraud, *Océans et gouttelettes quantiques*, 159 pages (CNRS Éditions, Paris, 2007).

❍ N. Destainville and E. Joly, *Biologistes et physiciens, le dialogue est-il possible ?*, two parallel talks given at *Conférences exceptionnelles de l'Université Paul Sabatier*, Toulouse (27/03/2008).

❍ É. Suraud accompanied high-school students from Lycée Bellevue (Toulouse) to visit CERN in 2007.

❍ C. Sire co-organized a one day training and information session (laboratory visits, conferences, "scientific lunch"...) for high-school physics teachers at the Fédération IRSAMC (13/01/2009).

❍ C. Sire, *La physique hors des sentiers battus (Physics off the beaten track)*, popular talk presented on many occasions since 2005 (*Ouvertures de l'UPS*, *Fête de la Science*, high-schools, high-school teachers, students, public conferences... download the *pdf* version in French or English).

❍ C. Sire, *Histoire de la cosmologie moderne : 13.7 milliards d'années en 60 minutes (History of modern cosmology: 13.7 billion years in 60 minutes)*, popular talk presented on many occasions since 2005 (*Fête de la Science*, high-schools, high-school teachers, students, public conferences... download the *pdf* version in French).

❍ C. Sire, *Borel et von Neumann : Deux grands mathématiciens précurseurs de la théorie du poker (Borel and von Neumann : two famous mathematicians pioneering the theory of poker)*, article published on the poker blog of the French daily *Libération* (2007); see also the entry reviewing Ref. [ACL-197].

❍ C. Sire, among other scientists, gave three 30 minutes public talks on *Les échelles de temps en recherche fondamentale: les exemples du laser, des cristaux liquides, du transistor électronique, et des mémoires à magnétorésistance géante (Time-scales in fundamental research)*, place du Capitole, Toulouse (February 2009). See the report on the daily *Libération*-Toulouse web site. A shorter version of the talk was given to UPS M2 students, before C. Sire's lecture, as a sign of protest against recent disparaging political attacks targeting the French research and education system.

5

Équipe Fermions Fortement Corrélés (FFC)

The treatment of *strong correlations in fermionic systems* **is a notoriously difficult task. The current effort undertaken in our group to develop new analytical and numerical tools to tackle these issues addresses one of the major challenges in modern theoretical condensed matter physics. Such efforts are greatly motivated by the number of new fundamental concepts and unconventional phenomena that have emerged or are expected to in many electronic (or atomic) correlated systems.**

Funding: Since 2007, the FFC group has been funded by two *ANR contract* as well as several exchange programs (Argentina, Germany, Japan). Like the three other groups, the FFC group is also funded by the LPT on its own resources (computers, travel expenses...).

Postdocs: M. Capello (2006-2008), A. Ralko (2006-2008)

PhD students: A. Abendschein (2005-2008), D. Charrier (2006-2009), M. Moliner (2004-2009), G. Roux (2004-2007), D. Schwandt (2008-2011), F. Trousselet (2005-2009).

Insert 5.1 : *Funding of the FFC group and non-permanent members.*

Our scientific activity briefly described here is directly connected to the most active domains of research in the field of correlated systems such as frustrated quantum magnets, unconventional and high-T_c superconductors, quantum phase transitions, low-dimensional conductors, novel quantum Hall states, cold atoms loaded on optical traps, quantum information, etc. From the recent progress in numerical algorithms supplemented by the steady increase of super-computer power, one can foresee major breakthroughs in the resolution of canonical models of correlated fermions and hence, a more refined comparison with many of the related experimental systems.

The Strongly Correlated Fermions (FFC) group has a world-wide recognition in numerical techniques (F. Alet, S. Capponi, M. Mambrini and D. Poilblanc). P. Pujol who has joined the FFC group in 2006 brings a necessary and complementary expertise in analytic techniques.

5.1 Realistic description of magnetic materials

Low-dimensional antiferromagnets

S. Capponi, D. Poilblanc

Concerning low-dimensional magnetism, which typical description uses a simple Heisenberg model, it is known that some compounds allow more complicated interactions, such as Dzyaloshinskii-Moriya terms that break spin

SU(2) symmetry. By taking into account such terms, S. Capponi and D. Poilblanc have shown that one can have a more faithful description of thermodynamic measurements of the coupled dimer system $Cu_2(C_5H_{12}N_2)_2Cl_4$ [ACL-32]. In a following work done in collaboration with E. Orignac (Lyon) and R. Citro (Salerno, Italy), we have made some predictions concerning extra spectroscopic signatures (in Raman scattering experiments) due to these additional non-Heisenberg interactions [ACL-36].

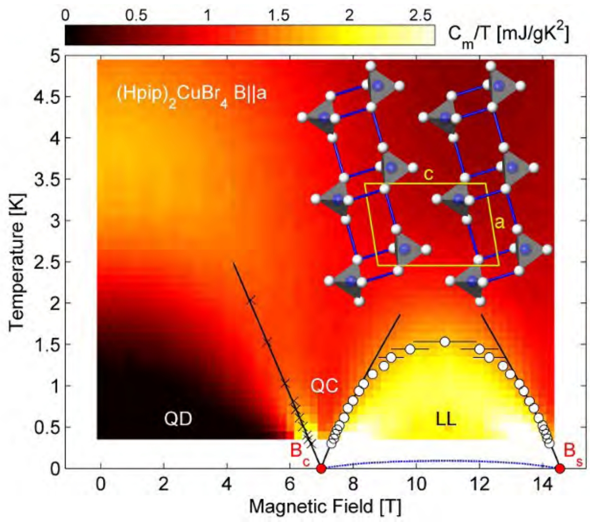


Figure 5.1 : Phase diagram of the spin-ladder compound $(C_5H_{12}N)_2Cuber_4$ obtained from magnetic specific data and showing quantum disordered (QD), quantum critical (QC) and Luttinger liquid (LL) regions (see Ref. [ACL-55]).

Still, we wish to emphasize that the simple Heisenberg model can provide a faithful and quantitative description of some spin-1/2 ladders, such as $(C_5H_{12}N)_2Cuber_4$. Its phase diagram in temperature and magnetic field has been studied experimentally and our numerical simulations combined with other theoretical tools have given an excellent quantitative agreement with the experimental data across the entire phase diagram [ACL-55]. In particular, a large area of the phase diagram displays so-called **Luttinger liquid physics** where the system possesses exotic properties.

Another way to investigate the ground-state of low-dimensional magnets is to probe the effect of adding non-magnetic impurities. In collaboration with F. Mila (Lausanne, Switzerland), we have investigated the effect of controlled doping of $SrCu_2(BO_3)_2$, a faithful realization of the Heisenberg spin-1/2 antiferromagnet on the Shastry-Sutherland lattice, with non-magnetic impurities [ACL-66]. We have shown that such doping generates bound-states below the spin gap that could be selectively probed with **Raman spectroscopy**. We hope that such experiments will be performed in the near future.

Influence of a strong magnetic field

A. Abendschein (PhD), S. Capponi, M. Moliner (PhD) and P. Pujol

The Shastry-Sutherland lattice (SSL) was considered more than 20 years ago by Shastry and Sutherland as an interesting example of a frustrated quantum spin system with an exact ground state. It can be described as a square lattice with antiferromagnetic J' couplings between nearest neighbors and additional antiferromagnetic couplings J between next-nearest neighbors in every second square.

This lattice attracted much attention after an experimental realization was identified in $SrCu_2(BO_3)_2$, a compound which exhibits a layered structure of $Cu(BO_3)$ planes separated by magnetically inert Sr atoms. The Cu^{2+} ions carry a spin $S = 1/2$ and are located on a lattice topologically equivalent to the SSL. The quantum SSL was widely studied both theoretically and experimentally. In particular, in the presence of a magnetic field, theoretical studies have predicted the existence of plateaux in the magnetization curve for rational values of the magnetization $M/M_{\rm sat} = 1/8$, 1/4, 1/3 and 1/2: T. Momoi and K. Totsuka showed that the stripe order of the dimer triplets explains the $M/M_{\rm sat} = 1/2$ and 1/3 plateaux and the latter was predicted to be the broadest. Experimentally, magnetization plateaux were first observed for $M/M_{\rm sat} = 1/8$, 1/4 and 1/3, but more recently various teams have reported evidences for additional plateaux. Qualitatively, S. Miyahara and K. Ueda explained the existence of all those plateaux as a consequence of the crystallization of excited triplets. In order to be more quantitative, A. Abendschein and S. Capponi have derived an effective model to describe the triplet dynamics and they show that indeed **additional plateaux are expected** [ACL-58].

Recently, rare-earth tetraborides RB_4 have been attracting new interest to the SSL. These compounds present a large total magnetic moment $\mathcal{J} > 1$, which justifies a *classical* model although magnetic anisotropies are likely to be relevant for a description of the experiments. For TbB_4 (which has a large $\mathcal{J} = 6$ magnetic moment), magnetization plateaux were found at $M/M_{\text{sat}} = 1/4, 1/3$ and $1/2$. The compound ErB_4 (with $\mathcal{J} = 15/2$) exhibits a magnetization plateau at $M/M_{\text{sat}} = 1/2$ for both $\mathbf{h}//[001]$ and $\mathbf{h}//[100]$. The compound TmB_4 also presents several magnetization plateaux for $\mathbf{h}//[001]$.

As a first step to understand the appearance of these plateaux in the large spin compounds, we have investigated classical Heisenberg spins on the Shastry-Sutherland lattice under an external magnetic field [ACL-63, ACTI-15]. A detailed study was carried out both analytically and numerically by means of classical Monte-Carlo simulations. Magnetization pseudo-plateaux were observed around 1/3 of the saturation magnetization for the particular magnetic coupling ratio $J'/J = 1/2$. For this value of the magnetization the spin configuration is in a collinear configuration. We showed that the existence of the pseudo-plateau is due to an **entropic selection** of a particular collinear state. A phase diagram that shows the domains of existence of those pseudo-plateaux in the (h, T) plane and an interesting variety of phase transitions was also obtained. We confirmed that the Shastry-Sutherland lattice behaves like the triangular lattice and it presents two quasi-long-range-ordered phase below and above the long-ranged-ordered phase. We also showed that the pseudo-plateau survives for a small variation of the magnetic coupling ratio around $J'/J = 1/2$. The phase diagram was found to present a new incommensurate umbrella phase in the low-temperature region, at least for $J'/J = 0.4$.

5.2 Strongly correlated fermions: from high-T_c superconductors to atomic gases

High-temperature superconductivity

D. Poilblanc, M. Capello (postdoc)

Recent Scanning Tunneling Microscopy (STM) experiments with unprecedented atomic resolution have revealed density of states modulations in many under-doped cuprates superconductors. Over a few years we have carried out a program of investigation of such **inhomogeneous** states of matter in models of two-dimensional correlated fermions using Gutzwiller projected wave functions within improved mean-field theories and advanced numerical techniques such as variational Monte Carlo simulations. A collaboration with École Polytechnique Lausanne (C. Weber and F. Mila) involving S. Capponi has initiated the project in 2006-2007. More recently, an ANR post-doc M. Capello and a collaborator from Krakow (Poland), M. Raczkowski, have been deeply involved in the project [ACL-29, ACL-38, ACL-52]. Among many fascinating results (see publication list), let us mention the discovery of a striped d-wave superconductor with anomalous properties. Together with D. Scalapino and T. Maier [ACL-51], we have also addressed the issue of a "retarded glue" in the mechanism of high-T_c superconductivity using Exact Diagonalizations and Dynamical Mean-Field Theory.

Doped frustrated Mott insulators

D. Poilblanc, F. Trousselet (PhD)

There is growing interest for doped Mott insulators or correlated itinerant electrons subject to magnetic frustration introduced by lattice geometry. Such an excitement has been reinforced by the recent discovery of superconductivity in a large number of pyrochlore compounds [1] (see Fig. 5.2 for an illustration) as well as in some Cobalt oxides with a triangular lattice [2]. Let us also cite LiV_2O_4, a $3d^{0.5}$ (i.e. quarter-filled) strongly correlated system with a frustrating spinel (pyrochlore) structure, displaying an anomalously high critical temperature.

1. M. Hanawa *et al.*, Phys. Rev. Lett. **87**, 187001 (2001).
2. K. Takada *et al*, Nature **422**, 53 (2003).

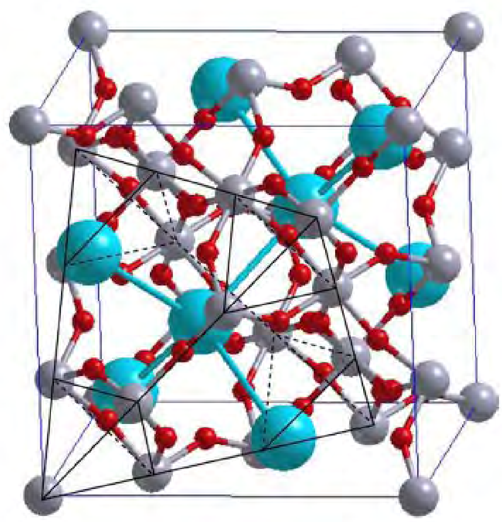


Figure 5.2 : The $Cd_2Re_2O_7$ compound is an ideal representation of a three-dimensional lattice of corner sharing tetrahedra.

The fact that superconductivity may be connected to the magnetic frustration present in these materials offers new promising routes of research. Hence, motivated by such experimental facts, in the FFC group we have carried out an important research activity on (generalized) Hubbard models on two-dimensional frustrated lattices (see F. Trousselet's thesis) and on doped frustrated magnets modeled by Quantum Dimer Models. The number of publications in renamed journals is an indication of the output of the research carried out in this area.

Cold atomic gases

S. Capponi

The observation of Bose-Einstein condensation (BEC) and Fermi degeneracy in ultracold atomic gases has opened a new area of research in atomic and molecular physics. Early experiments have focused on quantum phenomena associated to coherent matter waves and superfluidity (interference between condensates, atom lasers, quantized vortices and vortex lattices, etc.). More recently, emphasis has shifted towards strongly correlated systems following three major experimental developments: i) the realization of quasi-one- or -two-dimensional (quasi-1D/2D) atomic gases using strongly anisotropic confinement traps, ii) the possibility to tune the interaction strength by Feshbach resonances in the scattering amplitude between two atoms, iii) the generation of strong periodic potentials (analog to the crystalline lattice in solids) by optical standing waves. Thus quantum phenomena typical of condensed-matter physics have been observed in cold atomic gases: the Mott transition in bosonic and fermionic gases, the BCS-BEC crossover in superfluid fermionic gases, the Berezinskii-Kosterlitz-Thouless transition in quasi-2D bosonic systems, etc. These experiments are characterized by two distinguishing features: a detailed knowledge of the underlying microscopic Hamiltonian and a **complete control of the parameters** of the system (dimensionality, interaction strength, etc.) *via* external fields.

Ultracold atomic gases offer a unique opportunity to explore the **effect of spin degeneracy** since the atom total angular momentum F (often dubbed the atom "spin"), which includes both nuclear spin and total electron angular momentum, can be non-zero for bosons or larger than 1/2 for fermions. While the $2F+1$ hyperfine levels ($m_F = F, F-1, \cdots, -F$) are split in magnetic traps, they remain degenerate in optical traps and may give rise to novel quantum phenomena.

For a one-dimensional lattice, thanks to powerful analytical and numerical techniques, we have addressed some of these issues, namely the possibility of dominant **molecular superfluidity** instability in multicomponent fermionic systems [ACL-57] as well as a rich phase diagram for interacting spin-3/2 fermions [ACL-40, ACL-62].

More recently, we have considered the case of Lithium (^{6}Li) atoms for which a stable degenerate condensate made of three hyperfine states has been recently stabilized [3]. By taking into account realistic parameters, we predict that such a Fermi gas loaded on a one-dimensional optical lattice could exhibit various trionic phases (with bound states of three fermions) that distinguish themselves by the relative phases between the $2k_F$ atomic density waves fluctuations of the three species [SRP-2]. Moreover, at small enough

3. T.B. Ottenstein *et al.*, Phys. Rev. Lett. **101**, 203202 (2008).

densities or strong anisotropies in the interactions, we give further evidences for a decoupling and the stabilization of more conventional BCS phases.

5.3 Valence-bond description of quantum antiferromagnets

Valence-bond calculations

F. Alet, S. Capponi, M. Mambrini, D. Schwandt (PhD)

Understanding exotic quantum states

A great challenge is to unveil the nature of novel phases of matter arising at low temperature in quantum antiferromagnets. This is the precise arena where quantum fluctuations and frustration effects can combine in order to create exotic states which description challenges the conventional theories of condensed matter. This is particularly appealing as these states are observed or close to be realized in experimental systems. Addressing this problem of strong correlations is a theoretical challenge as we lack theoretical tools to understand the competition between various interactions, and to capture the complexity of the arising low-energy manifold.

To this end, we have started using the valence bond (VB) basis, which looks like old-school quantum mechanics but has in fact been reintroduced recently as it can provide a faithful representation of some exotic (i.e. non-magnetic) ground-states. For instance, one important novelty is the possibility to implement large-scale Quantum Monte Carlo (QMC) simulations directly in this overcomplete basis [4]. Using this approach, we have recently [SRP-1] revisited one of the gold standard models of quantum magnetism, namely the **2D SU(N) Heisenberg model**. While at low N the system develops long-range antiferromagnetic order, large-N calculations indicate that a Valence Bond Crystal (VBC) is formed. This can easily be understood in the VB language as short range VBs forming the VBC are favored by a factor N over longer-range singlets needed for the Néel order. We have generalized VB algorithms to the SU(N) symmetry with N *real*, allowing us to study the Néel-VBC quantum phase transition which we have shown to take place at $N = 4.57(5)$ and to be continuous. This is an important step as all previous approaches were limited to integer N and therefore not able to capture quantum criticality. This work calls for new theoretical developments to understand the nature of the Néel-VBC transition, a topic which is highly controversial since standard Landau-Ginzburg arguments predict a first-order transition.

Connections to quantum information

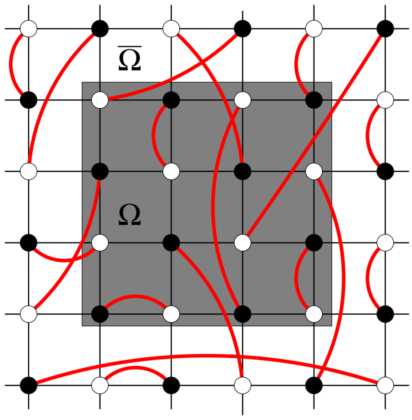
VB singlets are not only good candidates to describe exotic non-magnetic phases of matter, but are also the natural elementary bricks of entanglement as a singlet is maximally entangled. It is natural therefore that they give access to quantum information quantities. For instance, we have introduced the **valence-bond entanglement entropy** as a measure of quantum entanglement between two subsystems (see insert 5.2 and Ref. [ACL-27]). This new estimator allowed for the first time the study of how block entanglement scales with size in non-trivial 2D ground-states. The importance for condensed matter steams from the fact that this scaling can indicate the nature of the underlying phase (gapped, critical, topological etc.), as well as the location of quantum critical points, without any prior knowledge of the relevant correlations.

The non-orthogonality of the VB basis, which is often considered as a hurdle in numerical computations, can be turned into an advantage. We have recently shown that this specificity allows the computation of **fidelity** (or overlap) between different singlet (ground-)states [SRP-3]. The fidelity, which is also rooted in quantum information theory, is intrinsically complex to compute on large systems with other methods. The interest comes from the fact that quantum critical points induce a large **fidelity drop**, allowing for an automatic detection thereof. With QMC simulations in the VB basis, we have shown the validity of this scenario for the quantum phase transitions of the Heisenberg model on the CaVO lattice [SRP-3].

This line of research constitutes an important part of the *ANR "Jeunes Chercheurs" (Q-BONDS)*, in which the three young permanent researchers of the group are involved.

4. A. W. Sandvik, Phys. Rev. Lett. **95**, 207203 (2005); A. W. Sandvik and H.-G. Evertz, arXiv:0807.0682.

Valence Bonds as entanglement carriers



Divide a quantum spin 1/2 system in two parts Ω and $\bar{\Omega}$. The amount of entanglement between the two parts is usually quantified using the von Neumann entanglement entropy $S_{\rm vN} = -{\rm Tr}\rho \ln \rho$, where $\rho = {\rm Tr}_{\bar{\Omega}}|\Psi\rangle\langle\Psi|$ is the reduced density matrix of Ω. $S_{\rm vN}$ unfortunately is quite complex to compute for realistic systems.

As an alternative, we have introduced [ACL-27] the VB Entanglement Entropy, defined naturally in VB states as the **number of singlets shared by the two subsystems** (8 for instance in the figure). The VB Entanglement Entropy has all the properties of an entropy and also shares with $S_{\rm vN}$ the same size scaling when both can be compared. Most importantly, it is amenable to large-scale numerical computations thanks to novel VB algorithms, at odds with $S_{\rm vN}$. Finally, it also provides a long-awaited **geometrical interpretation of entanglement** in quantum spin systems.

Insert 5.2 : *Valence Bond Entanglement Entropy*

Quantum dimer models

D. Poilblanc, A. Ralko (postdoc)

Magnetic frustration plays a key role in a number of quantum antiferromagnets with a geometrically frustrated lattice structure (*e.g.* in some transition metal oxide Mott insulators) and commonly leads to the (dynamical) formation of spin singlets (or dimers).

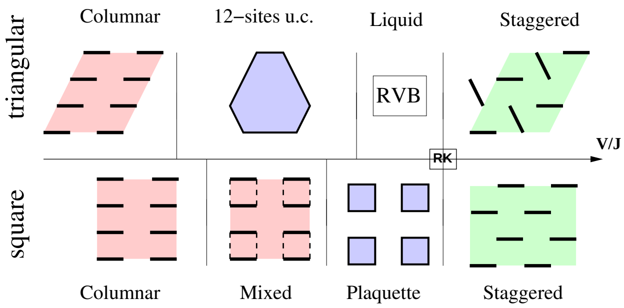


Figure 5.3 : *Schematic phase diagrams of the (undoped) QDM for both triangular and square lattices. $V/|J|$ is the ratio between the dimer repulsion and the dimer-flip amplitude. Only the triangular lattice is believed to exhibit a RVB liquid phase. A rich variety of crystalline phases, the VBCs, breaking lattice translation symmetry, are observed. Evidences for a mixed phase on the square lattice have been reported recently and might be generic of some frustrated quantum antiferromagnets.*

Generically, systems of quantum fluctuating dimers can often order to give rise to VBC breaking lattice symmetries or remain in an unconventional quantum disordered state, the spin liquid, breaking neither spin nor lattice symmetries.

The 2D Quantum Dimer Model (QDM) introduced by Rokhsar and Kivelson [5] plays an increasing role to understand frustrated and/or quantum-disordered spin systems. We have reexamined and extended the investigation of such models. Among the successful achievements are the discovery of a new mixed columnar-plaquette phase and of a new quantum critical point (on the triangular lattice) characterized by spinon Bose-condensation under the action of a magnetic field.

Classical dimer models

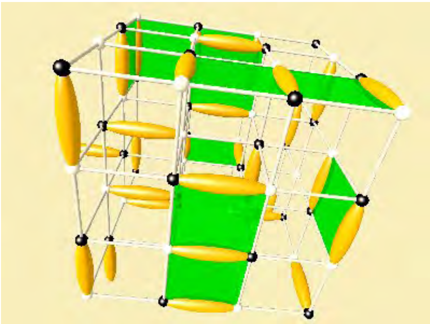
F. Alet, D. Charrier (PhD), P. Pujol, F. Trousselet (PhD)

A popular approach in the study of complex quantum many-body problems consists in starting from the classical limit where physics is well understood, and to introduce quantum fluctuations to see whether and how they can destabilize the classical order and induce new phases of matter. This is a standard procedure used for instance in the spin-wave approximation.

In the study of **classical dimer models**, we have taken steps in the reverse direction by considering the classical counterpart of QDMs (see

5. D. S. Rokhsar and S. A. Kivelson, Phys. Rev. Lett. **61**, 2376 (1988).

Simple models, unusual physics



The simplest interaction term in dimer models favors parallel dimers on a plaquette, for instance in 2D: $E = -\sum_{\square} = + \parallel$. On the figure, plaquettes with parallel dimers are shaded in green in this dimer covering of the cubic lattice. This interaction favors a crystalline phase where dimers are aligned in columns at low temperature. On the other hand, entropic effects give rise to a Coulomb phase at high temperature for bipartite lattices, with dipolar dimer correlations in 3D. An **unconventional direct second order phase transition** separates the crystal and Coulomb phases (see Ref. [ACL-15] and text).

Insert 5.3 : *Interacting dimer models*

Sec. 5.3.2). Surprisingly, the classical limit of QDMs (whence quantum kinetic terms vanish) reveals very rich physics. The key ingredient here is the hardcore nature of dimers which readily builds a level of frustration, even at the classical level. In some sense, classical dimer models are the Ising models of frustration. Thus it is no surprise that they can apply to other physical situations than frustrated magnets [6], as for instance in surface physics (see the recent adsorption experiments [7] and the theoretical interpretation of Ref. [ACL-60]).

In 2D, the entropic problem of dimer coverings is well-known to give rise to two different physics, depending on the biparticity of the lattice. If the lattice is bipartite (*e.g.* square lattice), the dimer correlations are critical whereas non-bipartite (eg. triangular) lattice display exponentially decaying correlations, which is the origin of the RVB liquid state in the equivalent QDM. In Ref. [ACL-28], we have shown that this intuitive result can be spoiled when interactions are present between dimers.

The inclusion of interactions in dimer coverings indeed gives rise to exotic physics, even in the simplest case (see Inset 5.3). In 3D, bipartite lattices harbor a Coulomb phase where dimer coverings behave exactly as a fictitious electromagnetic medium, with for instance dipolar dimer correlations as well as photon-like excitations [ACL-56]. Adding interactions between dimers can cause a **continuous phase transition** to an ordered crystalline phase. This phase transition, which we first studied by Monte Carlo simulations [ACL-15], is very unconventional in the sense that it **cannot be described by the standard Landau-Ginzburg-Wilson (LGW) approach** to phase transitions, where the effective action is expanded in terms of local order parameters. Understanding such "non-LGW" phase transitions is currently a hot topic in the context of strongly correlated quantum magnets and the transition observed in the 3D dimer model appears the simplest and the most robust to show such a phenomenology. Numerical simulations are eased by the classical nature of the problem, which allows to study in depth both quantitative [ACL-15] and qualitative [ACL-45] aspects of the transition, as well as variants of the model [ACL-65].

Providing a description of this continuous phase transition out of the LGW paradigm is a strong theoretical challenge – indeed standard approaches predict a generic first order transition between these two phases. We have offered a theoretical interpretation (supported by numerical simulations) in terms of a **Higgs confining transition** [ACL-46], which is found to be continuous. This scenario was also independently proposed [8]. It certainly is amusing to find that such involved gauge-theoretical descriptions are relevant and necessary to describe the behavior of an after all simple models of statistical physics. This confirms our initial statement of rich and universal physics in dimer models.

6. A. Sen, K. Damle, and A. Vishwanath, Phys. Rev. Lett. **100**, 097202 (2008).
7. M. O. Blunt *et al.*, Science **322**, 1077 (2008).
8. S. Powell and J. Chalker, Phys. Rev. Lett **101**, 155702 (2008).

6

Équipe Information et Chaos Quantiques (Quantware)

The Quantware team regroups researchers having an expertise in classical and quantum chaos, mesoscopic and many-body physics. The group has applied these methods and concepts to different branches of physics with experimental relevance, including in particular quantum information and computation. The group has also been investigating chaos-related problems in quantum optics, atomic physics, condensed matter, astrophysics and very recently, statistical physics of networks.

Permanent researchers of the Quantware include Daniel Braun (PR2), Robert Fleckinger (PR Emeritus), Klaus Frahm (PR2), Bertrand Georgeot (CR1 CNRS), Olivier Giraud (CR2 CNRS) and Dima L. Shepelyansky (DR1 CNRS, head of the group). Non permanent staff have included two post-docs who left at the end of 2008, Ignacio García-Mata and John Martin, and two PhD students, Ludovic Arnaud and Benoît Roubert.

Since 2007, the Quantware group has been funded by three ANR contracts, namely ANR contract for young researchers *INFOSYSQQ* (coordinator), ANR-NANO contract *MICONANO* (partner) and *NANOTERRA* (partner), and one European contract (*EuroSQIP*; partner). The Quantware group has had two postdoctoral fellowships funded by ANR, Europe, and CNRS; another postdoc will start in fall 2009.

Scientists who have visited the Quantware group for a period of at least one month since 2007 include Prof. P. Braun (Essen), M. V. Entin, L. I. Magarill, and O. Zhirov (RAS, Novosibirsk), A. Pikovsky (U. of Potsdam) and M. Znidaric (U. of Ljubljana).

The Quantware group has collaborations with LAAS, LCC, Observatoire Midi-Pyrénées (OMP) in Toulouse, researchers from Orsay, Grenoble, Lille in France, and scientists from Argentina, Belgium, South Korea, Germany, Italy, Russia, Slovenia and Switzerland.

During the last four years, the Quantware group has published 55 articles in referred journals and have contributed 31 invited talks. The main aspects of the scientific activity of the Quantware group during the 2007-2009 period are highlighted below. Three highlights marked by the group are imperfection effects in Shor algorithm [ACL-89, ACL-117], Loschmidt cooling of atomic matter waves [ACL-102, ACL-108] and delocalization in the Google matrix [ACL-124]. For more details, see the personal web pages of the members of the Quantware group.

6.1 Quantum Information

Quantum information and computation has been put forward recently as a mean to use properties of quantum mechanics to treat information in novel ways. The system considered is often a collection of two-level systems (qubits) on which local unitary transformations (quantum gates) are performed, enabling *e.g.* to build quantum algorithms outperforming classical ones, like the famous Shor and Grover algorithms. The work below was funded by the young researcher's ANR contract *INFOSYSQQ* and the European contract *EuroSQIP*.

Analysis of resources for quantum information

D. Braun, B. Georgeot, O. Giraud, J. Martin (postdoc), L. Arnaud (PhD student), B. Roubert (PhD student)

Interference is a quantum resource considered as very important in the literature, in par with entanglement. Surprisingly, although measures of entanglement do exist, there is no equivalent quantitative measure of interference enabling to evaluate it during a quantum process. Such a measure was proposed by the group in [ACL-78].

This measure was then used to systematically assess the role of interference in quantum processes. This allowed to show that important processes such as quantum state transfer along spin chains [ACL-93] and quantum cloning [ACL-115] can surprisingly be implemented without using interference. This means that this resource is not used in all quantum processes, which is also true for entanglement. In contrast, a more detailed study of quantum algorithms showed that interference is present in large quantities during these processes. We have studied algorithms producing efficiently random vectors [ACL-87] as well as the famous algorithms of Shor and Grover [ACL-103]. In all cases, a quantum algorithm using pure states needs a lot of interference, and often all the more since it is efficient compared to classical algorithms. This enables to show that interference is a quantum resource fully used by quantum algorithms.

Entanglement as a quantum resource has also been studied. In particular, the properties of entanglement of finite dimensional bipartite systems are still not well understood. In [ACL-113] we have studied the representability of systems of small dimension by superpositions of coherent states. This allows to develop a criterion for "classicality" of spin systems, which extends to these states a concept from quantum optics. A detailed study enabled to clarify the links with entanglement, and to show that for bipartite systems, classicality is a sufficient condition for separability. This gives a semiclassical criterion for separability, useful in view of the difficulty to determine if a quantum state is entangled or not.

We have also studied entanglement in the context of random quantum states. Such states have been put forward recently as an important resource of quantum information, which are useful in various quantum protocols. In a sense, they are the equivalent for quantum information of random numbers in classical information. Besides, they can also be used to model wavefunctions of physical systems. Ensembles of random vectors can be built that reproduce a certain physical property, and the analytical and numerical study of these ensembles enables to get results applying to physical systems sharing this property. Such methods have been used with great success in the field of quantum chaos using Random Matrix Theory, and only recently began to be applied to quantum information.

In [ACL-94, ACL-95] entanglement properties of random vectors were specified, enabling to obtain the distribution of entanglement measures. We also studied a more general class of random vectors, which present localization properties [ACL-92, ACL-119]. We were able to show that for such random vectors, the linear entropy, which approximates the entanglement entropy, is directly given as a simple function of the participation ratio, a measure of localization widely used in mesoscopic physics and quantum chaos. We have shown that these results can be applied beyond random vectors to describe physical systems with wavefunctions localized in space (e.g. electrons localized in a disordered potential as in the Anderson model), or in Hilbert space (e.g. interacting spin systems). We also found that the next orders in an expansion of the entanglement entropy are related to the moments of the wavefunction. In particular, for systems with an Anderson metal-insulator transition, or more generally for systems presenting intermediate spectral statistics between Random Matrix Theory and Poisson (characteristic of integrable systems), wavefunctions are multifractal and entanglement can be linked to the multifractal exponents. This allows to predict the entanglement produced by certain quantum algorithms, and also to shed new light on the behavior of entanglement in a metal-insulator phase transition. At last, these results allow to connect entanglement to other physical properties.

An application of these studies has consisted in proposing the implementation of nonlocality tests on condensed matter systems [ACL-112].

Quantum algorithms

D. Braun, B. Georgeot, O. Giraud, I. Garcia-Mata (postdoc), L. Arnaud (PhD student)

The existence of efficient quantum algorithms such as Shor's shows that quantum devices could in principle outperform classical ones. However there are not that many instances where a gain over classical computing can be shown to exist. Furthermore, it is so far not clear which kind of problems can be efficiently solved by a quantum processor, and how much gain is obtained compared to a classical processor. Our aim has been to propose new quantum algorithms, based on different approaches, where a gain over classical computation could be shown.

In [ACL-107] we investigated the possibility to efficiently calculate trace formulas for quantum maps. These formulas relate semiclassical eigenvalues of quantum operators – describing for instance quantum maps – to the periodic trajectories of the underlying classical map. We proposed quantum algorithms which yield quantum observables from classical trajectories, and which alternatively test the semiclassical approximation by computing classical actions from iterations of the quantum operator.

Most known quantum algorithms, such as the one above, rely on the use of the Quantum Fourier Transform, a quantum analog of the Fast Fourier Transform. But it is not the only transform which can be implemented efficiently on a quantum computer. Indeed, wavelet transforms, which are more and more used in classical image treatment and signal analysis, can be done by efficient quantum routines. Such transformations are able to describe multiscale properties of a signal, and are especially suited for analysis of multifractality. In [ACL-123] we have built a quantum algorithm using the quantum wavelet transform to efficiently extract multifractal properties of a quantum wavefunction. This not only gives a new useful algorithm, but opens the path to a new class of quantum algorithms based on different methods than the standard ones.

As mentioned above, there is a particular kind of quantum states whose generation by quantum circuits has attracted a lot of attention, namely random states, whose role is manifold in quantum information science. Efficient algorithms have been built which construct pseudo-random states. In [ACL-114], such pseudo-random states were compared to exact random states, showing that they describe very well many of their statistical properties, and can therefore be used reliably for various applications.

Previous algorithms have mainly focused on asymptotic regimes for large system sizes. They allow to estimate the potential gain of quantum computation over classical algorithms, regardless of the actual experimental situation. A second part of our work has been dedicated to the construction of quantum algorithms more specifically aimed at few-qubit systems. Such few-qubit quantum processors become available experimentally, and quantum algorithms should be optimized with that perspective. In [ACL-106] we have investigated the optimization of three-qubit circuits. We have proposed algorithms that allow to construct any quantum state on three qubits, starting either from a completely unentangled state or a maximally entangled state. We proved that our algorithms minimize the number of two-qubit gates involved, and classified three-qubit quantum states according to the resources needed to construct them.

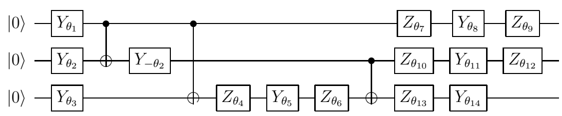


Figure 6.1 : *Quantum circuit for three-qubit state generation; lines are the qubits, boxes the quantum gates.*

On the basis of one of these algorithms, it was possible [SRP-9] to construct the quantum circuit depicted at Fig. 6.1. This circuit allows to construct any state from the unentangled ground state in an optimal way. In particular this circuit can be used to produce random states. Indeed, so far algorithms aimed at generating random states were constructing pseudo-random states with circuits optimized in the asymptotic limit. We have shown in [SRP-9] that our circuit of Fig. 6.1 produces true three-qubit random states in an optimal way, by calculating the exact analytic distribution of the angles of each gate.

At last, in [SRP-7], we have shown that it is possible to use triangular arrays of three Cu atoms deposed on surfaces to build logical qubits which are protected against magnetic noise. This opens the possibility of a new scalable implementation of quantum computers.

Effects of imperfections for Shor's algorithm

K. M. Frahm, D. L. Shepelyansky, I. Garcia-Mata (postdoc)

In the field of quantum computation Shor's factorization algorithm (1994) represents one of the most important potential applications of quantum computers because of the exponential efficiency gain compared to any known classical algorithm. It allows to factorize a large integer number N with $O(\ln^3 N)$ quantum gates while all known classical algorithms require a number of operations that grows exponentially with $\ln N$.

The main idea of Shor's algorithm is to prepare, by parallel quantum multiplications, a quantum state: $\sum_a |a\rangle\, |x^a\rangle$ where x is a small integer number relatively prime to N and x^a is taken modulo N. The first factor $|a\rangle$ represents the *control register* with n_l qubits ($0 \le a < 2^{n_l}$) and the second factor $|x^a\rangle$ is stored in the *computational register* with n_q qubits where typically n_q and n_l are chosen such that $N < 2^{n_q}$ and $n_l = 2\,n_q$. Applying a quantum Fourier transform to the control register one obtains a quantum state where the probability to measure a certain value of the control register is a strongly peaked function at certain values: $a_m = m\,2^{n_l}/r$ with r being the period defined as the minimal positive integer such that $x^r = 1$ modulo N and $m = 0, \ldots, r-1$. After a quantum measurement of the control register one obtains such a value a_m allowing to determine (with a certain probability) the period r and eventually to find a non-trivial factor of N.

We have studied [ACL-89, ACL-117] the effects of imperfections in the quantum multiplication gates, for various generic disorder models, and determined up to which critical imperfection strength Shor's algorithm remains operational. In Fig. 6.2, we show the effect of imperfections to the probability $W(c)$ to measure a certain control register value (with $c = a - a_m$ being the position relative to one of the peak-values of Shor's ideal algorithm) thus illustrating the melting of Shor's algorithm as a function of the imperfection strength.

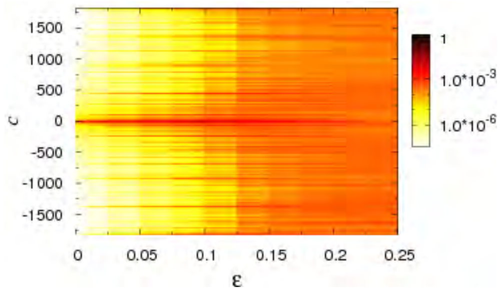


Figure 6.2 : *Quantum melting of Shor's algorithm induced by imperfections: color density plot of the global search probability $W(c)$ as a function of coupling strength ϵ for 9 qubits (from [ACL-89])*

Using the inverse participation ratio $\xi = \sum_c |W(c)|^{-2}$, we have determined the critical imperfection strength as a function of N and found a dependence $\epsilon_c = B/(\log_2(N))^\beta$ with exponents $\beta = 1.275$ or $\beta = 1.546$ depending on the imperfection model.

In our first work [ACL-89], we have emulated (on a classical computer) the quantum algorithm with a full control register and values up to $n_q = 10$ and $n_l = 20$ allowing to factorize numbers up to $N = 943$. However, using a wise reformulation of Shor's Algorithm it is possible to use a single control-qubit at the price of simulating the quantum measurement process at an earlier stage of the algorithm. We have determined [ACL-117] the critical imperfection strength for values up to $n_q = 18$ and $N = 205193$ which would have been completely impossible without the single control-qubit simplification.

Measurement and decoherence

D. Braun, J. Martin (postdoc)

Popular scientific belief holds that in a Schrödinger cat state the object is in two different states at the same time. Does it mean that one could do Young's double slit interference experiment with just one slit put into a quantum superposition of two different positions? Our theoretical setup was to place a single excited atom in a double well in a coherent superposition of "right" and "left", let the atom emit a single photon and detect that photon at a large distance, repeat the experiment many times and thus build the intensity distribution of the emitted light. Our calculations showed that by doing simply this, one will get nothing but the characteristic dipole pattern, just as if the atom were localized in a single position. However, if the external state of the atom can be post-selected in the energy basis (or equivalently, if the emitted light is filtered with a spectral resolution better than the tunnel splitting), a perfect double-slit interference pattern does indeed arise [SRP-8].

Moreover, it turned out that even the problem where the atom interacts with a single electro-magnetic mode is very interesting: in that case the tunneling of the atom can be drastically modified due to emission and re-absorption of a photon. This allows to coherently control quantum-tunneling of an atom trapped in a cavity. For a coherent initial state of the field in the cavity, collapse and revival of the tunneling effect can occur [ACL-97].

Possibly one of the most important spin-offs of the young field of quantum information is the development of "Quantum-Enhanced Measurements" (QEM). The idea is to use highly non-classical quantum states in order to measure quantities like the length of an optical cavity or the phase shift in an arm of an interferometer with unprecedented accuracy. These measurements are primers for many important applications, and successful implementation of QEMs would therefore have a large impact in many areas, such as improvement of frequency standards, gravitational wave detection, navigation, remote sensing, and measurement of very small magnetic fields (with applications to medical imaging).

The major goal in the field of QEM has been to beat the so-called "standard quantum limit" (SQL), in which the minimal amount of uncertainty allowed by Heisenberg's uncertainty relation is evenly distributed over two conjugate variables. Basically all of the schemes proposed so far make use of squeezed states where the uncertainty in one variable is reduced for the price of increasing the uncertainty in the other. This should allow in principle to achieve the so-called "Heisenberg limit", in which the minimal uncertainty scales as $1/N$ with the number N of quantum-constituents – an enormous increase in precision over the SQL in which the precision scales as $1/\sqrt{N}$. However, despite more than twenty years of intense work, only four experiments so far have demonstrated a slight improvement over the SQL, and they appear not to be scalable to substantially larger values of N.

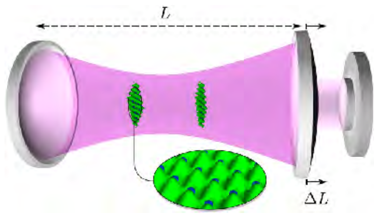


Figure 6.3 : *Measuring the length L of an optical cavity through a decoherence-enhanced measurement: N atoms (or ions) are trapped in two optical lattices perpendicular to the cavity axis. The atoms are prepared in a dark state relative to a given L. A slight change of L changes the true dark states, and the initial state is exposed to decoherence, detectable by photons leaking out through the semi-reflecting mirror at a rate proportional to N^2.*

In [SRP-8] we demonstrated that decoherence might be exploited for precision measurements, and in particular to reach or even surpass the Heisenberg limit. The basic idea behind this new measurement scheme is that decoherence becomes in general extremely fast for superpositions of quantum states which differ mesoscopically or even macroscopically. On the other hand, if the coupling of the quantum system to its environment enjoys a symmetry, entire decoherence free subspaces (DFS) can exist, in which even such macroscopic "Schrödinger cat states" are long-lived. But this means that the decoherence rate for such superpositions in a DFS must be extremely sensitive to changes in system parameters – and therefore allows for extremely precise measurements of such changes. While it appears that this would still call for the difficult preparation of large "Schrödinger cats", it turned out that also much easier to produce product states of pairs of atoms can allow to reach or even surpass the Heisenberg limit (reaching a scaling of $1/N^2$ in the latter case). We analyzed in detail the problem of the measurement of the length of an optical cavity (see Fig.6.3). We use ensembles of atoms trapped in two optical lattices perpendicular to the cavity axes. We showed that the system can be prepared in a DFS (a dark state in quantum optics parlance) relative to the actual position of the mirror, using a fraction of the quantum resources. A subsequent change of the mirror position can then be detected very sensitively by photons leaking out of the cavity. Compared to conventional interferometric length measurements, the scheme has the additional advantage, besides its exquisite sensitivity, of storing virtually no light directly in the cavity, such that the problem of radiation pressure noise on the mirror is entirely avoided.

6.2 Quantum synchronization

D. L. Shepelyansky

Recently, an impressive experimental progress has been reached in realization of a strong coupling regime of superconducting qubits with a microwave resonator. The spectroscopy of exchange of one to few microwave photons with one, two and even three superconducting qubits has been demonstrated to be in agreement with the theoretical predictions of the Jaynes-Cummings and Tavis-Cummings models even if certain nonlinear corrections have been visible. Thus the ideas of atomic physics and quantum optics find promising implementations with superconducting macroscopic circuits leading also to achievement of single artificial-atom lasing in a microwave range. In comparison to quantum optics models, a new interesting element of superconducting qubits is the dissipative nature of coupled resonator which opens new perspectives for quantum measurements.

Using method of quantum trajectories, we have studied [ACL-101, ACL-125] the behavior of two identical or different superconducting qubits coupled to a quantum dissipative driven resonator. Above a critical coupling strength the qubit rotations become synchronized with the driving field phase and their evolution becomes entangled even if two qubits may significantly differ from one another. Example of the radiation spectrum of one qubit is shown in Fig. 6.4: even if the qubit frequency has a significant 20 % shift it starts to radiate at the resonator frequency for sufficiently strong driving. Such entangled qubits can also radiate entangled photons that opens new opportunities for entangled wireless communication in a microwave range. This research is supported by EC FET project *EuroSQIP*.

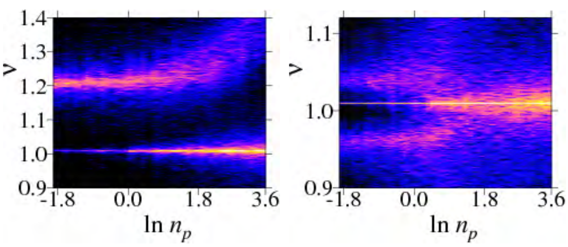


Figure 6.4 : *Spectral density $S(\nu)$ (shown by color) of qubit radiation as function of driving power given by the number of photons in resonator n_p. Left: qubit frequency 20 % larger than frequencies of resonator and driving; right: qubit frequency equal to the frequency of resonator showing vacuum Rabi splitting (from [ACL-101]).*

6.3 Ratchet transport at nanoscale

D. L. Shepelyansky

For systems without spatial inversion symmetry, the appearance of directed flow of particles induced by a time-periodic parameter variation with a zero-mean force is now commonly known as the ratchet effect. This phenomenon is ubiquitous in nature so that such flows appear in a variety of systems including asymmetric crystals and semiconductor surfaces under light radiation, vortexes in Josephson junction arrays, macroporous silicon membranes, microfluidic channels and others. A significant increase of interest to ratchets is related to the experimental progress in the investigation of molecular transport in biological systems like proteins characterized by asymmetry and non-equilibrium. At the same time, the nanotechnology development allowed to fabricate artificial asymmetric nanostructures with the two-dimensional electron gas

(2DEG) where it has been shown that infrared or microwave radiation creates a ratchet transport (see Fig. 6.5). The theoretical studies predict that the directionality of ratchet flow in such systems can be controlled by the polarization of radiation [ACL-88], which has been confirmed by recent experiments with a semi-disk Galton board for 2DEG in AlGaAs/GaAs heterojunctions by the group of Portal.

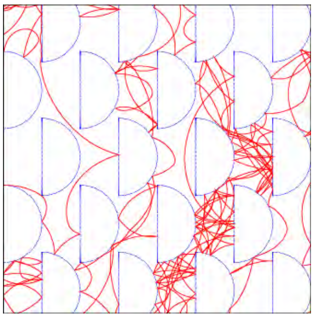


Figure 6.5 : *Example of semidisk Galton board of antidots experimentally realized by J.-C.Portal's group, LNCMI, Grenoble (Phys. Rev. B* **78***, 045431 (2008). For a microwave field polarized along x (y) electrons move to the left (right) (from [ACL-88]).*

The theory of ratchet transport of interacting particles has been developed in [ACL-109]. It was shown that the ratchet flow is preserved in the limit of strong interactions and can become even stronger compared to the non-interacting case. The developed kinetic theory gives a good description of these two limiting regimes. The numerical data show emergence of turbulence in the ratchet flow under certain conditions. The obtained results are well described by the analytical theory based on the kinetic equation for strongly interacting particles. This research is supported by the ANR projects *MICONANO* and *NANOTERRA*.

6.4 Anderson localization, interactions and nonlinearity

D. L. Shepelyansky, I. Garcia-Mata (postdoc)

In the past fifty years a large body of work by physicists and mathematicians was dedicated to the celebrated Anderson localization. The localization of linear waves is now well understood, at least at a physicist level of rigor. In contrast, the effects of nonlinearity on localization are not yet clarified and different opinions about the system behavior at large times appear in the literature.

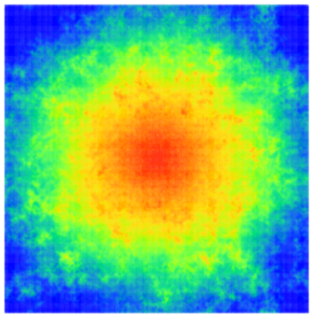


Figure 6.6 : *Probability spreading in 2d Anderson model with disorder and localization induced by nonlinear interactions of the type of Gross-Pitaevskii (from [ACL-118]).*

The active interest for the interplay of nonlinearity and localization has been much fostered by recent experimental studies. A remarkable experimental progress with Bose-Einstein condensates (BEC) in optical lattices stimulated the interest for investigations of the effects of nonlinearity on localization. At present the signatures of localization of BEC in one-dimensional (1D) optical disordered lattices have been detected by different experimental groups. The effects of nonlinearity on localization appear also for experiments with BEC in kicked optical lattices where the quantum chaos in the Chirikov standard map (kicked rotator) is investigated. They also comes out for propagation of nonlinear waves in disordered photonic lattices and the problem of lasing in random media.

In [ACL-99, ACL-118, SRP-5, SRP-6], we have studied numerically the effects of nonlinearity on the Anderson localization in lattices with disorder in one and two dimensions. The obtained results show that at moderate strength of nonlinearity an unlimited spreading over the lattice in time takes place with an algebraic growth of number of populated sites $\Delta n \propto t^{\nu}$. The numerical values of ν are found to be approximately $0.15 - 0.2$ and 0.25 for the dimension $d = 1$ and 2 respectively, in satisfactory agreement with the theoretical value $d/(3d + 2)$. We established the emergence of dynamical thermalization, characterized as an ergodic chaotic dynamical state with a Gibbs distribution over the modes [SRP-6]. The localization is preserved below a certain critical value of nonlinearity.

6.5 Chaos and cold atoms and ions

B. Georgeot, D. L. Shepelyansky, J. Martin (postdoc)

Recent experimental progress allowed to obtain precise control of atomic matter waves of ultracold atoms and Bose-Einstein Condensates (BEC) moving in optical lattices. This opened new pathways for experimental investigation of quantum coherence in the regime of quantum chaos. Such experiments can also be considered as quantum simulators of complex quantum dynamics, which led to the observation of new unexpected effects. In [ACL-85], we have studied the properties of one-dimensional chain of cold ions placed in a periodic potential of optical lattice and global harmonic potential of a trap. In close similarity with the Frenkel-Kontorova model, a transition from sliding to pinned phase takes place with the increase of the optical lattice potential for the density of ions incommensurate with the lattice period. Quantum fluctuations lead to a quantum phase transition and melting of pinned instanton glass phase at large values of dimensional Planck constant.

Such experiments also allow to reconsider ancient questions like time reversibility in physical systems. Indeed, the statistical theory of gases developed by Boltzmann leads to macroscopic irreversibility even if dynamical equations of motion are time reversible. This contradiction pointed out by Loschmidt is now known as the Loschmidt paradox. This paradox can be resolved with the help of the theory of dynamical chaos: in this regime, small perturbations grow exponentially with time, making the motion practically irreversible. This explanation is valid for classical dynamics, but in the quantum case the exponential growth takes place only during the rather short Ehrenfest time, and the quantum evolution remains stable and reversible in presence of small perturbations. Quantum reversibility in presence of various perturbations has been actively studied in recent years under the name of the Loschmidt echo. Experimental implementations of time reversibility for quantum dynamics or propagating waves have been realized with spin systems (spin echo), acoustic and electromagnetic waves, with various technological applications. However, time reversal of matter waves has not been performed so far.

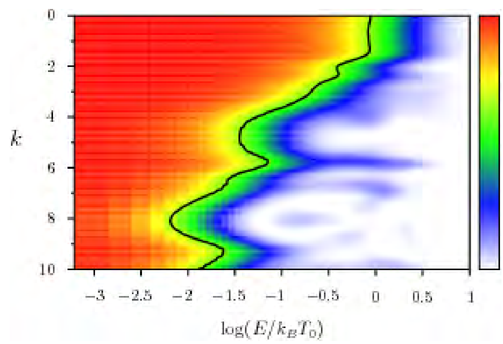


Figure 6.7 : Probability distribution of the wavefunction of cold atoms after time reversal, showing the Loschmidt cooling. Abscissa is energy of the atoms, vertical axis the chaos parameter, red color is maximal probability, white is minimal probability. The black curve is the final temperature of the returned atoms (from [ACL-102]).

In [ACL-102], we have presented a concrete experimental proposal of approximate time reversal of matter waves of ultracold atoms in the regime of quantum chaos. If the atoms were classical particles, they would never return back due to exponential instability of dynamical chaos. But the quantum dynamics is stable and thus a large fraction of the atoms returns back even if the time reversal is not perfect. This fraction of the atoms exhibits what we called “Loschmidt cooling” which can decrease their temperature by several orders of magnitude. Two experimental groups are now trying to perform this proposal.

In [ACL-108], using Gross-Pitaevskii equation, we have studied the time reversibility of BEC in kicked optical lattices, showing that in the regime of quantum chaos the dynamics can also be inverted. The accuracy of time reversal decreases with the increase of atom interactions in BEC, until it is completely lost. Surprisingly, quantum chaos helps to restore time reversibility. These predictions can be tested with existing experimental setups.

The last work in this direction [ACL-122] studies the coupling between a qubit and a BEC moving in a kicked optical lattice. This makes connection to our work on quantum information, and enables to identify several regimes depending on parameters; in particular, when the BEC size is smaller than the lattice period, the chaotic dynamics of the BEC is effectively controlled by the qubit state, giving an example of an exponentially sensitive control over a macroscopic state by internal qubit states.

The group proposal to observe Anderson localization with atomic matter waves in kicked optical lattice was realized experimentally by the group of J.-C. Garreau (Lille; featured in *Physics* **1**, 41 (2008)).

6.6 Applications to astrophysics

Wave chaos in rapidly rotating stars

B. Georgeot

The short-wavelength limit enables to obtain geometrical optic from electromagnetic waves or classical mechanics from quantum mechanics. In this limit, the system is described by trajectories of a Hamiltonian system and notions of chaos and regularity are well-defined.

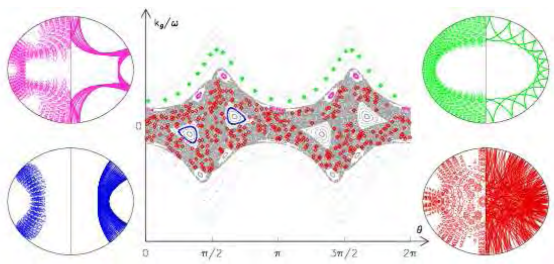


Figure 6.8 : *Acoustic rays, oscillation modes and phase space plot for a model of rapidly rotating star. Amplitudes of 4 typical modes, shown by level curves in the left half of the meridian plane of the star, are compared to 4 trajectories of acoustic rays (right half). Center: Poincaré surface of section visualizing chaotic and semi-integrable structures in phase space together with the 4 typical trajectories (colored diamonds).*

A new domain of application of these concepts has been recently developed. Indeed, acoustic waves also admit a short-wavelength limit, where the system is described by acoustic rays. Such acoustic waves can be observed in stars, using methods of stellar seismology. With the launching of the space missions COROT (December 2006) and KEPLER (2009), stellar seismology, which already revolutionized our knowledge of internal structure of the sun, is bound to do the same for other stars. In order to interpret the observed frequencies in term of constraints on stellar interiors, the physics of oscillation eigenmodes associated to these frequencies should be well understood. This is actually the case for acoustic modes of slowly rotating stars like the sun, which can be considered to be spherically symmetric. For such stars, acoustic rays cannot be chaotic. In contrast, current theories do not allow to understand the effects of centrifugal distortions, thus making the interpretation of the frequency spectrum of rapidly rotating stars a major challenge in present-day stellar seismology.

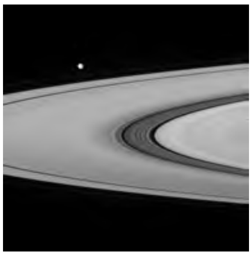
We have recently developed a mathematical formalism and numerical tools which allow to take into account for the first time the centrifugal distortions in the computation of acoustic modes. These first studies allowed us to show that the dynamics of acoustic rays allows to understand the structure of the frequency spectrum. Our studies showed that this dynamics can become chaotic as soon as the rotation becomes important. This explains why the methods developed in astrophysics for the case of slowly rotating stars cannot apply to rapidly rotating ones. The interpretation of observational spectra for such stars should thus make use of the concepts of quantum chaos. Indeed, the eigenfrequency spectrum is a superposition of regular frequency patterns and an irregular frequency subset respectively associated with near-integrable and chaotic phase space regions. This opens new perspectives for rapidly rotating star seismology and also provides a new and potentially observable manifestation of wave chaos in a large scale natural system.

Synchronization in rings of Saturn

D. L. Shepelyansky

The problem of sharp edges in rings of Saturn is an outstanding problem of planetary rings. Indeed, for example the outer B ring edge has a density drop by an order of magnitude on a distance $r_e \sim 10\,m$ that is enormously sharp compared to the edge distance to Saturn

(117580 km), the B ring width (25580 km) and the width of Cassini division (4620 km). This is especially surprising since the life time of the rings is extremely large being of about 10^{12} orbital periods and the particles inside the B ring are quite dense (e.g. there are particles of size 10 m down to 1 cm and smaller with a distance between them of about a few meters and less).



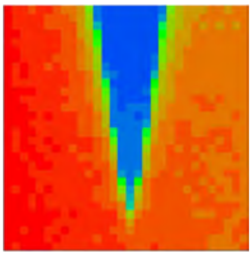


Figure 6.9 : Left: NASA image of Mimas and rings of Saturn. Right (from [ACL-120]): dependence of rescaled diffusion rate in ring B (red is maximum (one), blue is minimum (10^{-4})) on rescaled frequency in the ring (horizontal axis in interval $(0.85, 1.15)$) and driving force strength ϵ (vertical axis in interval $(0., 0.7)$, Mimas gives $\epsilon = 0.64$.)

In [ACL-120] we propose a new mechanism which explains the existence of enormously sharp edges in the rings of Saturn. This mechanism is based on the synchronization phenomenon due to which the epicycle rotational phases of particles in the ring, under certain conditions, become synchronized with the phase of external satellite, *e.g.* with the phase of Mimas in the case of the outer B ring edge. This synchronization eliminates collisions between particles and suppress the diffusion induced by collisions by orders of magnitude. The minimum of the diffusion is reached at the center of the synchronization regime corresponding to the ratio 2:1 between the orbital frequency at the edge of B ring and the orbital frequency of Mimas. This is illustrated in Fig. 6.9, which shows Mimas and the Great Division (left panel showing the image of NASA taken by Cassini mission) and the synchronization window from [ACL-120] (right panel). The synchronization theory gives the sharpness of the edge in few tens of meters that is in agreement with available observations. This work was highlighted by the web sites www.lenta.ru and www.gazeta.ru.

6.7 Chaos and complex systems

B. Georgeot, O. Giraud, D. L. Shepelyansky

Fractals in quantum chaos, isospectrality

New properties of isospectral billiards were investigated [ACL-77]. The properties of quantum fractals have been studied in [ACL-100, ACL-105], including fractal Weyl law and link between moments of multifractal wavefunctions and spectral statistics.

Delocalization transition for the Google matrix

The World Wide Web is an enormously large network with about 10^{11} web pages all over the world. Information retrieval in such a huge database is therefore a formidable task. An efficient method to this aim, known as the PageRank Algorithm (PRA), was put forward and formed the basis of the Google search engine. The PRA uses the PageRank vector, which is the eigenvector associated with the largest eigenvalue of the Google matrix, to rank the sites.

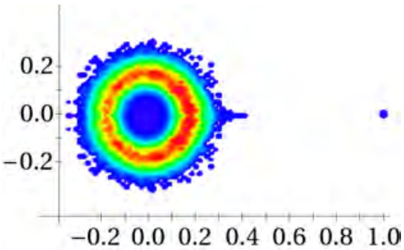


Figure 6.10 : Eigenvalues of Google matrices in the complex plane for a randomized University network. Color is proportional to the inverse participation ratio of the associated eigenvector, from minimal (blue) to maximal (red)(from [ACL-124]).

In [ACL-124], we have studied the localization properties of eigenvectors of the Google matrix, generated both from the World Wide Web and from the well-known Albert-Barabasi model of networks. We have established the emergence of a delocalization phase for the PageRank vector when network parameters are changed. In the phase of localized PageRank, a delocalization takes place in the complex plane of eigenvalues of the matrix, leading to delocalized relaxation modes. In the phase of delocalized PageRank, the efficiency of information retrieval by Google-type search is strongly affected since it does not produce anymore a clear ranking of the nodes.

7

Équipe Physique Statistique des Systèmes Complexes (PhyStat)

The PhyStat group addresses a large variety of problems using the analytical and numerical tools of statistical physics, and in particular, out of equilibrium statistical physics. Over the last ten years, it has developed a strong activity in the field of soft condensed matter physics (ionic fluids, polymers, lipidic films...) and biophysics of the cell membrane, collaborating and sharing contracts with several experimental groups of biologists and physicists. The PhyStat group also has a strong expertise in the applications of stochastic processes in various contexts (diffusing processes in random media, theory of signals, theory of competition, optimization problems...), and the physics of long-range interacting systems (with applications to turbulence, astrophysics, chemotaxis...).

The PhyStat group is headed by David S. Dean (PR1 & IUF) and the other permanent researchers are Pierre-Henri Chavanis (CR1), Nicolas Destainville (MCF), Manoel Manghi (MCF), John Palmeri (CR1), and Clément Sire (DR2, head of LPT). Non permanent staff includes two post-docs, Sahin Buyukdagli and Luca Delfini, and four PhD students, Thomas Portet (LPT-IPBS collaboration), Lorand Horvath (LPT-University of Cluj-Napoca collaboration), Julien Sopik (PhD obtained in June 2007), and Clément Touya.

Funding: since 2007, the PhyStat group has been funded by one *ANR contract NANO (SIMONANOMEM; coordinator)*, one *European contract (NANOBORON; minority partner)*, one *Appel d'Offres du Conseil Scientifique de l'UPS*, one CNRS grant *Interface physique, biologie et chimie : soutien à la prise de risque*, one CEA grant *contrat Équipe (CENEC)*, and one fellowship from the *Institut Universitaire de France (IUF)*. The PhyStat group currently has two postdoctoral fellowships funded respectively by ANR and CNRS. In addition, PhD fellowships have been awarded by the doctoral school *Sciences de la Matière* and the doctoral school *Biologie – Santé – Biotechnologies* of the University of Toulouse, and by the *Délégation Générale pour l'Armement* (DGA). Like the three other groups, the PhyStat group is also funded by the LPT from its own resources (computers, travel expenses...).

Main visitors: prominent scientists who have visited the PhyStat group for a period of at least one month since 2007 include Prof. Alan J. Bray (Manchester U., UK), Ron R. Horgan (Cambridge U., UK), Paul Krapivsky (Boston U., USA), David Lancaster (Westminster U., UK), Roland R. Netz (TU Munich, Germany), and Sidney Redner (Boston U., USA). They were funded by visiting professor fellowships from the University of Toulouse, CNRS guest scientist fellowships, or by means of the IUF grant.

Insert 7.1 : *Funding of the PhyStat group and its main foreign visitors.*

In addition, the PhyStat group typically hosts one or two Master students per year, during their three-month research projects.

The PhyStat group has several ongoing collaborations with scientific institutions

❍ **In Toulouse:** Institut de Pharmacologie et Biologie Structurale (IPBS; 2 independent collaborations), Institut de Mathématiques de Toulouse (IMT), Laboratoire de Microbiologie et Génétique Moléculaires (LMGM), Observatoire Midi-Pyrénées (OMP).

❍ **In France:** CEA-Saclay, ENS Lyon, ENS Paris, Université de Marseille, Université de Montpellier, Université Paris-Sud Orsay, Université Paris VI Pierre et Marie Curie, Université de Rennes.

❍ **Abroad:** Max Planck Institut – Stuttgart, Technische Universität München (Germany), Synchrotron Trieste, Università di Firenze, Università di Padova, Università di Roma "La Sapienza" (Italy), University of Osaka (Japan), Faculté des Sciences d'Agadir (Morocco), University of Ljubljana (Slovenia), École Nationale d'Ingénieurs de Tunis (Tunisia), London Research Institute, University of Cambridge, University of Manchester, University of Oxford, University of Sheffield, University of Westminster (UK), Carnegie Mellon University, National Health Institute – Bethesda, University of Boston, University of California – Merced, University of California – Santa Barbara (USA).

Insert 7.2 : *Main ongoing collaborations with institutions in Toulouse, France, and abroad (only the hosting university is cited in the two last cases).*

The main sources of funding of the PhyStat group and our medium-term foreign visitors are listed in Insert 7.1. The PhyStat group has ongoing collaborations with many local, French, or foreign institutions, which are listed in Insert 7.2.

D. S. Dean is a current fellow of the *Institut Universitaire de France (IUF; 2007-2012)*, and two members of the PhyStat group have received the Bronze Medal of CNRS in the past (C. Sire in 1994; P. H. Chavanis in 2000; both in section 02 – theoretical physics).

During the last four years, the PhyStat group has published more than **120 articles in refereed international journals** and has contributed to more than **50 conferences (32 invited talks)**. The main aspects of the scientific activity of the PhyStat group during the period 2007-2009 are highlighted in the next three sections. More details can be found on the personal web pages of the members of the PhyStat group.

7.1 Biophysics and soft condensed matter

Despite the inherent complexity of many soft matter, biomimetic, and biological systems (due to interactions $\sim k_B T$, thus large fluctuations, and strong correlations), a deeper fundamental understanding of the physical mechanisms at play could lead to potentially huge payoffs. Areas as important as human health and the worldwide supply of abundant clean water could benefit in the long term from far-reaching advances in comprehension obtained by applying the tools of Statistical Physics to such systems. In this section, we present recent work carried out at LPT PhyStat group, at the interface between physics and biology. This work has already provided greater insight into the thermal denaturation of DNA, the cluster phases of membrane proteins, electropermeabilization of membranes, fluctuation induced interactions in lipid membranes, and ion transport in nanopores.

DNA melting transition

M. Manghi, J. Palmeri, N. Destainville

The thermal denaturation of double-stranded DNA is a physical process in the course of which the double strand, or helix, can open locally thanks to thermal fluctuations that create an opening of successive base pairs, called a denaturation bubble. In the literature, DNA is essentially modeled as a one-dimensional system whose denaturation is described by a 1D Ising model in a "temperature dependent magnetic field" (Poland-Sheraga model) or by an unbinding transition in an orthogonal dimension (Peyrard-Bishop-Dauxois model).

Theory of thermal denaturation of DNA

Recently, J. Palmeri, M. Manghi and N. Destainville [ACL-192] have studied this denaturation process theoretically by illuminating the role of the **coupling between the**

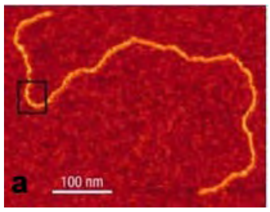
3D non-uniform statistical bending inside a DNA polymer and the **opening and closing of the base pairs** linking the two strands. Within a bubble the two fluctuating single strands are much more flexible than an unopened helix and therefore DNA can explore a much larger number of geometrical configurations when in the bubble state. The DNA geometry will in turn influence the bubble creation process. This mutual influence naturally leads to our coupled theoretical model (Ising-Discrete Worm-like chain model), permitting one to calculate, for example, the denaturation temperature above which the double strand tends to a completely open state (in most previous statistical models, this temperature was put in by hand to analyze experiments). More precisely, the melting temperature is determined by a balance between the energetic cost of opening a base-pair (H-bonds breaking) and the entropic gain in allowing the chain to fluctuate more easily. The statistical properties (end-to-end distance, persistence length) have been calculated as a function of temperature, T, reproducing qualitatively experimental data of DNA solution viscosity measurements. This study has been completed by exploring the influence of the chain length on the melting profile (fraction of open base-pairs *vs* T) [ACL-209, ACL-235] and the role of other chain degrees of freedom such as stretching and torsion [ACL-235].

This work [ACL-192] was recently featured on the scientific news section of CNRS *Institut de Physique* web site.

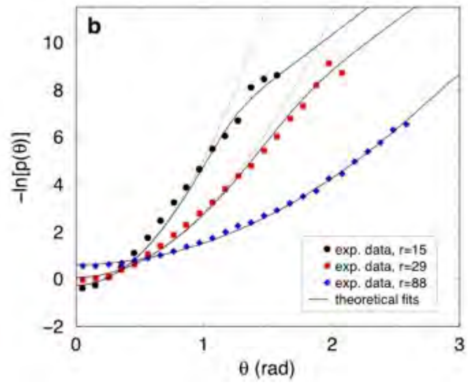
DNA adsorbed on surfaces

Atomic Force Microscopy (AFM) is widely used to observe double-stranded DNA adsorbed on surfaces. In recent experiments by Wiggins *et al.*, “anomalies” have been detected in the distribution of bending angles along DNA $p(\theta)$, which measures its flexibility: an over-abundance of large angles was found which is not predicted by the traditional *worm-like chain model* for DNA chains (Insert 7.3). The model has been applied to DNA adsorbed on surfaces by N. Destainville, M. Manghi and J. Palmeri [ACL-236], and these anomalies are related to the presence of **small denaturation bubbles** (or **kinks**) facilitated by the presence of the substrate which modifies the electrostatic interactions between DNA base-pairs. They predict that these anomalies exist in 3D but are too weak to be detected and reconcile the apparent discrepancy between observed 2D and 3D elastic properties. Hence, conclusions about 3D properties of DNA (and its companion proteins and enzymes) do not directly follow from 2D experiments by AFM.

Snapshot of a DNA observed by AFM on a mica surface (experiments by Wiggins *et al.* (2006)).



Experimental bending angle distribution (symbols) for three different values of the distance along the chain. It shows a deviation from the Worm Like Chain model (parabola) for large angles which is well fitted by the theory (solid line).



***Insert 7.3 :** DNA adsorbed on surfaces*

Cluster phases of membrane proteins

N. Destainville

N. Destainville studies the dynamical organization of assemblies of bio-membrane proteins. A cell contains several thousand of different proteins species that ensure a large variety of functions. To accomplish their task, they must interact with their parters that often lie in the membrane themselves. To account for the rapidity of the response to an external stimulus, it is generally believed that parters must be co-localized in advance in small membrane **micro-domains**, of size $\sim 100\,\mathrm{nm}$. To explain this compartmentalization, two models are usually invoked: lipid rafts, resulting from a lipidic micro-phase separation, and the "fence-and-picket model" for non-raft proteins, which supposes the delimitation of membrane domains by actin filaments of the cytoskeleton. In this context, N. Destainville proposed a new paradigm explaining the existence of micro-domains, based upon an **analogy with cluster phases in colloidal physics**. The coexistence of effective short-range attractive forces and longer-range repulsive ones ensures the existence, at equilibrium, of proteins clusters of a few tens or hundred of proteins, which play the role of the above-mentioned compartments. The interactions taken into account are mediated by the lipidic membrane in which the proteins dwell, and are on the order of the thermal energy $k_B T$.

These cluster phases have been studied by numerical [ACL-211] as well as analytical [ACL-212] means. It has been shown that the mean-cluster size grows proportionally to the protein concentration ϕ and that the mean diffusion coefficient of proteins is inversely proportional to ϕ. These results have been discussed in the context of biological membranes in the review article [ACL-214]. Work is in progress to study the role of the great diversity of membrane proteins and to test these predictions at the experimental level, in collaboration with the group of L. Salomé at the Institut de Pharmacologie et Biologie Structurale (Toulouse).

Electropermeabilization

D. S. Dean, T. Portet

Electropermeabilization is the phenomenon via which biological membranes are rendered permeable to the passage of molecules and even macro-molecules by the application of an electric field [ACL-185, ACL-189, ACL-231, ACL-234, SRP-11]. This effect is extensively exploited in medicine, specifically in the field of cancer and genetic therapy. In chemotherapy, the permeabilizing effect of the electric field enables the treatment of cancers in a much more targeted way (only the region of the tumor is subjected to the field) and the enhanced permeability due to the electric field means that much lower doses of chemotherapeutic drugs can be administered, greatly reducing side effects. Electropermeabilization is also a promising candidate for gene therapy treatments and does not entail the same risks as viral mediated gene transfer [ACL-185, ACL-231]. The PhyStat group has launched a collaboration with the team of M.-P. Rols at the IPBS Toulouse, one of the world leading experimental groups in the field. Currently, a PhD student (T. Portet) is being co-supervised by D. S. Dean and M.-P. Rols.

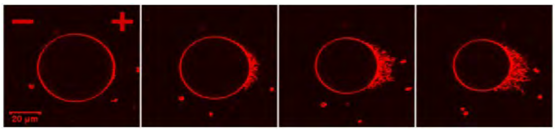


Figure 7.1 : Confocal images of a lipid giant unilamellar vesicle subjected to electric pulses (360 V/cm; 0.5 Hz; 5 ms duration), exhibiting size decrease and the formation of tubular structures facing the anode. 6 pulses are applied between each snapshot.

We have shown that giant unilamellar vesicles subjected to electropermeabilizing pulses tend to shrink [ACL-234]. The vesicles lose lipids from the main body via three mechanisms (i) the formation of pores, (ii) the budding off of micro-vesicles and (iii) the formation of vesicle tubules (see Fig. (7.1). These novel experimental results can be partly explained in a model where we assume lipid loss is proportional to the area where the lysis tension of the lipid membrane is exceeded (due to the addition of that coming from the Maxwell stress tensor of the applied field). We have also been studying the permeabilization of cells in the presence of plasmid DNA (4.7 kb). This problem is of practical importance (gene therapy) and also the underlying physics is rich (permeabilization of the membrane, interaction of DNA with the membrane and the electrophoretic transport of the DNA) [ACL-189]. We have modeled the transport of DNA in the region of a cell which is assumed to have a pore formed by electroporation. The model explains experiments carried out at the IPBS and confirms that the major obstacle to gene transfer is the actin cytoskeleton of the cell interior [SRP-11].

Fluctuation induced interactions

D. S. Dean, M. Manghi

Pseudo Casimir effects arise via the thermal fluctuations of classical fields such as those describing the order parameter of classical systems near critical points, the director fluctuations in liquid crystals and the height fluctuations of lipid membranes. We have studied the effective interactions between regions of lipid membranes of varying elasticity and bending rigidity. In [ACL-170] we showed that regions of differing mechanical properties (due to differing lipid types) could have attractive or repulsive interactions between them, meaning that the nature of the phase transition in membranes formed from lipid mixtures could be drastically modified by membrane height fluctuations. A thermal Casimir effect between large striped membrane regions of differing mechanical properties was demonstrated in [ACL-190].

In soft matter systems, where relaxation times can be large, it makes sense to ask how the Casimir force evolves out of equilibrium. To study this problem we considered a formulation of the Casimir effect where the energy of interaction of the fluctuating field with the boundaries or objects placed in the field is specified [ACL-232]. We were able to study the effect of these soft boundary conditions on systems of two and even three parallel plates. In the case of soft boundary conditions, whether or not the fluctuations exist outside the two external plates drastically affects the force on the central plate and can even change its sign. In [ACL-245], using this boundary energy formalism, we were able to compute the force on objects and surfaces in fluctuating fields out of equilibrium for a very general class of dissipative dynamics. In [ACL-242] the thermal Casimir or zero frequency van der Waals interaction between slabs of random dielectric media was studied. This calculation represents the first ever analysis of the Casimir effect in disordered systems. Two important physical points were found: (i) the long range force is self-averaging and is given by a description in terms of effective dielectric constants; (ii) the short range force is a random variable, dominated by the closest opposing layers.

Ion partitioning and transport in nanoporous membranes

J. Palmeri, M. Manghi, D. S. Dean, L. Horvath (PhD student), S. Buyukdagli (postdoc)

Using macroscopic mean field, field theoretic, and microscopic molecular dynamical (MD) simulation methods, our goal is to better understand the physical and physicochemical phenomena involved in nano-confined aqueous solutions, especially the role of "solute-solute" and "solute-interface" interactions in nanofiltration [ACL-140, ACL-193, COD-3, ACL-142]. We focus on effects due to the specific characteristics of molecules and ions (size, charge, polarizability) by studying their distribution, correlations, and fluctuations near interfaces and in nanopores [TH-14, TH-15, ACTI-20, AFF-30].

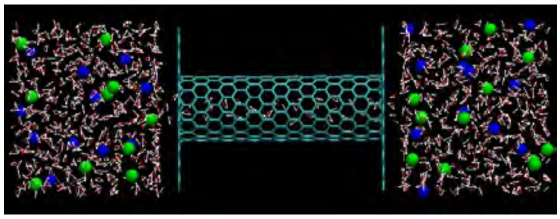


Figure 7.2 : *MD Snapshot of a nanopore with 1M Na Cl in water [TH-15].*

7.2 Stochastic processes and disordered systems

Many systems in Nature can be well described by effective random processes. From the diffusing trajectories of dust particles or proteins on the cell membrane (see Section 7.1), to financial signals, statistical physics has developed efficient tools to model a large class of physical, biological, or social signals, thereby giving a better qualitative and quantitative understanding of extremely complex systems. In the present section, we review a series of recent fundamental results obtained at LPT in the field of stochastic processes and disordered systems, and illustrate some of their applications.

Persistence and extreme value statistics

D. S. Dean, C. Sire

The persistence $P(M,t)$ of a general temporal signal $x(t)$ is the probability that this signal always remains above (or below) a certain threshold M from time 0 up to time t. In the period 1996-2001, C. Sire, S. N. Majumdar (CR1 at LPT in 1999-2004, now DR2 at LPTMS Orsay), and their collaborators in Manchester and Jülich developed powerful methods to evaluate the large time asymptotics of the persistence (and hence the persistence exponent) for physically relevant signals, but **only** when M is equal to the mean of x. Persistence exponents have been measured in systems as different as breath figures, liquid crystals, laser-polarized Xe gas, fluctuating steps on a Si surface, and soap bubbles. The aforementioned theories are in very good agreement with experiments (and numerical simulations) in all these cases. The two following studies illustrate the deep connection between **persistence and extreme value statistics**.

General theory of persistence

Recently [ACL-195, ACL-223], C. Sire has obtained a very precise approximation for $P(M,t)$, for arbitrary M and t, from the sole knowledge of the two-time correlation function of the random process x (not necessarily Gaussian). This theory gives access to the distribution of the minimum (or the maximum) of a general signal during a time window of duration t, since $P(M,t)$ is exactly the probability that the minimum of x over the interval $[0,t]$ be larger than M. Many general results have been obtained [ACL-223] for the distribution of time intervals at which the signal crosses the threshold M, and the approximation of [ACL-195] either reproduces most of these exact results, or turns out to be an excellent approximation.

Random matrices and persistence

As an original example of persistence, D. S. Dean and S. N. Majumdar computed exactly the probability that an $N\times N$ Gaussian Hermitian/real symmetric random matrix has all its eigenvalues above a certain threshold M [ACL-167, ACL-216]. This persistence probability decays exponentially with the number of entries N^2, and the rate is exactly the persistent exponent. Generalizing the celebrated Wigner semi-circle law, they obtained the corresponding conditional density of states of the eigenvalues, in the large N limit.

Theory of competition

C. Sire, D. S. Dean

Physicists are now more then ever involved in the study of complex systems which do not belong to the traditional realm of their science. Finance (option pricing theory,...), human networks (Internet, airports,...), the dynamics of biological evolution and in general of competitive "agents" are just a few examples of problems recently addressed by statistical physicists. In this section, four recent studies concerning **the theory of competition** are summarized. All are intimately related to the persistence problem, extreme value statistics, and traveling wave theory.

The "leader" problem

C. Sire, D. S. Dean, and S. N. Majumdar have defined a very general kind of competition which arise as a simplification of some evolutionary biology models. N "agents" have random fitnesses v_i, and obtain a "score" $s_i(t) = s_i(0) + v_i t$ at time t, where the initial scores are random variables. At large enough time, the leader of the pack (the agent with the highest score) will ultimately be the one having initially the largest fitness. A natural question thus arises: **how many different leaders were there during the competition?** In most practical examples of a general finite-time competition (see the case of poker tournaments below), one observes numerically that the total number of leaders behaves like $\log N$, and that the proportionality constant is universal. In [ACL-178], these results have been rigorously and explicitly derived and the authors obtained the full distribution of the number of leaders starting from N players.

Universal dynamics of poker tournaments

Poker tournaments, although *a priori* controlled by purely human factors (fear, bluff...), are a perfect laboratory to test the possible application of statistical physics methods to social systems: contrary to most other challenging systems (finance, social networks, epidemics...), they are **perfectly isolated** from the influence of the outside world.

C. Sire has developed a numerical model which mimics the dynamics of a poker tournament with initially N players [ACL-197]. This model can be analytically solved and its results are in perfect agreement with data gathered from actual Internet tournaments or live World Championships. The average duration of the tournament and the number of successive "chipleaders" (the player with the biggest fortune at a given time) are both found to be proportional to $\log N$, in agreement with the general result of [ACL-178]. The distribution of the fortune of the current chip-leader is universal and follows the Gumbel law, well-known in the context of extreme value statistics. The most spectacular result concerns a faithful description of the rank of a player at a given time, as a function of his current fortune, which is illustrated in Fig. 7.3. This work has received important media coverage (Scientific American, PhysOrg.com, and many others).

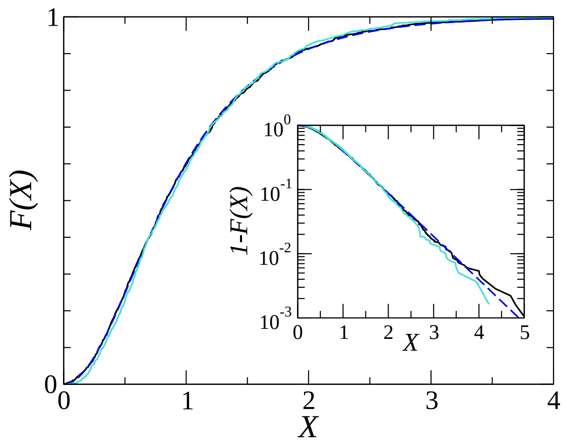


Figure 7.3 : *Plot of the fraction $F(X)$ of players who are poorer than a given player owning X times the average fortune. $F(X)$ does not depend explicitly on time (scale invariance). The solution of the model (blue dashes; no parameter fit) agrees perfectly with data collected from 22 Internet tournaments (black) and the full 2006 season of the Word Poker Tour (light blue).*

Baseball team standings and streaks

C. Sire and S. Redner (Boston) have modeled sport leagues [ACL-241] to quantify the distribution of a team's wins and losses in major-league baseball over the past century, and also to argue that long winning and losing streaks are of purely statistical origin. The data further reveal that the past half-century of baseball has been more competitive than the preceding half-century, and the analysis points to subtle effects due to the finite number of matches in a season.

Contest based on a random polymer

C. Sire has defined and solved a two-player game inspired by a model of a directed polymer on the Cayley tree (the tree of possible moves) [ACL-224]. The fact that the two players have antagonist goals is reminiscent of the notion of **frustration** common in disordered physical systems. The solution involves extreme value statistics and front wave propagation, including a subtle non linear front velocity selection mechanism.

Diffusion in random media

D. S. Dean, C. Sire, J. Sopik (PhD student), and C. Touya (PhD student)

Diffusion in random media is an interesting subject in its own right and also because systems exhibiting structural glass transitions often behave like systems with quenched disorder (which is dynamically induced). Other applications are to theories of absorption/growth processes (like DLA), where renormalization group techniques developed for diffusion in random media have been successfully adapted [ACL-177].

Diffusion in non-Gaussian random potentials

In the past, there have been many studies of the diffusion of a particle in a short range Gaussian potential ϕ. In finite dimensions, the diffusion constant of the particle is always non-zero at finite temperatures and no transition between a normal and sub-diffusive regime can occur. However, for a potential which is a function of a Gaussian potential $V = V(\phi)$, a transition can occur and this transition can be identified as the divergence of the mean occupation time in local minima [ACL-194]. An example is the potential $V(\phi) = \phi^2/2$, which physically arises when one considers dipoles in a random Gaussian electric field [ACL-246]. This model in dimension $D = 1$ and a particular variant in $D = 2$ can be treated analytically. The effective diffusion constant vanishes as $\kappa_e \sim (1-\beta^2)^{\frac{1}{2}}$ ($\beta = 1/k_BT$), in a way reminiscent of that predicted by mode-coupling theories of the glass transition. The low temperature exponent characterizing the sub-diffusion was also computed using a version of the replica method applied to the first-passage time problem. In higher dimensions, analytic results are not available and one must resort to approximation schemes. A self-similar renormalization group approach [ACL-217] was applied to the mathematically related problem of diffusion in a medium of random diffusivity, where the diffusion equation has the form $\dot{p} = \nabla \cdot \kappa(\mathbf{x}) \nabla p$. If one assumes that $\kappa = \kappa(\phi(\mathbf{x}))$ where ϕ is Gaussian, the self similar RG yields the result:

$$\kappa_e^{(p)} = \left\langle \kappa(\mathbf{x})^{1-\frac{2}{D}} \right\rangle^{\frac{1}{\left(1-\frac{2}{D}\right)}} \tag{7.1}$$

This result is a widely used approximation in the field of effective permeabilities (for random dielectrics and porous media) and this form is sometimes referred to as the Landau-Lifshitz-Matheron conjecture. From Eq. (7.1), using a mathematical relation between the two problems, we computed the effective diffusion constant for diffusion in a random potential $V(\phi)$. For quadratic V, this result gives the celebrated Volger-Fulcher-Tammann divergence of the relaxation time $\tau \sim 1/\kappa_e$ as one approaches the glass transition. A final result of this analysis concerns a tentative link with the diffusion constant of interacting Langevin particles. The potential seen by a particle is the sum over the pairwise interactions. Treating this potential as effectively random, the self-similar RG predicts the self-diffusion constant of the particles to be $\kappa_e = \exp(2\beta s_{ex}/D)$, where s_{ex} is the excess entropy. This sort of result has been observed in the literature on molecular dynamics simulations, but has not been understood theoretically.

Average number of critical points of Gaussian random fields

Gaussian random fields are of particular importance, as they can be argued to occur spontaneously in systems with a large number of degrees of freedom by appealing to the central limit theorem. The study of the distribution of critical points of complex and random fields occurs in a number of physical problems ranging from string theory (where the local minima of the string landscape correspond to possible universes), theories of the structural glass and spin glass transition (the onset of the glass transition is often identified with the point where the critical points in the free energy landscape become dominated by minima), theoretical studies of hard optimization problems and the problem of protein folding. In [ACL-186], we were able to compute the average number of critical points of a Gaussian potential, on a high dimensional space, at fixed value of the potential and at fixed number of negative eigenvalues at the critical point. This work presents a significant technical advance as the only previous results which existed were for the total average number of critical points and for the average number of local minima.

7.3 Statistical physics of systems with long range interactions

Systems with long-range interactions are numerous in nature and present the remarkable property of self-organizing spontaneously into coherent structures. This corresponds to galaxies in astrophysics (stellar systems), large scale vortices in geophysical and astrophysical flows (two-dimensional turbulence), aggregates of bacteria in biology (chemotaxis), and clusters in the HMF toy model. Interestingly, it is possible to understand the structure and organization of these very different systems in terms of similar arguments of statistical mechanics and kinetic theory.

The Hamiltonian Mean Field (HMF) model

P. H. Chavanis, L. Delfini (postdoc)

The HMF model describes the evolution of N rotators coupled through an attractive cosine interaction. The Hamiltonian reads

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N} p_j^2 + \frac{1}{2}\sum_{i,j=1}^{N} [1 - \cos(\theta_i - \theta_j)], \tag{7.2}$$

where θ_i represents the orientation of the i-th rotator and p_i stands for the conjugated momentum. To monitor the evolution of the system, it is customary to introduce the magnetization, an order parameter defined as $M = |\sum_i \mathbf{m}_i|/N$, where $\mathbf{m}_i = (\cos\theta_i, \sin\theta_i)$.

For $t \to +\infty$, this system is expected to reach a statistical equilibrium state described by the Boltzmann distribution. However, numerical simulations of the N-body system show a more complex behavior (see Fig. 7.4 from [ACL-230]). Indeed, the system **gets stuck in a quasi-stationary state (QSS) that differs from the Boltzmann distribution**. This discovery was a surprise in the statistical mechanics community and different approaches such as the generalized thermodynamics of Tsallis have been proposed to account for these QSS. In fact, the same phenomenon was previously observed in self-gravitating systems and 2D turbulence where an explanation in terms of a statistical mechanics of the Vlasov equation was proposed a long-time ago by D. Lynden-Bell[1]. This approach was not well-known by the statistical mechanics community and P. H. Chavanis [ACL-158] has contributed to popularizing it.

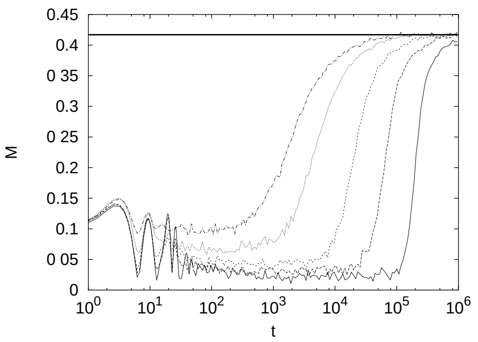


Figure 7.4 : *Evolution of the magnetization $M(t)$ for different values of the particle number N [ACL-230]. For $t \to +\infty$, the system relaxes towards the Boltzmann distribution (solid line). However, before reaching this statistical equilibrium state, it remains frozen in a QSS (plateau), whose lifetime diverges as $N \to +\infty$.*

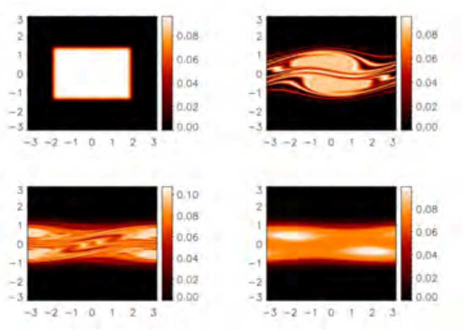


Figure 7.5 : *Numerical simulation of the Vlasov equation in phase space starting from an initial distribution function $f(\theta, v, t = 0)$ taking only two values $f = f_0$ or $f = 0$ [ACTI-24]. This figure reveals the complicated mixing process leading to a QSS on a coarse-grained scale, corresponding to violent collisionless relaxation.*

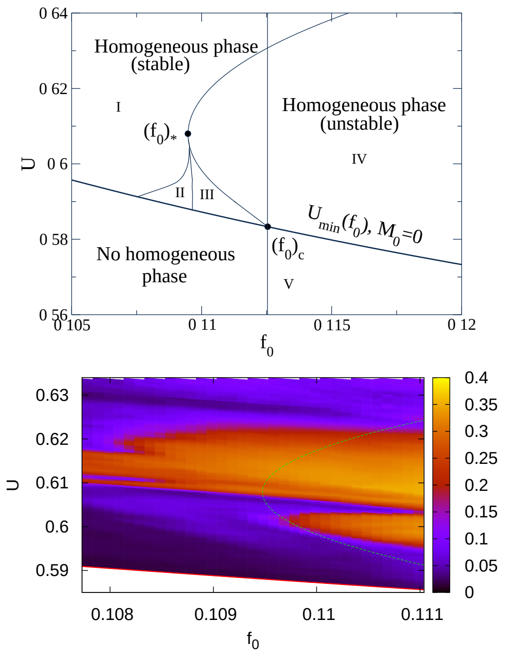
Using the Lynden-Bell theory of **violent relaxation** (see Fig. 7.5), P. H. Chavanis and his colleagues [ACL-158, ACL-180, ACTI-24, ACL-230] have determined the out-of-equilibrium phase diagram of the HMF model (see Insert 7.4). The prediction depends on two control parameters: the energy U and the value f_0 of the initial distribution function. Varying these parameters, an out-of-equilibrium phase transition occurs [ACL-158, ACL-180], where the QSS can be either un-magnetized (the system of rotators is spatially homogeneous) or magnetized ($M \neq 0$; inhomogeneous). A more detailed analysis [ACTI-24, ACL-230] shows that there exists on the same diagram **first and second order phase transitions** that merge at a tricritical point $((f_0)_*, U_*) = (0.10947, 0.608)$. Furthermore, the phase diagram displays an interesting phenomenon of **phase re-entrance** [ACL-158]: if f_0 lies in the small interval $[0.10947, 0.1125]$, by decreasing progressively the energy, the QSS is successively homogeneous, inhomogeneous, and homogeneous again.

Recently, this theoretical prediction has been confronted with direct numerical simulations of the N-body Hamiltonian system [ACL-230]. The phase re-entrance phenomenon is confirmed (see Insert 7.4). This is remarkable because phase re-entrance occurs in a very small range of parameters which would have been difficult to find without the theoretical prediction. The existence of first and second order phase transitions has also been confirmed numerically. However, the simulations show that the picture is more complicated than the prediction of the Lynden-Bell theory. In particular, there exists a secondary zone of phase re-entrance in the magnetized region and a persistence of magnetized states in the un-magnetized region. These anomalies are probably the result of an *incomplete relaxation* as observed in other domains [ACL-149], but it is difficult to make predictions when the evolution of the system is non-ergodic.

On longer timescales, the system is expected to converge towards the Boltzmann distribution due to correlation/finite N effects ("collisions"). P. H. Chavanis and his colleagues [ACL-206] have investigated numerically this phase of slow

1. D. Lynden-Bell, Mon. Not. R. Astron. Soc. **136**, 101 (1967).

collisional relaxation. They have found that, in the collisional regime, the distribution function $f(\theta, p, t)$ is well-fitted by q-Gaussian distributions (Tsallis distributions) with an index $q(t)$ evolving in time. When the $q(t)$-parameter reaches a critical value $q_c(U)$, the distribution becomes Vlasov unstable [ACL-206, ACL-244] [2] and a dynamical phase transition takes place which rapidly drives the system towards the Boltzmann distribution. This corresponds to the sudden transition from the non-magnetized QSS to the magnetized equilibrium state that can be observed on Fig. 7.4.



Out-of-equilibrium phase diagram of the HMF model in the framework of Lynden-Bell's theory of violent relaxation [ACL-158, ACTI-24] (top), and as obtained from direct numerical simulations (bottom), which confirms the main theoretical predictions (phase re-entrance, first and second order phase transitions...).

***Insert 7.4 :** Theoretical and numerical phase diagram of the HMF model.*

Thermodynamics of self-gravitating Brownian particles and chemotaxis of bacterial populations

P. H. Chavanis, C. Sire, J. Sopik (PhD student)

In biology, many organisms (bacteria, amoebae, cells,...) or social insects (ants, swarms,...) interact through the process of chemotaxis. Chemotaxis is a long-range interaction that accounts for the morphogenesis and self-organization of biological systems. A first successful model of chemotactic aggregation is provided by the Keller-Segel (KS) model [3]:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D_* \nabla \rho - \chi \rho \nabla c), \qquad (7.3)$$

$$\frac{\partial c}{\partial t} = D_c \Delta c - kc + h\rho. \qquad (7.4)$$

It consists in two coupled differential equations that govern the evolution of the density of cells (or other biological entities) $\rho(\mathbf{r}, t)$ and the evolution of the secreted chemical $c(\mathbf{r}, t)$. Eq. 7.3 is a drift-diffusion equation. The cells diffuse with a diffusion coefficient D_* and they also move in a direction of a gradient of the chemical (chemotactic drift). The second equation Eq. 7.4 in the KS model is a reaction-diffusion equation. The chemical is produced by the bacteria with a rate h and is degraded with a rate k. It also diffuses with a diffusion coefficient D_c. When chemotactic attraction prevails over diffusion, the KS model describes a *chemotactic collapse* leading to aggregates or Dirac peaks (see Fig. 7.6).

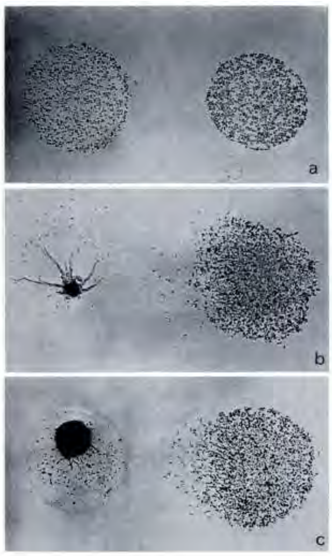


***Figure 7.6 :** An experimental example of chemotactic collapse.*

The first equation of the KS model can be

2. [ACL-244] was recently highlighted in *Europhysics News* **40**, 13 (2009).
3. E. Keller and L. A. Segel, J. Theor. Biol. **26**, 399 (1970).

interpreted as a mean field Smoluchowski equation describing a system of Brownian particles in interaction. On the other hand, in the limit of large diffusivity of the chemical, and when the degradation of the chemical can be neglected, the second equation reduces to a Poisson equation $D_c\Delta c = -h\rho$. In that case, we find that the simplified KS model becomes equivalent to the Smoluchowski-Poisson (SP) system

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left[\frac{1}{\xi}\left(\frac{k_B T}{m}\nabla\rho + \rho\nabla\Phi\right)\right], \quad (7.5)$$

$$\Delta\Phi = G\rho, \quad (7.6)$$

describing a system of overdamped self-gravitating Brownian particles in the mean field approximation. We have the correspondence: $D_* = k_B T/\xi m$, $\chi = 1/\xi$, $c = -\Phi$, $\lambda = G$. In particular, the **concentration of the secreted chemical** $c(\mathbf{r}, t) = -\Phi(\mathbf{r}, t)$ in biology plays the role of the **gravitational potential** (with the opposite sign) in astrophysics.

P. H. Chavanis and C. Sire [ACL-157, ACL-159, ACL-182, ACL-183, ACL-174, ACL-175, ACL-196, ACL-220, ACL-222] have performed a detailed analytical and numerical study of these equations. The extension of these studies to a multi-species system has been done with J. Sopik [ACL-143]. The theoretical problem is very rich because several regimes can occur depending on the value of the temperature, the dimension of space and whether the system is in a bounded or an unbounded domain. Typically, three types of evolution are possible: (i) convergence towards an equilibrium state for $t \to +\infty$. (ii) collapse in finite or infinite time. (iii) evaporation. P. H. Chavanis and C. Sire have performed a detailed study of the equilibrium phase diagram in order to determine under which conditions the system can achieve an equilibrium state. When no equilibrium state exists, the system can either collapse or evaporate. In that case, the strategy is to look for self-similar solutions describing the evolution of the system. Despite the mathematical complexity of the problem, it has been possible to provide analytical solutions for all the phases of the dynamics. In particular, in two dimensions, it is possible to compute exactly (*i.e.* for any particle number N) the diffusion coefficient of self-gravitating Brownian particles [ACL-174, ACL-183]:

$$D(T) = \frac{k_B T}{\xi m}\left(1 - \frac{T_c}{T}\right), \quad (7.7)$$

involving the critical temperature

$$k_B T_c = (N-1)\frac{G m^2}{4}. \quad (7.8)$$

The classical Einstein relation is recovered for $G = T_c = 0$. This expression shows that the system evaporates for $T > T_c$ and undergoes a finite time collapse for $T < T_c$.

P. H. Chavanis and C. Sire have also developed a kinetic theory of chemotaxis leading to hydrodynamic equations including a friction force [ACL-198, ACL-156, ACL-221]. The KS model is recovered in the limit of strong friction and leads to point wise blow-up. Alternatively, when the friction coefficient is reduced, the aggregates are replaced by a filamentary structure. These filaments are observed in experiments of blood vessel formation and they have been proposed to explain vasculogenesis. They are also observed in cosmology, where the evolution can be described by the Euler-Poisson system.

Other works

P. H. Chavanis

P. H. Chavanis has developed other aspects of the dynamics and thermodynamics of systems with long-range interactions. He studied the lifetime of metastable states of self-gravitating systems (such as globular clusters) and showed that it scales like e^N, with $N \sim 10^6$. Therefore, even if these systems are only local entropy maxima, they are very robust in practice [ACL-127]. Extending the Chandrasekhar theory of relativistic white dwarf stars in d dimensions, he showed that white dwarf stars become unstable in a space of dimension $d \geq 4$ [ACL-181]. He also developed an analogy between relativistic stars with a linear equation of state and black holes, and discovered a critical dimension $d_c = 9.96404372...$ for self-gravitating radiation (photon stars) in general relativity [ACL-203]. With F. Bouchet, he described the evolution of collisionless stellar systems on the coarse-grained scale [ACL-128]. With B. Dubrulle *et al.*, he developed the statistical mechanics of 3D axisymmetric magnetohydrodynamics and granular flows [ACL-128, ACL-148, ACL-243]. With M. Lemou, he developed the kinetic theory of point vortices [ACL-184, ACL-201].

8

Équipe Systèmes de Fermions Finis – Agrégats (AGRÉGATS)

The core activity of the AGRÉGATS group concerns the description of the dynamics of clusters and molecules subject to violent electromagnetic perturbations, such as delivered by short and intense laser pulses or highly charged ionic projectiles. During the last few years, we have extended our previous works on free systems to the case of systems in contact with polarizable environments. Beyond their intrinsic fundamental interest, these studies open up the way to remarkable applications in various domains of science among which the most prominent ones are certainly the tailoring of nanosystems on surfaces, with all potential applications to nanotechnologies, and the understanding of irradiation damages in living tissues, with all potential long term oncology implications.

During the last few years the new activities of the group were mostly developed along three complementing lines:

❍ Formal developments for the correct description of ionization dynamics in the framework of **Time Dependent Density Functional Theory (TDDFT)**.

❍ Methodological developments for the construction of **dynamical hierarchical approaches** to describe the **coupled response of the system *and* the environment**

❍ Technical and numerical extension of the **non adiabatic** description of electron dynamics to the case of **organic systems**.

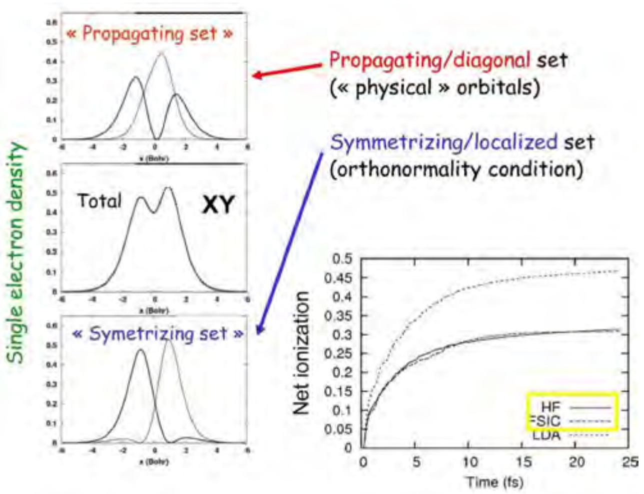
All three aspects have been successfully worked out over the last few years and will be discussed below in more detail. In parallel to these (sometimes heavy) theoretical developments we have continued to analyze some detailed aspects of coupled electron and ion dynamics in free irradiated metal clusters, motivated by new challenging experimental developments. This concerns mostly the growing availability of extreme light (extremely short pulses, extremely high photon frequencies) and the new experimental data on properties of (possibly time resolved, possibly angular resolved) distributions of emitted electrons.

The group has a long standing and active collaboration with Prof. P. G. REINHARD from Erlangen University (Germany) with whom, in particular, the whole set of computational platforms has been developed. Other important collaborations are running with theorists from Rostock (Germany), Dubna (Russia) and Valencia (Spain) as well as with experimentalists from Rostock (Germany) and Lyon (joined ANR project).

8.1 Dynamical self-interaction correction

J. Messud (PhD student), P. M. Dinh, É. Suraud

A correct treatment of ionization processes in Time Dependent Density Functional Theory (TDDFT) is still raising sizable difficulties, especially from the formal side. Indeed, standard DFT approaches rely on the Local Density Approximation (LDA) which is plagued by the well known self interaction problem (self interaction of an electron with itself through the total density from which the electron potential is built). There is thus a crucial need to overcome this problem in order to recover proper ionization properties, especially when considering explicit time dependent processes. A key point thus concerns a clean formulation of the Self Interaction Correction (SIC) method on top of the standard Local Density Approximation (LDA) of Time Dependent Density Functional Theory, (TDDFT, see [1] and references therein, for recent reviews on the topic). While the problem is well studied in the static domain, time dependent versions of the theory have only been developed in the framework of further approximations, especially within the Optimized Effective Potential (OEP) strategy. The first task was thus a clean reformulation of Time Dependent SIC (TDSIC) in which an explicit account of orthonormalization was included in the theory [ACL-272, ACL-275]. The TDSIC equations are rather involved and in order to be able to have a proper time propagation we have been led to introduce two sets of single electron orbitals. Such a strategy amounts to exploit the usually left over degree of freedom of unitary transform amongst electronic orbitals in time propagation, an idea which had never been put forward. The result led, to the best of our knowledge, to the first complete calculation of full TDSIC, which is thus providing a benchmark for the development of further approximations [ACL-272, ACL-275].



Example of application of full TDSIC to the irradiation of a model dimer molecule. Time dependent ionization is shown in the lower right panel where exchange only TDSIC is compared to the time dependent Hartree-Fock calculation which is then the benchmark calculation. LDA fails badly as expected. The left panels illustrate the double set strategy again on a model dimer and in terms of densities. Orthonormality is ensured through the so called symmetrizing set which turns out to provide rather Localized wavefunctions while "physical" orbitals used for time propagation diagonalize the SIC Hamiltonian (adapted from [ACL-272, ACL-275]).

Insert 8.1 : *Illustration of ionization in TDSIC and double set strategy.*

This double set strategy also turned out to be extremely useful for the stationary limit as it provided the basic idea for developing efficient and simple approximations of the OEP methods built on top of SIC. This allowed to propose a new, efficient SIC-OEP scheme which turns out to provide remarkably accurate results from a rather simple treatment [ACL-273]. The double set scheme furthermore shed some light on the long standing difficulties associated to the more or less localized nature of electronic orbitals: indeed one set provides rather localized orbitals (which allow to properly ensure orthonormalization) while the second one leads to more delocalized orbitals typical of bonding orbitals. The full TDSIC and its simplified SIC-OEP version have been applied with success to various physical systems including metal clusters, organic molecules and quantum dots. An illustration of TDSIC and the double set strategy is given in Insert 8.1.

1. M. A. Marques *et al.*, *Time Dependent Density Functional Theory*, Lect. Notes in Physics **706**, Springer, Berlin (2006); S. Kuemmel and L. Kronik, Rev. Mod. Phys. **80**, 3 (2008).

The next step to come is to develop a simplified and robust version of the theory to be used in large scale calculations. These formal investigations have been quite fruitful in terms of publications with half a dozen papers published or submitted and a few more to come.

8.2 Hierarchical modeling

G. Bousquet (PhD student), S. Vidal (PhD student), É. Suraud, P. M. Dinh

The physical motivation of our investigations was the understanding of the dynamics of clusters and molecules in contact with an environment, a situation which occurs in numerous physical contexts, ranging from surface physics to water-embedded biological systems. While environments may help controlling experimental conditions, such as for example on surfaces, they also make the description of the system much more involved, precisely due to the presence of the environment which may play a non negligible role in the response of the system to an external perturbation such as an irradiation. A proper account of the dynamical degrees of freedom of the environment is nevertheless not taken into account in standard approaches. We have thus been led to develop a more sophisticated model accounting for such degrees of freedom. This aspect becomes absolutely crucial when charges are involved, either because of dealing with charged species or as a result of an irradiation process. The many results obtained demonstrated *a posteriori* the key importance of this aspect, whatever the dynamical regime under consideration.

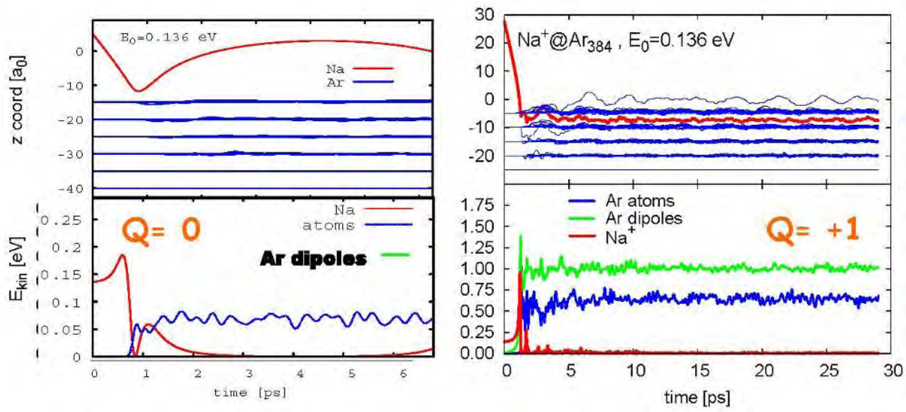


Illustration of the importance of charge effects and of the explicit account of dynamical polarizabilities of atoms environment in the case of the deposit of a Na atom or Na+ ion on an Ar surface (same deposition kinetic energy). Upper panels show cluster and substrate positions in time (along deposition direction) and lower panels kinetic energies thereof and energy stored in substrate dipoles. The positive charge leads to inclusion of the ion inside the substrate and to substantial excitation of Ar dipoles, the total associated (internal) excitation energy being about 40% larger than the total Ar kinetic energy in this case. Similar effects have been observed in the case of violent irradiations of embedded metal clusters in which high charge states have been attained. (adapted from [ACL-270]).

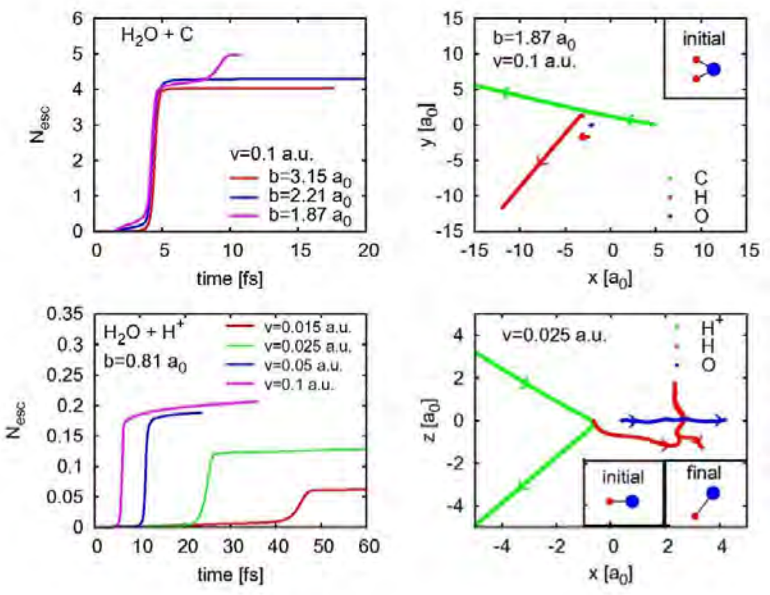
Insert 8.2 : *Illustration of dynamical QM/MM in charged system deposits.*

We originally developed hierarchical modeling for the case of metal clusters in contact with an insulating material, typically a rare gas or a MgO substrate [ACL-261, ACL-262, ACL-263, ACL-264, ACL-265, ACL-266, ACL-267, ACL-268, ACL-269, ACL-270]. While the cluster is treated in full TDLDA (for electrons) coupled to classical Molecular Dynamics (MD) for cluster ions, the environment is described at a lower level of sophistication in the spirit of QM/MM (Quantum Mechanics/Molecular Mechanics) approaches of quantum chemistry (see for example [2] and references therein for a review). The idea is to treat atoms of the environment as classical particles but, at variance with earlier approaches, we complement the description by attributing dynamical dipoles to each atom of the environment, which turns out to be a key issue for the

2. J. Gao and D. Truhlar, Ann. Rev. Phys. Chem. **53**, 467 (2002).

description of irradiation processes (see [SRP-17] and references therein, including our own papers, for a summary of these investigations). An illustration of our dynamical QM/MM calculations is given in Insert 8.2 exhibiting the key role of internal degrees of freedom of the surface and our capability to treat charged clusters.

While we continued to investigate our model in the case of cluster/substrate combinations we also started to consider its extension to the case of organic molecules in contact with polar molecules. The description of water is a well explored field and we have identified a few approaches compatible with our strategy. Still, discussions with several colleagues working on the irradiation of small organic/bio molecules led us to postpone the implementation of this extension of our hierarchical modeling to the benefit of more detailed studies of very small systems, which were more urgently interesting experimental colleagues. This indeed turns out to provide valuable prototype cases for irradiation studies even when very small. In such cases the system is fully treated at TDLDA-MD level. Such calculations, in addition to their intrinsic physical interest, will furthermore serve as benchmarks for hierarchical approaches to come. We have in particular focused on the simplest water molecules clusters. The first results are currently being prepared for publication on this topic.



Examples of fully non adiabatic TDLDA-MD calculations of the irradiation of water molecules either by a proton or by a neutral Carbon atom at various impact velocities.

Left panels show the net ionization (+4 units for the 4 carbon electrons in the case of Carbon projectile) and for various kinematical conditions. Right panels show examples of ionic motion in some specific cases. Trajectories are shown in the reaction plane.

Insert 8.3 : *Illustration of non adiabatic TDLDA-MD in irradiated organic molecules.*

8.3 Non adiabatic TDLDA-MD

Z. P. Wang (PhD student), P. M. Dinh,
U. F. Ndongmouo (postdoc), É. Suraud

We have developed non adiabatic TDLDA-MD calculations (electronic Time Dependent Local Density Approximation coupled to ionic Molecular Dynamics) since more than a decade in the simple case of metal clusters and applied our formalism to a bunch of dynamical scenarios with a particular emphasis on laser irradiations but also with some collisional calculations (see [3] or [4] and references therein for reviews). The extension of the method to organic molecules is in principle straightforward but requires some technical fine-tuning. Surprisingly enough such fully non adiabatic calculations allowing to cover any dynamical regimes had not been realized before. Only simplified situations in which either ions are kept fixed (very energetic collisions) or electrons "follow" ions at Born-Oppenheimer level

3. F. Calvayrac *et al.*, Phys. Rep. **337**, 493 (2000).
4. P. G. Reinhard and É. Suraud, *Introduction to Cluster Dynamics*, Wiley, New-York (2003).

were available for such systems.

The major effort to be done in our approach concerned the validation of pseudopotentials especially designed for our grid representation of electronic wavefunctions. Pseudopotentials imply a minimum length scale associated to the atomic core size which, in turn, determines a minimum grid spacing. As long as only one material is present, any well behaved (smooth enough) pseudopotential is applicable. In the case of mixed systems (as typical organic molecules) one has to retune pseudopotentials to a common (and sufficiently large) minimum length. Such a fine-tuning was successfully done for the standard elements, C, N, O, and H, to be used in our target molecules. Of course the retuning implies some compromises. But these are beneficial to attain representations which allow robust calculations over long times and in the non-linear domain.

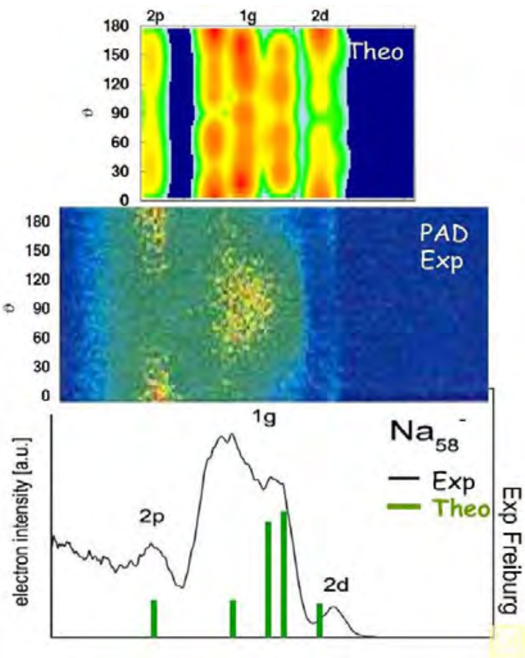
The new set of pseudopotentials was then used to study the dynamics of small organic systems especially under laser irradiation and collisions with charged or neutral projectiles. The full non adiabatic coupling between electrons and ions is here crucial as it allows to cover any dynamical regime in the field, namely charged or neutral projectiles at low or high velocity, a possibility which, to the best of our knowledge, is a "premiere" in the field[5]. The results of this first set of calculations are currently being prepared for publications. Three papers have already been submitted and some more are to come [SRP-14, SRP-15, SRP-16]. A typical example of our calculations is presented in Insert 8.3.

These calculations also provide benchmark results for the hierarchical modeling. The SIC was in these calculations still handled in a simplified way (Average Density SIC, ADSIC[6]), which allows to properly treat electronic dynamics but fails at describing molecular dissociation quantitatively. More sophisticated TDSIC will be included in a forthcoming step and will then allow to upgrade the treatment from qualitative to quantitative description of dissociation.

8.4 Detailed analysis of the dynamics of free irradiated clusters

S. Vidal (PhD student), P. M. Dinh, É. Suraud

The new developments in laser technology (attosecond pulses, Free Electron Laser frequencies) as well as in the detailed analysis of the electronic response of irradiated clusters (angular resolved photoelectron spectra, time resolved photoelectron spectra) have motivated us to pursue our studies on free irradiated clusters [ACL-248, ACL-251, ACL-252, ACL-254, ACL-258].



Example of analysis of the Photoelectron Angular Distribution in moderate size sodium clusters. Both single electron energies (bottom panel) and angular distributions (two upper panels) are indicated with comparison between experiments and calculations as indicated. Good agreement is found between experiments and theory.

Insert 8.4 : *Illustration of angular distributions of photoelectrons.*

We are currently attacking the opening domain of FEL frequencies in which ionization mechanisms strongly differ from the ones in the

5. M. P. Gaigeot *et al.*, J. Phys. B **40**, 1 (2007); J. Kohanoff and E. Artacho, AIP Conf. Proc. **1080**, 78 (2008).
6. C. Legrand *et al.*, J. Phys. B **35**, 1115 (2002).

optical domain. We have thus started to compute the response of clusters and molecules to very high laser frequencies, focusing on the detailed analysis of the properties of emitted electrons. We are in particular considering the angular distributions of photoelectrons, for which a few highly detailed experimental results start to be available in the optical domain. An example of such an analysis, in the optical domain is presented in Insert 8.4 for illustration. Such angular distributions are also interesting to explore in the case of irradiated deposited species. Such calculations are underway in the case of simple metal clusters deposited on either an Ar or a MgO surface.

9

Scientific production

This chapter lists the full scientific production of the LPT during the past four years. The diversity of subjects treated at LPT translates into an equally large variety of scientific journals and conferences where LPT scientists publish or present their work. The 18 active scientists at LPT are all "publiant/publishing" according to the criteria of the *AERES*.

Following the AERES **recommendation, the scientific production of LPT is listed according to the following categories:**

❍ **Articles published in refereed journals** (ACL; page 68): **278**
FFC: 66 – Quantware: 59 – PhyStat: 121 – Agrégats: 32

❍ **Articles without reference (preprints)** (SRP; page 80): **21**
FFC: 4 – Quantware: 5 – PhyStat: 4 – Agrégats: 8

❍ **Invited talks in international and national conferences** (INV; page 81): **115**
FFC: 26 – Quantware: 31 – PhyStat: 32 – Agrégats: 26

❍ **Oral communications with a conference proceeding (international conferences)** (ACTI; page 87): **27**
FFC: 15 – Quantware: 1 – PhyStat: 9 – Agrégats: 2

❍ **Oral communications not leading to a conference proceeding** (COM; page 90): **32**
FFC: 8 – Quantware: 3 – PhyStat: 11 – Agrégats: 10

❍ **Posters in conferences** (AFF; page 91): **34**
FFC: 11 – Quantware: 11 – PhyStat: 9 – Agrégats: 3

❍ **Books or book chapters** (OS; page 93): **11**
FFC: 5 – Quantware: 3 – PhyStat: 1 – Agrégats: 2

❍ **Vulgarization publications** (OV; page 94): **11**
FFC: 1 – Quantware: 2 – PhyStat: 7 – Agrégats: 1

❍ **Books as Editor** (DO; page 95): **4**
FFC: 1 – Quantware: 1 – PhyStat: 1 – Agrégats: 1

❍ **Commercial and Open Source softwares** (COD; page 95): **3**
FFC: 1 – Quantware: 1 – PhyStat: 1 – Agrégats: 0

❍ **Habilitation thesis to supervise researches** (HDR; page 96): **2**
FFC: 1 – Quantware: 0 – PhyStat: 1 – Agrégats: 0

❍ **PhD thesis completed or in progess** (TH; page 96): **23**
FFC: 7 – Quantware: 3 – PhyStat: 8 – Agrégats: 5

Some statistical data on LPT refereed publications:

❍ The **average number of authors** on a LPT ACL/SRP publication is just below 3: 1.3 permanent researcher at LPT, 0.25 LPT postdoc or PhD student (excluding LPT visitors), 1.4 non LPT researcher (including LPT visitors) [1]. The names of LPT permanent researchers are underlined and those of LPT postdocs/PhD students are dash-underlined in the publication list below.

❍ Since 2005, more than **250 authors** have participated to LPT publications (including LPT permanent staff, postdocs, and PhD students working at the LPT). They work in **130 different institutions outside Toulouse** [2] and **6 laboratories on the UPS campus** [3].

❍ Percentage of LPT publications since 2005 having **at least one author from a foreign institution**[2] **(21 countries)**: Germany 20.5 %, USA 8 %, Switzerland 7.5 %, UK 7 %, Italy & Russia 4.5 %, Canada & Japan & Poland 2 %...

❍ The following publication list includes, among others, 35 articles published in *Physical Review Letters* (+8 submitted), and 1 in *Nature Physics*.

❍ The roughly **1100 publications** of the 18 active permanent researchers presently working at the LPT have gathered more than **19000** citations [4] and at least 90/45 articles have received more than 50/80 citations (mean – and median – age of the 18 LPT active researchers as on 1st January 2010: 42).

The references in light green are linked to their ArXiv preprint in *pdf* or to the corresponding journal web site (subscription needed in this case), and can thus be directly consulted from the *pdf* version of the present document. Most LPT publications since 2006 are also referenced on CNRS HAL repository.

9.1 Articles published in refereed journals

Fermions Fortement Corrélés

[ACL-1] N. Laflorencie, D. Poilblanc, and M. Sigrist, *Critical properties of doped spin-Peierls chains*, *Physical Review B* **71**, 212403 (2005).

[ACL-2] D. Poilblanc and D. J. Scalapino, *Gap function $\Phi(k,\omega)$ for a two-leg t–J ladder and the pairing interaction*, *Physical Review B* **71**, 174403 (2005).

[ACL-3] D. Poilblanc, *Stability of inhomogeneous superstructures from renormalized mean-field theory of the t–J model*, *Physical Review B* **72**, 060508(R) (2005).

[ACL-4] D. C. Cabra, M. D. Grynberg, P. C. W. Holdsworth, A. Honecker, P. Pujol, J. Richter, D. Schmalfuss, and J. Schulenburg, *Quantum kagome antiferromagnet in a magnetic field: Low-lying non-magnetic excitations versus valence-bond crystal order*, *Physical Review B* **71**, 144420 (2005).

[ACL-5] C. Castelnovo, C. Chamon, C. Mudry, and P. Pujol, *Quantum three-coloring dimer model and the disruptive effect of quantum glassiness on its line of critical points*, *Physical Review B* **72**, 104405 (2005).

1. FFC: 1.3/0.33/2.1; Quantware: 1.3/0.33/0.8; PhyStat: 1.2/0.11/1.1; Agrégats: 1.6/0.37/2.4. Publications of the LPT groups heavily involved in numerical simulations logically involve more authors.

2. Analyzing non exhaustive search results on ISI Web of Sciences.

3. Institut de Pharmacologie et Biologie Structurale (2 independent collaborations), Institut de Mathématiques de Toulouse, Laboratoire de Microbiologie et Génétique Moléculaires, Laboratoire de Chimie et Physique Quantiques, Laboratoire National des Champs Magnétiques Intenses, Observatoire Midi-Pyrénées.

4. Rough estimates obtained from ISI Web of Sciences based on LPT scientists individual records, without taking into accounts overlaps (1.3 permanent LPT researcher/article in 2005-2009). LPT publications are systematically signed under the affiliation Laboratoire de Physique Théorique since 2004 only.

[ACL-6] C. Castelnovo, C. Chamon, C. Mudry, and P. Pujol, *From quantum mechanics to classical statistical physics: generalized Rokhsar-Kivelson Hamiltonians and the "Stochastic Matrix Form" decomposition*, Annals of Physics **318/2**, 316 (2005).

[ACL-7] D. Carpentier, P. Pujol, and K.-U. Giering, *Random quantum Ising chains with competing interactions*, Physical Review E **72**, 066101 (2005).

[ACL-8] F. Alet, S. Wessel, and M. Troyer, *Generalized directed loop method for Quantum Monte Carlo simulations*, Physical Review E **71**, 036706 (2005).

[ACL-9] P. Sengupta, L. P. Pryadko, F. Alet, M. Troyer, and G. Schmid, *Supersolids versus phase separation in two-dimensional lattice bosons*, Physical Review Letters **94**, 207202 (2005).

[ACL-10] C. Yasuda, S. Todo, K. Hukushima, F. Alet, M. Keller, M. Troyer, and H. Takayama, *Néel temperature of quasi-low-dimensional Heisenberg antiferromagnets*, Physical Review Letters **94**, 217201 (2005).

[ACL-11] F. Alet, J. L. Jacobsen, G. Misguich, V. Pasquier, F. Mila, and M. Troyer, *Interacting classical dimers on the square lattice*, Physical Review Letters **95**, 235702 (2005).

[ACL-12] G. Roux, S. R. White, S. Capponi, A. Läuchli, and D. Poilblanc, *Doped two-leg ladder with ring exchange*, Physical Review B **72**, 014523 (2006).

[ACL-13] F. Alet, A. M. Walczak, and M. P. A. Fisher, *Exotic quantum phases and phase transitions in correlated matter*, Physica A **369**, 122 (2006).

[ACL-14] M. Al Hajj, F. Alet, S. Capponi, M.-B. Lepetit, J.-P. Malrieu, and S. Todo, *Parity law of the singlet-triplet gap in graphitic ribbons*, European Physical Journal B **51**, 517 (2006).

[ACL-15] F. Alet, G. Misguich, V. Pasquier, R. Moessner, and J. L. Jacobsen, *Unconventional continuous phase transition in a three dimensional dimer model*, Physical Review Letters **97**, 030403 (2006).

[ACL-16] F. Alet, Y. Ikhlef, J. L. Jacobsen, G. Misguich, and V. Pasquier, *Classical dimers with aligning interactions on the square lattice*, Physical Review E **74**, 041124 (2006).

[ACL-17] D. Poilblanc, A. Laeuchli, M. Mambrini, and F. Mila, *Spinon deconfinement around a vacancy in frustrated quantum antiferromagnets*, Physical Review B **73**, 100403(R) (2006).

[ACL-18] T. Vekua, D. C. Cabra, A. Dobry, C. Gazza, and D. Poilblanc, *Magnetization plateaux induced by a coupling to the lattice*, Physical Review Letters **96**, 117205 (2006).

[ACL-19] G. Roux, S. R. White, S. Capponi, and D. Poilblanc, *Zeeman effect in superconducting two-leg ladders: irrational magnetization plateaus and exceeding the Pauli limit*, Physical Review Letters **97**, 087207 (2006).

[ACL-20] C. Weber, D. Poilblanc, S. Capponi, F. Mila, and C. Jaudet, *Bond-order modulated staggered flux phase for the t–J model on the square lattice*, Physical Review B **74**, 104506 (2006).

[ACL-21] D. Poilblanc, F. Alet, F. Becca, A. Ralko, F. Trousselet, and F. Mila, *Doping quantum dimer models*, Physical Review B **74**, 014437 (2006).

[ACL-22] M. Mambrini, A. Läuchli, D. Poilblanc, and F. Mila, *Plaquette valence bond ordered phase in the J_1-J_2-J_3 Heisenberg $S = 1/2$ antiferromagnet on the square lattice*, Physical Review B **74**, 014437 (2006).

[ACL-23] M. Indergand, A. Läuchli, S. Capponi, and M. Sigrist, *Modeling bond-order wave instabilities in doped frustrated antiferromagnets: Valence bond solids at fractional filling*, Physical Review B **74**, 064429 (2006).

[ACL-24] C. Castelnovo, C. Chamon, C. Mudry, and P. Pujol, *High-temperature criticality in strongly constrained quantum systems*, Physical Review B **73**, 144411 (2006).

[ACL-25] A. H. Castro Neto, P. Pujol, and E. Fradkin, *Ice: a strongly correlated proton system*, Physical Review B **74**, 024302 (2006).

[ACL-26] M. Picco, A. Honecker, and P. Pujol, *Strong disorder fixed points in the two-dimensional random-bond Ising model*, Journal of Statistical Mechanics, 09006 (2006).

[ACL-27] F. Alet, S. Capponi, N. Laflorencie, and M. Mambrini, *Valence bond entanglement entropy*, Physical Review Letters **99**, 117204 (2007).

[ACL-28] F. Trousselet, P. Pujol, F. Alet, and D. Poilblanc, *Criticality of a classical dimer model on the triangular lattice*, Physical Review E **76**, 041125 (2007).

[ACL-29] M. Raczkowski, D. Poilblanc, R. Frésard, and A. M. Oleś, *Spin-rotationally symmetric domain flux phases in underdoped cuprates*, Physical Review B **75**, 094505 (2007).

[ACL-30] M. Indergand, C. Honerkamp, A. Läuchli, D. Poilblanc, and M. Sigrist, *Plaquette valence bond order in the 1/4-filled extended Hubbard model on the checkerboard lattice*, Physical Review B **75**, 045105 (2007).

[ACL-31] G. Roux, E. Orignac, P. Pujol, and D. Poilblanc, *Bosonization and DMRG study of FFLO phase and irrational magnetization plateaus in coupled chains*, Physical Review B **75**, 245119 (2007).

[ACL-32] S. Capponi and D. Poilblanc, *Thermodynamic properties of the coupled dimer system* $Cu_2(C_5H_{12}N_2)_2Cl_4$, Physical Review B **75**, 092406 (2007).

[ACL-33] D. Poilblanc, K. Penc, and N. Shannon, *Doped singlet-pair crystal in the Hubbard model on the checkerboard lattice*, Physical Review B **75**, 220503(R) (2007).

[ACL-34] A. Ralko, F. Mila, and D. Poilblanc, *Phase separation and flux quantization in the doped quantum dimer model on the square and triangular lattices*, Physical Review Letters **99**, 127702 (2007).

[ACL-35] D. Poilblanc, *Exotic Mott phases of the extended t–J model on the checkerboard lattice at commensurate densities*, Physical Review B **76**, 115104 (2007).

[ACL-36] E. Orignac, R. Citro, S. Capponi, and D. Poilblanc, *Breathers and Raman scattering in a two-leg ladder with staggered Dzialoshinskii-Moriya interaction*, Physical Review B **76**, 144422 (2007).

[ACL-37] G. Roux, E. Orignac, S. R. White, and D. Poilblanc, *Diamagnetism of two-leg ladders and probing the nature of commensurate phases*, Physical Review B **76**, 195105 (2007).

[ACL-38] M. Raczkowski, M. Capello, D. Poilblanc, R. Frésard, and A. Oleś, *Unidirectional d-wave superconducting domains in the two-dimensional t–J model*, Physical Review B **76**, 140505(R) (2007).

[ACL-39] S. Capponi and F. F. Assaad, *Spin-nematic phases in models of correlated electron systems: a numerical study*, Physical Review B **75**, 045115 (2007).

[ACL-40] S. Capponi, G. Roux, P. Azaria, E. Boulat, and P. Lecheminant, *Confinement versus deconfinement of Cooper pairs in one-dimensional spin-3/2 fermionic cold atoms*, Physical Review B **75**, 100503(R) (2007).

[ACL-41] A. Abendschein and S. Capponi, *Contractor-Renormalization approach to frustrated magnets in magnetic field*, Physical Review B **76**, 064413 (2007).

[ACL-42] C. Castelnovo, C. Chamon, C. Mudry, and P. Pujol, *Zero-temperature Kosterlitz-Thouless transition in a two-dimensional quantum system*, Annals of Physics **322/4**, 903 (2007).

[ACL-43] C. Brünger, F. F. Assaad, S. Capponi, F. Alet, D. N. Aristov, and M. N. Kiselev, *Spin gap and string order parameter in the ferromagnetic Spiral Staircase Heisenberg Ladder: a quantum Monte Carlo study*, Physical Review Letters **100**, 017202 (2008).

[ACL-44] K. S. D. Beach, M. Mambrini, and F. Alet, *Comment on "Quantum Monte Carlo scheme for frustrated Heisenberg antiferromagnets"*, Physical Review B **77**, 146401 (2008).

[ACL-45] G. Misguich, V. Pasquier, and F. Alet, *Correlations and order parameter at a Coulomb-crystal phase transition*, Physical Review B **78**, 100402(R) (2008).

[ACL-46] D. Charrier, F. Alet, and P. Pujol, *Gauge theory picture of an ordering transition in a dimer model*, Physical Review Letters **101**, 167205 (2008).

[ACL-47] F. Alet, D. Braun, and G. Misguich, *Comment on "Regional versus global entanglement in resonating-valence-bond states"*, Physical Review Letters **101**, 248901 (2008).

[ACL-48] A. Ralko, D. Poilblanc, and R. Moessner, *Generic mixed columnar-plaquette phases in Rokhsar-Kivelson models*, Physical Review Letters **100**, 037201 (2008).

[ACL-49] D. Poilblanc, *Superconductivity: beyond convention*, Nature Physics **4**, 16 (2008).

[ACL-50] D. Poilblanc, *Properties of holons in the Quantum Dimer Model*, Physical Review Letters **100**, 157206 (2008).

[ACL-51] T. A. Maier, D. Poilblanc, D. J. Scalapino, *Pairing glue in the Hubbard and t–J models*, Physical Review Letters **100**, 237001 (2008).

[ACL-52] M. Capello, M. Raczkowski, and D. Poilblanc, *Stability of RVB hole stripes in high-temperature superconductors*, Physical Review B **77**, 224502 (2008).

[ACL-53] A. Ralko, F. Becca, and D. Poilblanc, *Magnetic field-induced transition in a quantum magnet described by the Quantum Dimer Model*, Physical Review Letters **101**, 117204 (2008).

[ACL-54] F. Trousselet, D. Poilblanc, and R. Moessner, *Mixed columnar-plaquette crystal of correlated fermions on the 2D pyrochlore lattice at fractional filling*, Physical Review B **78**, 195101 (2008).

[ACL-55] Ch. Rüegg, K. Kiefer, B. Thielemann, D. F. McMorrow, V. Zapf, B. Normand, M. Zvonarev, P. Bouillot, C. Kollath, T. Giamarchi, S. Capponi, D. Poilblanc, D. Biner, K. W. Krämer, *Thermodynamics of the spin Luttinger-liquid in a model ladder material*, Physical Review Letters **101**, 247202 (2008).

[ACL-56] A. Läuchli, S. Capponi, and F. F. Assaad, *Dynamical dimer correlations at bipartite and non-bipartite Rokhsar-Kivelson points*, Journal of Statistical Mechanics, P010110 (2008).

[ACL-57] S. Capponi, G. Roux, P. Lecheminant, P. Azaria, E. Boulat, and S. R. White, *Molecular superfluid phase in one-dimensional multicomponent fermionic cold atoms*, Physical Review A **77**, 013624 (2008).

[ACL-58] A. Abendschein and S. Capponi, *Effective theory of magnetization plateaux in the Shastry-Sutherland lattice*, Physical Review Letters **101**, 227201 (2008).

[ACL-59] M. Mambrini, *Hard-core dimer aspects of the SU(2) singlet wave function*, Physical Review B **77**, 134430 (2008).

[ACL-60] J. L. Jacobsen and F. Alet, *Semiflexible fully packed loop model and interacting rhombus tilings*, Physical Review Letters **102**, 145702(2009).

[ACL-61] M. Capello and D. Poilblanc, *Many-body calculation of the spatial extent of the wave-function of a non-magnetic impurity in a d-wave high-temperature superconductor using the t–J model*, Physical Review B **79**, 224507 (2009).

[ACL-62] G. Roux, S. Capponi, P. Lecheminant, and P. Azaria, *Spin 3/2 fermions with attractive interactions in a one-dimensional optical lattice: phase diagrams, entanglement entropy, and effect of the trap*, European Physical Journal B **68**, 293 (2009).

[ACL-63] M. Moliner, D. C. Cabra, A. Honecker, P. Pujol, and F. Stauffer, *Magnetization process in the classical Heisenberg model on the classical Shastry-Sutherland lattice*, Physical Review B **79**, 144401 (2009).

[ACL-64] M. Raczkowski and D. Poilblanc, *Supersolid Phases of a Doped Valence-Bond Quantum Antiferromagnet: Evidence for a Coexisting Superconducting Order Parameter*, Physical Review Letters **103**, 027001 (2009).

[ACL-65] G. Chen, J. Gukelberger, S. Trebst, F. Alet, and L. Balents, *Coulomb gas transitions in three-dimensional classical dimer models*, Physical Review B **80**, 045112 (2009).

[ACL-66] S. Capponi, D. Poilblanc, and F. Mila, *Theory of the Raman spectra of the Shastry-Sutherland antiferromagnet $SrCu_2(BO_3)_2$ doped with nonmagnetic impurities*, Physical Review B, in press (2009).

Information et Chaos Quantiques

[ACL-67] G. G. Carlo, G. Benenti, G. Casati, and D. L. Shepelyansky, *Quantum ratchets in dissipative chaotic systems*, Physical Review Letters **94**, 164101 (2005).

[ACL-68] O. Kern, G. Alber, and D. L. Shepelyansky, *Quantum error correction of coherent errors by randomization*, European Physical Journal D. **32**, 153 (2005).

[ACL-69] M. Terraneo, B. Georgeot, and D. L. Shepelyansky, *Quantum computation and analysis of Wigner and Husimi functions: toward a quantum image treatment*, Physical Review E **71**, 066215 (2005).

[ACL-70] J. W. Lee and D. L. Shepelyansky, *Quantum chaos algorithms and dissipative decoherence with quantum trajectories*, Physical Review E **71**, 056202 (2005).

[ACL-71] J. W. Lee, D. V. Averin, G. Benenti, and D. L. Shepelyansky, *Model of a deterministic detector and dynamical decoherence*, Physical Review A **72**, 012310 (2005).

[ACL-72] G. G. Carlo, G. Benenti, and D. L. Shepelyansky, *Dissipative quantum chaos: transition from wave packet collapse to explosion*, Physical Review Letters **95**, 164101 (2005).

[ACL-73] O. Giraud, B. Georgeot, and D. L. Shepelyansky, *Quantum computing of delocalization in small-world networks*, Physical Review E **72**, 036203 (2005).

[ACL-74] O. Giraud and B. Georgeot, *Intermediate quantum maps for quantum computation*, Physical Review A **72**, 042312 (2005).

[ACL-75] D. Braun, *Entanglement from thermal blackbody radiation*, Physical Review A **72**, 062334 (2005).

[ACL-76] O. Giraud, *Periodic orbits and two-point correlation form factor for barrier billiards*, Communications in Mathematical Physics **260**, 183 (2005).

[ACL-77] O. Giraud, *Finite geometries and diffractive orbits in isospectral billiards*, Journal of Physics A **38**, L477 (2005).

[ACL-78] D. Braun and B. Georgeot, *Quantitative measure of interference*, Physical Review A **73**, 022314 (2006).

[ACL-79] O. V. Zhirov and D. L. Shepelyansky, *Quantum synchronization*, European Physical Journal D **38**, 375 (2006).

[ACL-80] O. V. Zhirov and D. L. Shepelyansky, *Dissipative decoherence in the Grover algorithm*, European Physical Journal D **38**, 405 (2006).

[ACL-81] J. Lages and D. L. Shepelyansky, *Suppression of quantum chaos in a quantum computer hardware*, European Physical Journal D **74**, 026208 (2006).

[ACL-82] D. Braun, *Decoherence in a system of many two-level atoms*, Physical Review Letters **96**, 230502 (2006).

[ACL-83] D. Braun, *Indirect decoherence in optical lattices and cold gases*, European Physical Journal D **42**, 103 (2006).

[ACL-84] D. Braun, *Invariant integration over the orthogonal group*, Journal of Physics A **39**, 14581 (2006).

[ACL-85] I. García-Mata, O. V. Zhirov, and D. L. Shepelyansky, *Frenkel-Kontorova model with cold trapped ions*, European Physical Journal D **41**, 325 (2007).

[ACL-86] A. D. Chepelianskii and D. L. Shepelyansky, *Magnetization of ballistic quantum dots induced by a linear-polarized microwave field*, European Physical Journal B **55**, 261 (2007).

[ACL-87] L. Arnaud and D. Braun, *Distribution of interference in random quantum algorithms*, Physical Review A **75**, 062314 (2007).

[ACL-88] A. D. Chepelianskii, M. V. Entin, L. I. Magarill, and D. L. Shepelyansky, *Photogalvanic current in artificial asymmetric nanostructures*, European Physical Journal B **56**, 323 (2007).

[ACL-89] I. García-Mata, K. M. Frahm, and D. L. Shepelyansky, *Effects of imperfections for Shor's factorization algorithm*, Physical Review A **75**, 052311 (2007).

[ACL-90] I. García-Mata, A. R. R. Carvalho, F. Mintert, and A. Buchleitner, *Entanglement-screening by nonlinear resonances*, Physical Review Letters **98**, 120504 (2007).

[ACL-91] B. Georgeot, *Complexity of chaos and quantum computation*, Mathematical Structures in Computer Science **17**, 1221 (2007).

[ACL-92] O. Giraud, J. Martin, and B. Georgeot, *Entanglement of localized states*, Physical Review A **76**, 042333 (2007).

[ACL-93] A. O. Lyakhov, D. Braun, and C. Bruder, *Role of interference in quantum state transfer through spin chains*, Physical Review A **76**, 022321 (2007).

[ACL-94] O. Giraud, *Distribution of bipartite entanglement for random pure states*, Journal of Physics A **40**, 2793 (2007).

[ACL-95] O. Giraud, *Purity distribution for bipartite random pure states*, Journal of Physics A **40**, F1053 (2007).

[ACL-96] A. D. Chepelianskii, A. S. Pikovsky, and D. L. Shepelyansky, *Synchronization, zero-resistance states and rotating Wigner crystal*, European Physical Journal B **60**, 225 (2007).

[ACL-97] J. Martin and D. Braun, *Coherent control of atomic tunneling*, Journal of Physics B **41**, 115502 (2008).

[ACL-98] J. Martin and D. Braun, *Spontaneous emission from a two-level atom tunneling in a double-well potential*, Physical Review A **77**, 032102 (2008).

[ACL-99] A. S. Pikovsky and D. L. Shepelyansky, *Destruction of Anderson localization by a weak nonlinearity*, Physical Review Letters **100**, 094101 (2008).

[ACL-100] D. L. Shepelyansky, *Fractal Weyl law for quantum fractal eigenstates*, Physical Review E **77**, 015202(R) (2008).

[ACL-101] O. V. Zhirov and D. L. Shepelyansky, *Synchronization and bistability of qubit coupled to a driven dissipative oscillator*, Physical Review Letters **100**, 014101 (2008).

[ACL-102] J. Martin, B. Georgeot, and D. L. Shepelyansky, *Loschmidt cooling by time reversal of atomic matter waves*, Physical Review Letters **100**, 044106 (2008).

[ACL-103] D. Braun and B. Georgeot, *Interference versus success probability in quantum algorithms with imperfections*, Physical Review A **77**, 022318 (2008).

[ACL-104] I. García-Mata and D. L. Shepelyansky, *Quantum phase estimation algorithm in presence of static imperfections*, European Physical Journal D **47**, 151 (2008).

[ACL-105] J. Martin, O. Giraud, and B. Georgeot, *Multifractality and intermediate statistics in quantum maps*, Physical Review E **77**, 035201(R) (2008).

[ACL-106] M. Znidaric, O. Giraud, and B. Georgeot, *Optimal number of controlled-NOT gates to generate a three-qubit state*, Physical Review A **77**, 032320 (2008).

[ACL-107] B. Georgeot and O. Giraud, *Quantum computing of semiclassical formulas*, Physical Review E **77**, 046218 (2008).

[ACL-108] J. Martin, B. Georgeot, and D. L. Shepelyansky, *Time reversal of Bose-Einstein condensates*, Physical Review Letters **101**, 074102 (2008).

[ACL-109] A. D. Chepelianskii, M. V. Entin, L. I. Magarill, and D. L. Shepelyansky, *Ratchet transport of interacting particles*, Physical Review E **78**, 041127 (2008).

[ACL-110] F. Lignières and B. Georgeot, *Wave chaos in rapidly rotating stars*, Physical Review E **78**, 016215 (2008).

[ACL-111] J. Martin and T. Bastin, *Detuning effects in the vertical cold-atom micromaser*, European Physical Journal D **48**, 301 (2008).

[ACL-112] D. Braun and M.-S. Choi, *Hardy's test versus the CHSH test of quantum non-locality: fundamental and practical aspects*, Physical Review A **78**, 032114 (2008).

[ACL-113] O. Giraud, P. Braun, and D. Braun, *Classicality of spin states*, Physical Review A **78**, 042112 (2008).

[ACL-114] L. Arnaud and D. Braun, *Efficiency of producing random unitary matrices with quantum circuits*, Physical Review A **78**, 062329 (2008).

[ACL-115] B. Roubert and D. Braun, *Role of interference in quantum cloning*, Physical Review A **78**, 042311 (2008).

[ACL-116] F. Alet, D. Braun, and G. Misguich, *Comment on "Regional versus global entanglement in Resonating-Valence-Bond states*, Physical Review Letters **101**, 248901 (2008).

[ACL-117] I. García-Mata, K. M. Frahm, and D. L. Shepelyansky, *Shor's factorization algorithm with a single qubit and imperfections*, Physical Review A **78**, 062323 (2008).

[ACL-118] I. García-Mata and D. L. Shepelyansky, *Delocalization induced by nonlinearity in systems with disorder*, Physical Review E **79**, 026205 (2009).

[ACL-119] O. Giraud, J. Martin, and B. Georgeot, *Entropy of entanglement and multifractal exponents for random states*, Physical Review A **79**, 032308 (2009).

[ACL-120] D. L. Shepelyansky, A. S. Pikovsky, J. Schmidt, and F. Spahn, *Synchronization mechanism of sharp edges in rings of Saturn*, Monthly Notices of the Royal Astronomical Society, **395**, 1934 (2009).

[ACL-121] F. Lignières and B. Georgeot, *Asymptotic analysis of high-frequency acoustic modes in rapidly rotating stars*, Astronomy & Astrophysics, **500**, 1173 (2009).

[ACL-122] J. Martin, B. Georgeot, and D. L. Shepelyansky, *Chaotic dynamics of a Bose-Einstein condensate coupled to a qubit*, Physical Review E **79**, 066205 (2009).

[ACL-123] I. García-Mata, O. Giraud, and B. Georgeot, *Quantum computation of multifractal exponents through the quantum wavelet transform*, Physical Review A **79**, 052321 (2009).

[ACL-124] O. Giraud, B. Georgeot, and D. L. Shepelyansky, *Delocalization transition for the Google matrix*, Physical Review E **80**, 026107 (2009).

[ACL-125] O. V. Zhirov and D. L. Shepelyansky, *Quantum synchronization and entanglement of two qubits coupled to a driven dissipative resonator*, Physical Review B **80**, 014519 (2009).

Physique Statistique des Systèmes Complexes

[ACL-126] P. H. Chavanis, *Statistical mechanics of geophysical turbulence: application to Jovian flows and Jupiter's great red spot*, Physica D **200**, 257 (2005).

[ACL-127] P. H. Chavanis, *On the lifetime of metastable states in self-gravitating systems*, Astronomy and Astrophysics **432**, 117 (2005).

[ACL-128] P. H. Chavanis and F. Bouchet, *On the coarse-grained evolution of collisionless stellar systems*, Astronomy and Astrophysics **430**, 771 (2005).

[ACL-129] N. Leprovost, B. Dubrulle, and P. H. Chavanis, *Thermodynamics of MHD flows with axial symmetry*, Physical Review E **71**, 036311 (2005).

[ACL-130] P. H. Chavanis, J. Vatteville, and F. Bouchet, *Dynamics and thermodynamics of a simple model similar to self-gravitating systems: the HMF model*, European Physical Journal B **46**, 61 (2005).

[ACL-131] P. H. Chavanis and M. Lemou, *Relaxation of the distribution function tails for systems described by Fokker-Planck equations*, Physical Review E **72**, 061106 (2005).

[ACL-132] V. Desoutter and N. Destainville, *Flip dynamics in three-dimensional random tilings*, Journal of Physics A **38**, 17 (2005).

[ACL-133] N. Destainville, M. Widom, R. Mosseri, and F. Bailly, *Random tilings of high symmetry: I. Mean-field theory*, Journal of Statistical Physics **120**, 799 (2005).

[ACL-134] M. Widom, N. Destainville, R. Mosseri, and F. Bailly, *Random tilings of high symmetry: II. Boundary conditions and numerical studies*, Journal of Statistical Physics **120**, 837 (2005).

[ACL-135] D. S. Dean, D. J. Lancaster, and S. N. Majumdar, *The statistical mechanics of traveling salesman type problems*, Journal of Statistical Mechanics, L01001 (2005).

[ACL-136] D. S. Dean, I. T. Drummond, R. R. Horgan, and S. N. Majumdar, *Equilibrium statistics of a slave estimator in Langevin processes*, Physical Review E **71**, 031103 (2005).

[ACL-137] D. S. Dean and R. R. Horgan, *The thermal Casimir effect in lipid bilayer tubules*, Physical Review E **71**, 041907 (2005).

[ACL-138] D. S. Dean and R. R. Horgan, *The field theory of symmetrical layered electrolytic systems and the thermal Casimir effect*, Journal of Physics C **17**, 3473 (2005).

[ACL-139] D. S. Dean, D. Lancaster, and S. N. Majumdar, *The statistical mechanics of combinatorial optimization problems with site disorder*, Physical Review E **72**, 026125 (2005).

[ACL-140] X. Lefebvre and J. Palmeri, *Nanofiltration theory: good co-ion exclusion approximation for single salts*, Journal of Physical Chemistry B **109**, 5525 (2005).

[ACL-141] S. Touil, S. Tingry, J. Palmeri, S. Bouchtalla, and A. Deratani, *Preparation and characterization of a cyclodextrin containing membranes : application to the selective extraction of xylene isomers*, Polymer **46**, 9615 (2005).

[ACL-142] J. Palmeri, *NanoFlux predicts and scales-up nano processes*, Filtration+Separation **42**, 15 (2005).

[ACL-143] J. Sopik, C. Sire, and P. H. Chavanis, *Self-gravitating Brownian systems and bacterial populations with two or more types of particles*, Physical Review E **72**, 026105 (2005).

[ACL-144] P. H. Chavanis and C. Sire, *On the interpretations of Tsallis functional in connection with Vlasov-Poisson and related systems: Dynamics vs thermodynamics*, Physica A **356**, 419 (2005).

[ACL-145] P. H. Chavanis, *Coarse-grained distributions and superstatistics*, Physica A **359**, 177 (2006).

[ACL-146] P. H. Chavanis, *Hamiltonian and Brownian systems with long-range interactions: I. Statistical equilibrium states and correlation functions*, Physica A **361**, 55 (2006).

[ACL-147] P. H. Chavanis, *Hamiltonian and Brownian systems with long-range interactions: II. Kinetic equations and stability analysis*, Physica A **361**, 81 (2006).

[ACL-148] N. Leprovost, B. Dubrulle, and P. H. Chavanis, *Dynamics and thermodynamics of axisymmetric flows: Theory*, Physical Review E **73**, 046308 (2006).

[ACL-149] P. H. Chavanis, *Quasi-stationary states and incomplete violent relaxation in systems with long-range interactions*, Physica A **365**, 102 (2006).

[ACL-150] P. H. Chavanis, *Dynamical stability of collisionless stellar systems and barotropic stars: the nonlinear Antonov first law*, Astronomy and Astrophysics **451**, 109 (2006).

[ACL-151] P. H. Chavanis, *Curious behavior of the diffusion coefficient and friction force for the strongly inhomogeneous HMF model*, European Physical Journal B **52**, 47 (2006).

[ACL-152] P. H. Chavanis, *Relaxation of a test particle in systems with long-range interactions: diffusion coefficient and dynamical friction*, European Physical Journal B **52**, 61 (2006).

[ACL-153] P. H. Chavanis, *Nonlinear mean-field Fokker-Planck equations and their applications in physics, astrophysics, and biology*, Comptes Rendus de Physique **7**, 318 (2006).

[ACL-154] P. H. Chavanis, *Newtonian gravity in d dimensions*, Comptes Rendus de Physique **7**, 331 (2006).

[ACL-155] P. H. Chavanis and B. Dubrulle, *Statistical mechanics of the shallow-water system with an a priori potential vorticity distribution*, Comptes Rendus de Physique **7**, 442 (2006).

[ACL-156] P. H. Chavanis, *Jeans type instability for a chemotactic model of cellular aggregation*, European Physical Journal B **52**, 433 (2006).

[ACL-157] P. H. Chavanis, *Phase transitions in self-gravitating systems*, International Journal of Modern Physics B **20**, 3113 (2006).

[ACL-158] P. H. Chavanis, *Lynden-Bell and Tsallis distributions for the HMF model*, European Physical Journal B **53**, 487 (2006).

[ACL-159] P. H. Chavanis, *Phase separation of bacterial colonies in a limit of high degradation. Analogy with Jupiter's great red spot*, European Physical Journal B **54**, 525 (2006).

[ACL-160] N. Destainville and L. Salomé, *Quantification and correction of systematic errors due to detector time-averaging in single molecule tracking experiments*, Biophysical Journal **90**, L17 (2006).

[ACL-161] N. Meilhac, L. Le Guyader, L. Salomé, and N. Destainville, *Detection of confinement and jumps in single protein membrane trajectories*, Physical Review E **73**, 011915 (2006).

[ACL-162] N. Destainville, *Numerical entropy and phason elastic constants of plane random tilings with any 2D-fold symmetry*, European Physical Journal B **52**, 119 (2006).

[ACL-163] N. Pouget, C. Turlan, N. Destainville, L. Salomé, and M. Chandler, *IS911 transposome assembly as analyzed by tethered particle motion*, Nucleic Acids Research **34**, 4313 (2006).

[ACL-164] D. S. Dean and R. R. Horgan, *Renormalization of membrane rigidity by long-range interactions*, Physical Review E **73**, 011906 (2006).

[ACL-165] D. S. Dean and D. Lancaster, *The statistical mechanics of multi-index matching problems with site disorder*, Physical Review E **74**, 041122 (2006).

[ACL-166] D. S. Dean and S. N. Majumdar, *Phase Transition in a Generalized Eden Growth Model on a Tree*, Journal of Statistical Physics **124**, 1351 (2006).

[ACL-167] D. S. Dean and S. N. Majumdar, *Large deviations of extreme eigenvalues of random matrices*, Physical Review Letters **97**, 160201 (2006).

[ACL-168] M. Manghi, X. Schlagberger, and R. R. Netz, *Propulsion with a rotating elastic nanorod*, Physical Review Letters **96**, 068101 (2006).

[ACL-169] M. Manghi, X. Schlagberger, Y. W. Kim, and R. R. Netz, *Hydrodynamic effects in driven soft matter*, Soft Matter **2**, 653 (2006).

[ACL-170] D. S. Dean and M. Manghi, *Fluctuation-induced interactions between domains in membranes*, Physical Review E **74**, 021916 (2006).

[ACL-171] N. Ben Amar, H. Saidani, J. Palmeri, and A. Deratani, *Quels paramètres prendre en compte pour la modélisation de l'effet de la température sur les performances en nanofiltration ? Cas des solutés neutres*, Récents Progrès en Génie des Procédés **93**, P61-1 (2006).

[ACL-172] A. Deratani, S. Touil, J. Palmeri, S. Tingry, and S. Bouchtalla, *Pertraction of xylene isomers using cyclodextrin-containing membranes : mass transport mechanism and modeling*, Desalination **200**, 103 (2006).

[ACL-173] N. Ben Amar, H. Saidani, J. Palmeri, and A. Deratani, *Temperature dependence of water and neutral solutes transport in nanofiltration membranes*, Desalination **199**, 46 (2006).

[ACL-174] P. H. Chavanis and C. Sire, *Virial theorem and dynamical evolution of self-gravitating Brownian particles in an unbounded domain : I. Overdamped models*, Physical Review E **73**, 066103 (2006).

[ACL-175] P. H. Chavanis and C. Sire, *Virial theorem and dynamical evolution of self-gravitating Brownian particles in an unbounded domain : II. Inertial models*, Physical Review E **73**, 066103 (2006).

[ACL-176] J. Sopik, C. Sire, and P. H. Chavanis, *Dynamics of the Bose-Einstein condensation : analogy with the collapse dynamics of a classical self-gravitating Brownian gas*, Physical Review E **74**, 011112 (2006).

[ACL-177] D. S. Dean, C. Sire, and J. Sopik, *Distance traveled by random walkers before absorption in a random medium*, Physical Review E **73**, 066130 (2006).

[ACL-178] C. Sire, S. N. Majumdar, and D. S. Dean, *Exact solution of a model of time-dependent evolutionary dynamics in a rugged fitness landscape*, Journal of Statistical Mechanics, L07001 (2006).

[ACL-179] P. H. Chavanis, *Kinetic theory with angle-action variables*, Physica A **377**, 469 (2007).

[ACL-180] A. Antoniazzi, D. Fanelli, J. Barré, P. H. Chavanis, T. Dauxois, and S. Ruffo, *A maximum entropy principle explains quasi-stationary states in systems with long-range interactions: the example of the Hamiltonian Mean-Field model*, Physical Review E **75**, 011112 (2007).

[ACL-181] P. H. Chavanis, *White dwarf stars in d dimensions*, Physical Review D **76**, 023004 (2007).

[ACL-182] P. H. Chavanis, *Critical mass of bacterial populations and critical temperature of self-gravitating Brownian particles in two dimensions*, Physica A **384**, 392 (2007).

[ACL-183] P. H. Chavanis, *Exact diffusion coefficient of self-gravitating Brownian particles in two dimensions*, European Physical Journal B **57**, 391 (2007).

[ACL-184] P. H. Chavanis and M. Lemou, *Kinetic theory of point vortices in two dimensions: analytical results and numerical simulations*, European Physical Journal B **59**, 217 (2007).

[ACL-185] C. Favard, D. S. Dean, and M.-P. Rols, *Electrotransfer as a non viral method of gene delivery*, Current Gene Therapy **7**, 67 (2007).

[ACL-186] A. J. Bray and D. S. Dean, *The statistics of critical points of Gaussian fields on large dimensional spaces*, Physical Review Letters **98**, 150201 (2007).

[ACL-187] L. F. Cugliandolo, D. S. Dean, and H. Yoshino, *Non-linear susceptibilities of spherical models*, Journal of Physics A **40**, 4285 (2007).

[ACL-188] D. S. Dean, I. T. Drummond, and R. R. Horgan, *Effective transport properties for diffusion in random media*, Journal of Statistical Mechanics, P07013 (2007).

[ACL-189] J.-M. Escoffre, D. S. Dean, M. Hubert, M.-P. Rols, and C. Favard, *Membrane perturbation by an external electric field: a mechanism to permit molecular uptake*, European Biophysics Journal **36**, 973 (2007).

[ACL-190] D. S. Dean and R. R. Horgan, *Path integrals for stiff polymers applied to membrane physics*, Physical Review E **76**, 041102 (2007).

[ACL-191] D. S. Dean and D. Lancaster, *Fluctuations in the site disordered traveling salesman problem*, Journal of Physics A **40**, 13837 (2007).

[ACL-192] J. Palmeri, M. Manghi, and N. Destainville, *Thermal denaturation of fluctuating DNA driven by bending entropy*, Physical Review Letters **99**, 088103 (2007).

[ACL-193] N. Ben Amar, H. Saidani, A. Deratani, and J. Palmeri, *Effect of temperature on the transport of water and neutral solutes across nanofiltration membranes*, Langmuir **23**, 2937 (2007).

[ACL-194] C. Touya and D. S. Dean, *Dynamical transition for a particle in a squared Gaussian potential*, Journal of Physics A **40**, 919 (2007).

[ACL-195] C. Sire, *Probability distribution of the maximum of a smooth temporal signal*, Physical Review Letters **98**, 020601 (2007).

[ACL-196] P. H. Chavanis and C. Sire, *Logotropic distributions*, Physica A **375**, 140 (2007).

[ACL-197] C. Sire, *Universal statistical properties of poker tournaments*, Journal of Statistical Mechanics, P08013 (2007).

[ACL-198] P. H. Chavanis and C. Sire, *Kinetic and hydrodynamic models of chemotactic aggregation*, Physica A **384**, 199 (2007).

[ACL-199] P. H. Chavanis, *Hamiltonian and Brownian systems with long-range interactions: III. The BBGKY hierarchy for spatially inhomogeneous systems*, Physica A **387**, 787 (2008).

[ACL-200] P. H. Chavanis, *Hamiltonian and Brownian systems with long-range interactions: IV. General kinetic equations from the quasilinear theory*, Physica A **387**, 1504 (2008).

[ACL-201] P. H. Chavanis, *Kinetic theory of 2D point vortices from a BBGKY-like hierarchy*, Physica A **387**, 1123 (2008).

[ACL-202] P. H. Chavanis, *Nonlinear mean field Fokker-Planck equations. Application to the chemotaxis of biological populations*, European Physical Journal B **62**, 179 (2008).

[ACL-203] P. H. Chavanis, *Relativistic stars with a linear equation of state: analogy with classical isothermal spheres and black holes*, Astronomy and Astrophysics **483**, 673 (2008).

[ACL-204] P. H. Chavanis, *Hamiltonian and Brownian systems with long-range interactions: V. Stochastic kinetic equations and theory of fluctuations*, Physica A **387**, 5716 (2008).

[ACL-205] P. H. Chavanis, *Statistical mechanics of 2D turbulence with a prior vorticity distribution*, Physica D **237**, 1998 (2008).

[ACL-206] A. Campa, P. H. Chavanis, A. Giansanti, and G. Morelli, *Dynamical phase transitions in Hamiltonian long-range systems and Tsallis distributions with time dependent index*, Physical Review E **78**, 040102(R) (2008).

[ACL-207] P. H. Chavanis, *Two-dimensional Brownian vortices*, Physica A **387**, 6917 (2008).

[ACL-208] R. Monchaux, P. H. Chavanis, A. Chiffaudel, P. P. Cortet, F. Daviaud, P. Diribarne, and B. Dubrulle, *Fluctuation-Dissipation Relations and statistical temperatures in a turbulent von Karman flow*, Physical Review Letters **101**, 174502 (2008).

[ACL-209] J. Palmeri, M. Manghi, and N. Destainville, *Thermal denaturation of fluctuating finite DNA chains: The role of bending rigidity in bubble nucleation*, Physical Review E **77**, 011913 (2008).

[ACL-210] N. Destainville, *Theory of fluorescence correlation spectroscopy at variable observation area for two-dimensional diffusion on a meshgrid*, Soft Matter **4**, 1288 (2008).

[ACL-211] N. Destainville, *Cluster phases of membrane proteins*, Physical Review E **77**, 011905 (2008).

[ACL-212] N. Destainville and L. Foret, *Thermodynamics of nano-cluster phases: a unifying theory*, Physical Review E **77**, 051403 (2008).

[ACL-213] N. Destainville, A. Saulière, and L. Salomé, *Comment to the paper of Michael J. Saxton: "A Biological Interpretation of Transient Anomalous Subdiffusion. I. Qualitative Model"*, Biophysical Journal **95**, 3117 (2008).

[ACL-214] N. Destainville, F. Dumas, and L. Salomé, *What do diffusion measurements tell us about membrane compartmentalization? Emergence of the role of interprotein interactions*, Journal of Chemical Biology **1**, 37 (2008).

[ACL-215] N. Destainville and V. Desoutter, *Slow flip dynamics of three-dimensional rhombus tilings: failure of the Langevin approach*, Applied Mathematics & Information Sciences **2**, 83 (2008).

[ACL-216] D. S. Dean and S. N. Majumdar, *Extreme value statistics of eigenvalues of Gaussian random matrices*, Physical Review E **77**, 041108 (2008).

[ACL-217] D. S. Dean and C. Touya, *Self similar renormalization group applied to diffusion in non-Gaussian potentials*, Journal of Physics A **41**, 335002 (2008).

[ACL-218] M. Manghi and M. Aubouy, *Adsorption of polyelectrolytes from semidilute solutions on an oppositely charged surface*, Physical Chemistry Chemical Physics **10**, 1697 (2008).

[ACL-219] S. Touil, J. Palmeri, S. Tingry, S. Bouchtalla, and A. Deratani, *Generalized dual mode modeling of xylene isomer sorption in polyvinylalcohol membranes containing alpha cyclodextrin*, Journal of Membrane Science **317**, 2 (2008).

[ACL-220] P. H. Chavanis and C. Sire, *Critical mass of bacterial populations in a generalized Keller-Segel model: Analogy with the Chandrasekhar limiting mass of white dwarf stars*, Physica A **387**, 1999 (2008).

[ACL-221] P. H. Chavanis and C. Sire, *Jeans type analysis of chemotactic collapse*, Physica A **387**, 4033 (2008).

[ACL-222] C. Sire and P. H. Chavanis, *Critical dynamics of self-gravitating Langevin particles and bacterial populations*, Physical Review E **78**, 061111 (2008).

[ACL-223] C. Sire, *Crossing intervals of non-Markovian Gaussian processes*, Physical Review E **78**, 011121 (2008).

[ACL-224] C. Sire, *Contest based on a directed polymer in a random medium*, Physical Review E **78**, 061106 (2008).

[ACL-225] F. Baldovin, P. H. Chavanis, and E. Orlandini, *Microcanonical quasi-stationarity of long-range interacting systems in contact with a heat bath*, Physical Review E **79**, 011102 (2009).

[ACL-226] P. H. Chavanis, *Dynamical and thermodynamical stability of two-dimensional flows : variational principles and relaxation equations*, European Physical Journal B **70**, 73 (2009).

[ACL-227] P. H. Chavanis, *Kinetic theory of stellar systems, two-dimensional vortices and HMF model*, Theoretical and Computational Fluid Dynamics, in press (2009).

[ACL-228] P. H. Chavanis, *A stochastic Keller-Segel model of chemotaxis*, Communications in Nonlinear Science and Numerical Simulation **15**, 60 (2010).

[ACL-229] P. H. Chavanis, *Statistics of the gravitational force in various dimensions of space: from Gaussian to Lévy laws*, European Physical Journal B **70**, 413 (2009).

[ACL-230] F. Staniscia, P. H. Chavanis, G. De Ninno and D. Fanelli, *Out-of-equilibrium phase reentrance(s) in long-range interacting systems*, Physical Review E **80**, 021138 (2009).

[ACL-231] J.-M. Escoffre, T. Portet, L. Wasungu, J. Tessié, D. S. Dean and M.-P. Rols, *What is (still not) known of the mechanism by which electroporation mediates gene transfer and expression in cells and tissues*, Molecular Biotechnology **41**, 286 (2009).

[ACL-232] D. S. Dean, *Thermal Casimir effect with soft boundary conditions*, Physical Review E **79**, 011108 (2009).

[ACL-233] D. S. Dean, R. R. Horgan, A. Naji, and R. Podgornik, *One-dimensional counterion gas between charged surfaces: Exact results compared with weak- and strong-coupling analysis*, Journal of Chemical Physics **130**, 094504 (2009).

[ACL-234] T. Portet, F. Camps, I. Febrer, J.-M. Escoffre, C. Favard, M.-P. Rols, and D. S. Dean, *Visualization of lipid expulsion during the shrinkage of giant vesicles under electropulsation*, Biophysical Journal **96**, 4109 (2009).

[ACL-235] M. Manghi, J. Palmeri, and N. Destainville, *Coupling between denaturation and chain conformations in DNA: stretching, torsion, bending and finite size effects*, Journal of Physics: Condensed Matter **21**, 034104 (2009).

[ACL-236] N. Destainville, M. Manghi, and J. Palmeri, *Microscopic mechanism for experimentally observed anomalous elasticity of DNA in 2D*, Biophysical Journal, **96**, 4464 (2009).

[ACL-237] N. Ben Amar, H. Saidani, J. Palmeri, and A. Deratani, *Effect of temperature on the rejection of neutral and charged solutes by the Desal 5 DK nanofiltration membrane*, Desalination **246**, 294 (2009).

[ACL-238] N. Ben Amar, N. Kechaou, J. Palmeri, A. Deratani, and A. Sghaier, *Comparison of tertiary treatment by Nanofiltration and Reverse Osmosis for water reuse in Denim textile industry*, Journal of Hazardous Materials, **170**, 111 (2009).

[ACL-239] H. Saidani, N. Ben Amar, J. Palmeri, and A. Deratani, *Interplay between the transport of solutes across nanofiltration membranes and the thermal properties of the thin active layer*, Langmuir, in press (2009).

[ACL-240] J. Palmeri, N. Ben Amar, H. Saidani, and A. Deratani, *Process Modeling of Brackish and Seawater Nanofiltration*, *Desalination and Water Treatment*, in press (2009).

[ACL-241] C. Sire and S. Redner, *Understanding baseball team standings and streaks*, *European Physical Journal B* **67**, 473 (2009).

[ACL-242] D. S. Dean, R. R. Horgan, A. Naji, and R. Podgornik, *Thermal Casimir effect between random layered dielectrics*, *Physical Review A* **79**, 040101 (2009).

[ACL-243] D. Bonamy, P. H. Chavanis, F. Daviaud, B. Dubrulle, and M. Renouf, *Non-linear steady states in dense granular flows*, *European Physical Journal B* **68**, 619 (2009).

[ACL-244] P. H. Chavanis and L. Delfini, *Dynamical stability of systems with long-range interactions: application of the Nyquist method to the HMF model*, *European Physical Journal B* **69**, 389 (2009). Highlighted in *Europhysics News* **40**, 13 (2009).

[ACL-245] D. S. Dean and A. J. Gopinathan, *The non-equilibrium behavior of fluctuation induced forces*, submitted to *Journal of Statistical Mechanics*, L08001 (2009).

[ACL-246] C. Touya, D. S. Dean, and C. Sire, *Dipole diffusion in a random electrical potential*, *Journal of Physics A* **42**, 375001 (2009).

Systèmes de Fermions Finis – Agrégats

[ACL-247] M. Ma, P. G. Reinhard, and É. Suraud, *Dynamics of H_9^+ in intense laser pulses*, *European Physical Journal D* **33**, 49 (2005).

[ACL-248] É. Suraud and P. G. Reinhard, *Vlasov dynamics in finite fermion systems*, *Transport Theory and Statistical Physics* **34**, 417 (2005).

[ACL-249] B. Gervais, É. Giglio, E. Jacquet, A. Ipatov, P. G. Reinhard, and É. Suraud, *Simple DFT model of clusters embedded in a rare gas matrix*, *Journal of Chemical Physics* **121**, 8466 (2005).

[ACL-250] F. Fehrer, M. Mundt, P. G. Reinhard, and É. Suraud, *Modeling Na clusters in Ar matrices*, *Annalen der Physik (Leipzig)* **14**, 411 (2005).

[ACL-251] P. G. Reinhard and É. Suraud, *Dynamics of orientations in an ensemble of Na_7^+ clusters*, *European Physical Journal D* **34**, 145 (2005).

[ACL-252] P. M. Dinh, P. G. Reinhard, and É. Suraud, *Time resolved fission in metal clusters*, *Journal of Physics B* **38**, 1637 (2005).

[ACL-253] F. Fehrer, P. G. Reinhard, É. Suraud, É. Giglio, B. Gervais, and A. Ipatov, *Linear and non linear response of embedded clusters*, *Applied Physics A* **82**, 151 (2006).

[ACL-254] K. Andrae, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Pump and probe analysis of metal cluster dynamics*, *Computational Material Science* **35**, 169 (2006).

[ACL-255] M. Belkacem, F. Mégi, P. G. Reinhard, É. Suraud, and G. Zwicknagel, *Coulomb explosion of simple metal clusters in intense laser fields*, *Physical Review A* **73**, 051201 (2006).

[ACL-256] F. Fehrer, P. G. Reinhard, and É. Suraud, *Coupled plasmon and phonon dynamics in embedded Na clusters*, *Applied Physics A* **82**, 145 (2006).

[ACL-257] C. Legrand, É. Suraud, and P. G. Reinhard, *Semi-classical description of small Na clusters and dynamics*, *Journal of Physics B* **39**, 2481 (2006).

[ACL-258] V. O. Nesterenko, P. G. Reinhard, T. Halfmann, and É. Suraud, *Exploration of electronic quadrupole states in atomic clusters by 2 photons processes*, *Journal of Physics B* **39**, 3905 (2006).

[ACL-259] M. Belkacem, F. Mégi, É. Suraud, P. G. Reinhard, and G. Zwicknagel, *A Molecular Dynamics description of clusters in strong laser fields*, *European Physical Journal D* **40**, 247 (2006).

[ACL-260] J. Navarro, P. G. Reinhard, and É. Suraud, *Small fermionic systems, the common methods and challenges*, *European Physical Journal A* **30**, 333 (2006).

[ACL-261] P. M. Dinh, F. Fehrer, P. G. Reinhard, and É. Suraud, *Charge and size effects on the deposition of Na on Ar*, *International Journal of Quantum Chemistry* **107**, 2828 (2007).

[ACL-262] P. M. Dinh, F. Fehrer, P. G. Reinhard, and É. Suraud, *Dynamics of cluster deposition on Ar surfaces*, European Physical Journal D **45**, 415 (2007).

[ACL-263] P. M. Dinh, F. Fehrer, G. Bousquet, P. G. Reinhard, and É. Suraud, *Shape dynamics during deposit of simple metal clusters on rare gas matrices*, Physical Review A **76**, 043201 (2007).

[ACL-264] M. Baer, L. V. Moskaleva, M. Winkler, P. G. Reinhard, N. Roesch, and É. Suraud, *Structure and optical properties of Na clusters deposited on MgO(001)*, European Physical Journal D **45**, 507 (2007).

[ACL-265] F. Fehrer, P. M. Dinh, M. Baer, P. G. Reinhard, and É. Suraud, *Hindered Coulomb explosion of embedded Na clusters – stopping, shape dynamics and energy transport*, European Physical Journal D **45**, 447 (2007).

[ACL-266] F. Fehrer, P. M. Dinh, É. Suraud, and P. G. Reinhard, *Dynamics of cluster deposition on Ar surface*, European Physical Journal D **45**, 415 (2007).

[ACL-267] F. Fehrer, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Structural properties and optical response of Na clusters in Ne, Ar, and Kr matrices*, Physical Review B **75**, 235418 (2007).

[ACL-268] M. Baer, G. Bousquet, P. M. Dinh, F. Fehrer, P. G. Reinhard, and É. Suraud, *Dynamics of metal clusters in rare gas*, International Journal of Modern Physics B **21**, 2439 (2007).

[ACL-269] F. Fehrer, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Embedded metal clusters in strong laser fields*, Computational Material Science **42**, 203 (2008).

[ACL-270] F. Fehrer, P. M. Dinh, É. Suraud, and P. G. Reinhard, *Deposition Dynamics of Na monomers and dimers on an Ar(001) substrate*, Surface Science **602**, 2699 (2008).

[ACL-271] P. M. Dinh, J. Messud, P. G. Reinhard, and É. Suraud, *Self Interaction Correction in a simple model*, Physics Letters A **372**, 5598 (2008).

[ACL-272] J. Messud, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Time-dependent density-functional theory with self-interaction correction*, Physical Review Letters **101**, 096404 (2008).

[ACL-273] J. Messud, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Improved Slater approximation to SIC-OEP*, Chemical Physics Letters **461**, 316 (2008).

[ACL-274] P. M. Dinh, P. G. Reinhard, and É. Suraud, *Dipole excitations of Ar substrate in contact with Na clusters*, Surface Science **602**, 2699 (2008).

[ACL-275] J. Messud, P. M. Dinh, P. G. Reinhard, and É. Suraud, *On the exact treatment of Time Dependent Self-Interaction Correction*, Annals of Physics (NY) **324**, 955 (2009).

[ACL-276] Z. P. Wang, P. M. Dinh, P. G. Reinhard, É. Suraud, G. Bruny, C. Montano, S. Feil, S. Eden, H. Abdoul-Carime, B. Farizon, M. Farizon, S. Ouaskit, and T. D. Maerk, *Microscopic studies of atom-water collisions*, International Journal of Mass Spectrometry **285**, 143 (2009).

[ACL-277] P. M. Dinh, P. G. Reinhard, and É. Suraud, *Dynamics of clusters and molecules in contact with an environment*, Physics Reports, in press (2009).

[ACL-278] J. Messud, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Generalized Slater and static polarizabilities*, Chemical Physics Letters, in press (2009).

9.2 Articles without references (preprints)

Fermions Fortement Corrélés

[SRP-1] K. S. D. Beach, F. Alet, M. Mambrini, and S. Capponi, *The SU(N) Heisenberg model on the square lattice: a continuous-N quantum Monte Carlo study*, submitted to Physical Review B (2009).

[SRP-2] P. Azaria, S. Capponi, and P. Lecheminant, *Three-component Fermi gas in a one-dimensional optical lattice*, submitted to Physical Review Letters (2009).

[SRP-3] D. Schwandt, F. Alet, and S. Capponi, *Quantum Monte Carlo simulations of fidelity at magnetic quantum phase transitions*, submitted to Physical Review Letters (2009).

[SRP-4] H. Nonne, P. Lecheminant, S. Capponi, G. Roux, and E. Boulat, *Haldane charge conjecture in one-dimensional multicomponent fermionic cold atoms*, submitted to Physical Review Letters (2009).

Information et Chaos Quantiques

[SRP-5] I. García-Mata and D. L. Shepelyansky, *Nonlinear delocalization on disordered Stark ladder*, submitted to Europhysics Letters (2009).

[SRP-6] M. Mulansky, K. Ahnert, A. Pikovsky, and D. L. Shepelyansky, *Dynamical thermalization of disordered nonlinear lattices*, submitted to Physical Review Letters (2009).

[SRP-7] B. Georgeot and F. Mila, *Chirality of triangular antiferromagnetic clusters as a qubit*, submitted to Physical Review Letters (2009).

[SRP-8] D. Braun and J. Martin, *Decoherence-enhanced measurements*, submitted to Nature Physics (2009).

[SRP-9] O. Giraud, M. Znidaric, and B. Georgeot, *Quantum circuit for three-qubit random states*, submitted to Physical Review A (2009).

Physique Statistique des Systèmes Complexes

[SRP-10] P. H. Chavanis, *Virial theorem for rotating self-gravitating Brownian particles and two-dimensional point vortices*, submitted to Europhysics Letters (2009).

[SRP-11] J.-M. Escoffre, C. Favard, T. Portet, C. Rosazza, E. Phez, D. S. Dean, and M.-P. Rols, *Time scales of electro-mediated membrane permeabilisation and DNA uptake in cells revealed by direct imaging with high temporal resolution*, submitted to Proceedings of the National Academy of Sciences (2009).

[SRP-12] D. S. Dean, R. R. Horgan, A. Naji, and R. Podgornik, *The effects of dielectric disorder on van der Waals interactions in slab geometries*, submitted to Physical Review E (2009).

[SRP-13] A. Naji, D. S. Dean, J. Sarabadani, R. R. Horgan, and R. Podgornik, *Thermal Casimir-van der Waals interaction between randomly charged dielectrics*, submitted to Physical Review Letters (2009).

Systèmes de Fermions Finis – Agrégats

[SRP-14] Z. P. Wang, P. M. Dinh, P. G. Reinhard, É. Suraud, and F. S. Zhang, *High-order harmonic generation and multi-photon ionization of ethylene in laser*, submitted to THEOCHEM (2009).

[SRP-15] Z. P. Wang, P. M. Dinh, P. G. Reinhard, É. Suraud, and F. S. Zhang, *DFT studies of ethylene in femtosecond laser pulses*, submitted to Physical Review A (2009).

[SRP-16] J. Messud, M. Bender, and É. Suraud, *Density Functional Theory and Kohn Sham schemes for self bound systems*, submitted to Physical Review Letters (2009).

[SRP-17] T. Fennel, K. H. Meiwes-Broer, J. Tiggesbaumker, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Laser-driven nonlinear cluster dynamics: from single- and multiphoton excitations to the strong-field domain*, submitted to Reviews of Modern Physics (2009).

[SRP-18] J. Messud, M. Bender, and É. Suraud, *Density functional theory and Kohn-Sham scheme for self-bound systems*, submitted to Physical Review C (2009).

[SRP-19] M. Bär, P. M. Dinh, L. V. Moskaleva, P.-G. Reinhard, N. Rösch, and É. Suraud, *Deposition of Na Clusters on MgO(001)*, submitted to *Physical Review B* (2009).

[SRP-20] J. Messud, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Time-dependent Generalized SIC-OEP formalism and Generalized SIC-Slater approximation*, submitted to Physical Review Letters (2009).

[SRP-21] M. Bär, P. M. Dinh, L. V. Moskaleva, P.-G. Reinhard, N. Rösch, and É. Suraud, *Angular distributions of electrons emitted from free and deposited Na_8 clusters*, submitted to *European Physical Journal D* (2009).

9.3 Invited talks in international and national conferences

Fermions Fortement Corrélés

[INV-1] D. Poilblanc, *Spectral functions in doped frustrated magnets*, invited talk at the *International Seminar and Workshop on "Strong Correlations and ARPES: Recent progress in theory and experiment"* (Dresden, Germany, April 2005).

[INV-2] D. Poilblanc, *Doped 2D frustrated magnets: spin-charge separation and non-conventional superconductivity*, invited talk at the *European Conference "Physics of Magnetism 05"* (Poznan, Poland, 24-27 June 2005); *Physica Status Solidi (b)* **243**, No. 1 (2006).

[INV-3] D. Poilblanc, *On confinement in frustrated quantum magnets*, invited talk at the *ICAM Advanced Workshop on "Strongly Correlated Electrons: Diverse Examples and Unifying Themes"* (Institut Scientifique de Cargèse, Cargèse, France, 8-20 August 2005).

[INV-4] S. Capponi, *Numerical Contractor Renormalization applied to strongly correlated systems*, invited plenary talk at the *International Workshop on Effective Models for Low-Dimensional Strongly Correlated Systems* (Peyresq, France, September 2005).

[INV-5] D. Poilblanc, *Doped 2D frustrated magnets: spin-charge separation and non-conventional superconductivity*, invited talk at the *International Conference on "Concepts in Electron Correlations"* (Hvar, Croatia, 30 September-5 October 2005).

[INV-6] D. Poilblanc, *Effective models for frustrated quantum antiferromagnets*, invited talk at the *International ESF "Highly Frustrated Magnetism" workshop on "Novel theoretical aspects of frustrated spin systems"* (CECAM, ENS-Lyon, France, 9-12 March 2006).

[INV-7] M. Mambrini, *Some Exotic phenomena in undoped and doped quantum frustrated magnets*, invited talk at the *International conference "Self-organized Strongly Correlated Electron Systems"* (Seillac, France, May 2006).

[INV-8] D. Poilblanc, *Checkerboard order in the t–J model on the square lattice*, invited talk at the *International Conference on Magnetism (ICM17)* (Kyoto, Japan, 20-25 August 2006); D. Poilblanc, C. Weber, F. Mila, and M. Sigrist, *Journal of Magnetism and Magnetic Materials* **310**, 523 (2007).

[INV-9] D. Poilblanc, *Exotic phenomena in doped frustrated magnets*, invited talk at the *International Conference on "Highly Frustrated Magnets"* (Osaka, Japan, 15-19 August 2006); D. Poilblanc, M. Mambrini, A. Läuchli, and F. Mila, *Journal of Magnetism and Magnetic Materials* **19**, 523 (2007).

[INV-10] F. Alet, *Introduction to Quantum Monte Carlo*, invited talk at the *ALPS Tutorial* (PSI Institute, Villigen, Switzerland, September 2006).

[INV-11] D. Poilblanc, *Spin-rotationally symmetric modulated flux phases in underdoped cuprates*, invited talk at the *5th International Conference "Stripes06" on "Macroscopic Quantum Phenomena in Complex Striped Matter"* (University of Roma "La Sapienza", Rome, Italy, 17-22 December 2006).

[INV-12] P. Pujol, *Effective model of low dimensional frustrated systems*, invited plenary talk at the *Workshop "Statistical physics and low dimensional systems"* (Nancy, France, May 2006).

[INV-13] D. Poilblanc, *Exotic phenomena under doping frustrated quantum magnets & dimer models: Numerical approaches*, invited talk at the *International focus workshop "Mobile Fermions and Bosons on Frustrated Lattices"* (MPIPKS Dresden, Germany, 11-13 January 2007).

[INV-14] D. Poilblanc, *Doped frustrated magnets*, invited lecture at the *International School and Workshop "Highly Frustrated Magnets and Strongly Correlated Systems: from Non-Perturbative Approaches to Experiments"* (ICTP Trieste, Italy, 30 July-17 August 2007).

[INV-15] F. Alet, *Valence bond entanglement entropy*, invited talk at the *Workshop "Highly Frustrated Magnets and Strongly Correlated Systems: from Non-Perturbative Approaches to Experiments"* (ICTP Trieste, Italy, 30 July-17 August 2007).

[INV-16] M. Mambrini, *Characterizing singlet states with SU(2) dimers*, invited talk at the *Workshop "Highly Frustrated Magnets and Strongly Correlated Systems: from Non-Perturbative Approaches to Experiments"* (ICTP Trieste, Italy, 30 July-17 August 2007).

[INV-17] S. Capponi, *Spin nematic phases in an itinerant correlated electronic system*, invited talk at the *Workshop "Highly Frustrated Magnets and Strongly Correlated Systems: from Non-Perturbative Approaches to Experiments"* (ICTP Trieste, Italy, 30 July-17 August 2007).

[INV-18] F. Alet, *Statistical physics of dimers*, invited plenary talk at the *Workshop "Statistical physics and low dimensional systems"* (Nancy, France, May 2008).

[INV-19] D. Poilblanc, *The physics of doped quantum dimer models* invited talk at the *International Workshop on "Entanglement in Spin and Orbital Systems"* (ESF "The Highly Frustrated Magnetism Network", Krakow, Poland, 18-22 June 2008).

[INV-20] P. Pujol, *Gauge theory picture of an ordering transition in a dimer model*, invited talk at the *Workshop "Topological Aspects of Solid State Physics"* (ISSP, Tokyo, Japan, June 2008).

[INV-21] D. Poilblanc, *Superconducting stripes in High-T_c cuprates* invited talk at the *6th International Conference of the STRIPES series, Stripes08* (Erice, Italy, 26 July-1 August 2008).

[INV-22] D. Poilblanc, *The physics of doped quantum dimer models* invited talk at the *International Conference on "Concepts in Electron Correlation"* (Hvar, Croatia, 24-30 September 2008).

[INV-23] D. Poilblanc, *Simulations of Qunatum Dimer Models* invited talk at the *International Conference on "Numerical Approaches to Quantum Many-Body Systems"* (Institute for Pure & Applied Mathematics at UCLA, Los Angeles, USA, 26-30 January, 2009).

[INV-24] D. Poilblanc, *Simulations of correlated fermions and constrained models* invited talk at the *International Workshop on "The Next Generation of Quantum Simulations"* (Richard B. Gump South Pacific Research Station, Moorea, French Polynesia, 2-7 May 2009).

[INV-25] D. Poilblanc, *Topological properties of effective models for frustrated spin systems* invited talk at the *International Workshop on "Topological Order: From quantum Hall systems to magnetic materials"* (Max-Planck Institut for the Physics of Complex Systems, Dresden, Germany, 29 June-24 July 2009).

[INV-26] D. Poilblanc, *Simulations of low-dimensional quantum magnets* invited talk at the *ICAM International Workshop on "Emergent Quantum Phenomena from the Nano- to the Macro- World"* (International Institute for Complex Adaptive Matter (ICAM-I2CAM), Institut d'Études Scientifiques de Cargèse, Corsica, France, 6-19 July 2009).

Information et Chaos Quantiques

[INV-27] D. Braun, *Reservoir Induced Entanglement*, invited talk at the *"KIAS-KAIST 2005 Workshop on Quantum Information Science"* (Seoul, South Korea, August 2005).

[INV-28] B. Georgeot, *Quantum computing of Poincaré recurrences and periodic orbits*, invited talk at the *9th International Conference on Squeezed States and Uncertainty Relations-ICSSUR' 2005* (Besançon, France, May 2005).

[INV-29] B. Georgeot, *Quantum computing for physics research*, invited talk at the *Xth International Workshop on Advanced Computing and Analysis Techniques in Physics Research-ACAT 2005* (Zeuthen, Germany, May 2005); B. Georgeot, *Quantum computers for physics research*, Nuclear Instruments and Methods in Physics Research A **559**, 6 (2006).

[INV-30] B. Georgeot, *Quantum algorithms and quantum chaos*, invited course at the *International School of Physics "Enrico Fermi" on Quantum Computers, Algorithms, and Chaos* (Varenna, Italy, July 2005).

[INV-31] B. Georgeot, *Quantum chaos and quantum computation*, invited talk at the *International Workshop "Energy Relaxation Versus Phase Relaxation in Many-Body Systems"* (Centro Internacional de Ciencias, Cuernavaca, Mexico, November 2005).

[INV-32] D. L. Shepelyansky, *EDIQIP highlights*, invited talk at the *conference "IST-FET QIPC Review"* (Innsbruck, Austria, 14-16 February 2005).

[INV-33] D. L. Shepelyansky, *Microwave control of transport in mesoscopic structures*, invited talk at the *2nd Workshop "Quantum Chaos and Localisation Phenomena"* (Inst. of Physics, Polish Academy of Sciences, Warsaw, Poland, 19-22 May 2005).

[INV-34] D. L. Shepelyansky, *Quantum chaos and realistic quantum computations*, invited talk at the *KIAS-KAIST 2005 Workshop on "Quantum Information Science"* (Seoul, South Korea, 22-24 August 2005).

[INV-35] B. Georgeot, *Quantum computation and complex dynamics*, invited course at the *International Workshop "Quantum Information, Computation, and Complexity"* (centre Emile Borel, Institut Henri Poincaré, Paris, February-March 2006).

[INV-36] B. Georgeot, *Quantum algoritms and chaotic systems*, invited talk at the *26th International Colloquium on Group Theoretical Methods in Physics* (City University of New York, USA, June 2006).

[INV-37] D. L. Shepelyansky, *Frenkel-Kontorova model with cold trapped ions*, invited talk at the *376 Heraues – Seminar, "At the Interface of Cold Atoms and Statistical Physics"* (Schloss Reisensburg, Gunzburg, Germany, 6-9 September 2006).

[INV-38] D. L. Shepelyansky, *Quantum computation and quantum chaos*, invited talk at the *Int. Conference "Quantum Mechanics and Chaos"* (Osaka City University, Osaka, Japan, 19-21 September 2006).

[INV-39] D. L. Shepelyansky, *Directed transport born from chaos*, invited talk at the *Conference "Chaos and Complex Systems 2006"* (Monastery of Novacella, Southern Tyrol, Italy, 9-12 October 2006).

[INV-40] D. L. Shepelyansky, *Quantum computation and quantum chaos*, invited talk at the *Bar-Ilan Meeting "Advances in Classical and Quantum Chaos"* (Bar-Ilan University, Israel, 12 December 2006).

[INV-41] D. Braun, *Decoherence in the N-spin boson model*, invited talk at the *"GdR Conference on Mesoscopic Physics"* (Aussois, France, March 2007).

[INV-42] B. Georgeot, *Results of the INFOSYSQQ project*, invited talk at the *Colloque Jeunes Chercheuses, Jeunes Chercheurs de l'ANR* (Orléans, France, April 2007).

[INV-43] D. L. Shepelyansky, *Directed transport and chaos in asymmetric nanostructures*, invited talk at the *International Conference "Chaos, Complexity and Transport: Theory and Applications"* (Le Pharo, Marseille, France, 4-8 June 2007).

[INV-44] D. L. Shepelyansky, *2D Electron transport in a microwave field*, invited talk at the *International Program "Statistical Physics of Systems out of Equilibrium"* (Institut Henri Poincaré, Paris, 10 September-14 December 2007).

[INV-45] D. Braun, *Decoherence — from fundamentals to quantum computing*, invited lecture at the *"Winter School on Quantum Information Science"* (Taitung, Taiwan, January 2008).

[INV-46] D. Braun, *Hardy non-locality versus Bell-CHSH inequalities*, invited talk at the *"GdR Conference on Quantum Information"* (Paris, France, October 2008).

[INV-47] B. Georgeot, *Quantum computing with few-qubit systems and imperfections*, invited talk at the *"EuroSQIP Meeting"* (Hindas, Sweden, 29-30 May 2008).

[INV-48] B. Georgeot, *Quantum information and computation, from dream to reality*, invited talk at the *International Symposium on Molecular Materials – MOLMAT 2008* (Toulouse, France, July 2008).

[INV-49] B. Georgeot, *Quantum chaos in quantum information and cold atom physics*, invited talk at the *International NATO Conference "Recent Advances in Nonlinear Dynamics and Complex System Physics"* (Tashkent, Uzbekistan, October 2008).

[INV-50] O. Giraud, *Classicality of spin states*, invited talk at the *"GdR Conference on Quantum Information"* (Paris, France, October 2008).

[INV-51] D. L. Shepelyansky, *Chirikov standard map*, invited talk at the *"Chirikov Memorial Seminar"* (Budker Institute of Nuclear Physics, Novosibirsk, 23 May 2008).

[INV-52] D. L. Shepelyansky, *Synchronization of qubits by resonator coupling*, invited talk at the *"EuroSQIP Meeting"* (Hindas, Sweden, 29-30 May 2008).

[INV-53] D. L. Shepelyansky, *Nonlinearity, localization, and quantum chaos*, invited talk at the *Workshop "Anderson Localization for the Nonlinear Schroedinger Equation (NLSE)?"* (Lewiner Insitute for Theoretical Physics, Technion, Haifa, Israel, 22-27 June 2008).

[INV-54] D. L. Shepelyansky, *Nonlinearity, interactions, and Anderson localization*, invited talk at the *Workshop "Mathematics and Physics of Anderson Localization: 50 Years After"* (Newton Institute, Cambridge, UK, 14 July-19 December 2008).

[INV-55] B. Georgeot, *INFOSYSQQ project*, invited talk (video forum) at the *Colloque Blanc de l'ANR* (Paris, France, February 2009).

[INV-56] D. L. Shepelyansky, *Interplay of nonlinearity, interactions and Anderson localization*, invited talk at the *Workshop "Anderson Localization in Nonlinear and Many-Body Systems"* (Max Planck Institute for the Physics of Complex Systems, Dresden, 16-20 March 2009).

[INV-57] D. L. Shepelyansky, *Delocalization by nonlinearity and interactions in systems with disorder*, invited talk at the *DPG Spring Meeting of the Condensed Matter Section; SYAL 1: Anderson Localization in Nonlinear and Many-Body Systems* (TU Dresden, 22-27 March 2009).

Physique Statistique des Systèmes Complexes

[INV-58] P. H. Chavanis, *Nonlinear mean field Fokker-Planck equations*, invited talk at the *Conference "News, Expectations and Trends in Statistical Physics (NEXT-SigmaPhi)"* (Kolymbari, Creta, 12-19 August 2005).

[INV-59] P. H. Chavanis, *Phase transitions in self-gravitating systems*, invited talk at the *Conference "Statistical Mechanics of Non-Extensive Systems"* (Paris, France, 24-25 October 2005)

[INV-60] D. S. Dean, *Slow dynamics and aging*, invited talk at the *Conference on Slow Dynamics and Aging* (Session on Granular Matter, Institut Henri Poincaré, Paris, France, March 2005).

[INV-61] D. S. Dean, *Thermodynamic approaches to granular media*, invited talk at the *Granular Physics Conference* (KITP, Santa Barbara, USA, June 2005).

[INV-62] D. S. Dean, *A physicist's perspective on optimization problems*, invited talk at the *FCOM Stochastic Computation* (Santander, Spain, June 2005).

[INV-63] D. S. Dean, *The statistics of a slave estimator for response in Langevin systems*, invited talk at the *Recent Progress in Glassy Physics* (Paris, France, September 2005).

[INV-64] D. S. Dean, *Field theoretic methods for transport in random media*, invited talk at the *Conference in honour of Prof. I. T. Drummond* (Cambridge, UK, September 2005).

[INV-65] D. S. Dean, *The statistical mechanics of combinatorial optimization problems with site disorder*, invited talk at the *ECCS'05 Cospico Satellite* (Paris, France, November 2005).

[INV-66] D. S. Dean, *Statistics of a slave estimator*, invited talk at the *Conference on Relaxation Dynamics of Macroscopic Systems* (Isaac Newton Institute, Cambridge, UK, January 2006).

[INV-67] D. S. Dean, *Phase transition in the Aldous Shields Growth Model*, invited talk at the *Conference on First-Passage and Extreme Value Problems in Random Processes* (Isaac Newton Institute, Cambridge, UK, June 2006).

[INV-68] N. Destainville, *Arctic phenomena in random tilings with fixed boundaries*, invited talk at the *DMV-Jahrestagung* (Bonn, Germany, 18-22 September 2006).

[INV-69] A. Ayral, A. Julbe, C. Guizard, J. Sanchez, G. M. Rios, and J. Palmeri, *Use of ceramic nanofilters for the treatment of solvents*, in *Proceedings of the International Workshop on Membranes in Solvent Filtration*, invited talk at the *International Workshop on Membranes in Solvent Filtration* (Leuven, Belgium, 23-24 March 2006).

[INV-70] P. H. Chavanis, *Nonlinear mean field Fokker-Planck equations*, invited talk at the *Conference "Complexity, Metastability and Nonextensivity"* (Catania, Italy, 1-4 July 2007); *AIP Conference Proceedings* **965**, 144 (2007).

[INV-71] P. H. Chavanis, *Systems with long-range interactions: interpretation of the different functionals*, invited talk at the *Conference "Dynamics and Thermodynamics of Systems with Long-range Interactions: Theory and Experiments"* (5-7 July 2007, Assisi, Italy); *AIP Conference Proceedings* **970**, 39 (2008).

[INV-72] N. Destainville, *Flip dynamics and connectivity in 3-dimensional tilings by rhombohedra*, invited talk at the *International Conference on Combinatorics* (Cracow, Poland, July 2007).

[INV-73] A. Deratani, H. Saidani, J. Palmeri, and N. Ben Amar, *Temperature effect on solutes transport in nanofiltration*, invited talk at the *Asian Membrane Society Conference* (Taipei, Taiwan, 16-18 August 200).

[INV-74] D. S. Dean, *Growth models on trees*, invited talk at the *Conference on Interfaces between Physics and Computer Science* (Jacobs University, Bremen, Germany, July 2007).

[INV-75] D. S. Dean, *Extreme value statistics of maximal eigenvalues of random matrices* invited talk at the *III BRUNEL Workshop on Random Matrix Theory* (Brunel, UK, December 2007).

[INV-76] P. H. Chavanis, *Kinetic theory of point vortices in two dimensions*, invited talk at the *IUTAM Symposium "150 Years of Vortex Dynamics"* (Copenhagen, Denmark, 13-16 October 2008).

[INV-77] P. H. Chavanis, *Kinetic theory of point vortices in two dimensions*, invited talk at the *International Conference on Statistical Physics (SigmaPhi2008)* (Kolymbari, Creta, 14-18 July 2008).

[INV-78] D. S. Dean, *Diffusion in non-Gaussian potentials in one dimension*, invited talk at the *Workshop on Statistical Physics and Low Dimensional Systems* (Nancy, France, 21-23 May 2008).

[INV-79] D. S. Dean, *Fluctuation induced interactions in one dimensional Coulomb gases*, invited talk at the *Conference Fluctuate 08* (Santa Barbara, USA, September 2008).

[INV-80] N. Destainville, *Methodological aspects of diffusion analysis by microscopy techniques*, invited talk at the *INSERM Workshop on Physical modeling and mathematical analysis in cellular biology* (St-Raphaël, France, 2008).

[INV-81] N. Destainville, *Mixing times of Markov chains, the multi-decomposition technique, flip dynamics in random tilings*, invited talk at the *Workshop on "Random Tilings, Random Partitions and Stochastic Growth Processes"* (Montréal, Canada, 1-6 September 2008).

[INV-82] N. Destainville, *Apports de la physique théorique à la compréhension de la matière vivante à l'échelle moléculaire*, invited talk at the *Troisième Workshop ITAV* (Toulouse, France, 25 September 2008).

[INV-83] N. Destainville, *Phases "clusters" de protéines membranaires : un nouveau mécanisme de confinement ?*, invited talk at the *GDR Physique de la cellule au tissu* (Sète, France, 2008).

[INV-84] C. Sire, *Poker and statistical physics*, invited talk at the *Conference on Algebraic Statistics, Machine Learning and Lattice Spin Models* (Cold Spring Harbor Laboratory, USA, 16-19 March 2008).

[INV-85] C. Sire, *The out of equilibrium physics of poker tournaments*, invited plenary talk at the *Workshop on Statistical Physics and Low Dimensional Systems* (Nancy, France, 21-23 May 2008).

[INV-86] J. Palmeri, *Brackish and seawater desalination using NF and RO membranes: transport theory, modeling, and process simulation*, invited talk at the *4-day Intensive Course, Middle East Desalination Research Center (MEDRC)* (Casablanca, Morocco, 2-5 February 2009).

[INV-87] J. Palmeri, L. Schrive, and A. Deratani, *Modélisation des procédés de nanofiltration avec le logiciel NanoFlux: applications nucléaires*, invited talk at the *Journées Thématiques "Membranes et Nucléaire" – Club Français des Membranes (CFM)* (Marcoule, France, 15-16 January 2009).

[INV-88] J. Palmeri and M. Metaiche, *Optimization of reverse osmosis and nanofiltration desalination systems*, invited talk at the *Scientific Workshop: Microsoft-CNRS Chair: Optimisation for Sustainable Development - École Polytechnique* (Palaiseau, France, 3 June 2009).

[INV-89] C. Sire, *Dynamics of self-gravitating Brownian particles*, invited talk at the *MGAT9 – Self-Gravitating Systems* session of the *12th Grossmann Meeting* (UNESCO, Paris, France, 12-18 July 2009).

Systèmes de Fermions Finis – Agrégats

[INV-90] É. Suraud, *Small fermionic systems: the common methods and challenges*, Invited talk at the *Workshop "World Consortium Initiative (WCI 3)"* (Texas A & M, College Station, Texas, USA, February 2005).

[INV-91] É. Suraud, *Au delà de TDDFT*, Invited talk at the *School "Density Functional Theory"* (Caen, France, June 2005).

[INV-92] É. Suraud, *Molecular dynamics for clusters*, Invited talk at the *XXIX Internal Workshop on "Condensed Matter Theories"* (Nara, Japan, September 2005). M. Belkacem, F. Mégi, P. G. Reinhard, É. Suraud, and G. Zwicknagel, *Molecular dynamics for clusters*, *Nova Science (Commack, NY), Condensed Matter Theories*, **20** (2006).

[INV-93] É. Suraud, *Electron emission and cluster dynamics*, Invited talk at the *Festschrift für Prof. P. G. Reinhard* (Erlangen, Germany, October 2005).

[INV-94] É. Suraud, *From mean field to molecular dynamics*, Invited talk at the *Simulations of Heavy-ion Collisions Conference* (Trento, Italy, April 2006).

[INV-95] É. Suraud, *Dynamics of metal clusters in rare gas matrices*, Invited talk at the *XXX Internal Workshop on "Condensed Matter Theories"* (Dresden, Germany, June 2006). M. Baer, G. Bousquet, P. M. Dinh, F. Fehrer, P. G. Reinhard, and É. Suraud, *Dynamics of metal clusters in rare gas clusters*, *International Journal of Modern Physics E* **15**, 1549 (2006).

[INV-96] É. Suraud, *Metal clusters and nuclei*, Invited talk at the *International Conference on "Nuclear Structure"* (Shanghai, China, June 2006). P. G. Reinhard and É. Suraud, *Metal clusters and nuclei*, *Nova Science (Commack, NY), Condensed Matter Theories* **21**, (2007).

[INV-97] É. Suraud, *Dynamics of embedded/deposited metal clusters*, Invited talk at the *XI European Workshop on "Quantum Systems in Chemistry and Physics"* (Saint Petersburg, Russia, August 2006).

[INV-98] É. Suraud, *From mean field to molecular dynamics*, Invited talk at the *International Workshop on "Femtosecond Physics"* (Marseille, France, March 2007).

[INV-99] É. Suraud, *Small fermionic systems: the common methods and challenges*, Invited talk at the *International Workshop on "Nuclear Theory" (IWNT26)* (Rila, Bulgaria, June 2007). P. G. Reinhard and É. Suraud, *Small Fermionic systems: the common methods and challenges*, *Proceedings IWNT26*, World Scientific, Singapore (2008).

[INV-100] É. Suraud, *Basis of electromagnetism*, Invited talk at the *Summer school in Physics* (Phnom-Penh, Cambodia, August-September 2007).

[INV-101] É. Suraud, *Dynamics of clusters and molecules in contact with an environment*, Invited talk at the *Clustertreffen 2007* (Berlin, Germany, September 2007).

[INV-102] É. Suraud, *Time-resolved analysis of large amplitude collective motion in metal clusters*, Invited talk at the *International Marie Curie Workshop on Fission* (Kazimirierz, Poland, September 2007). P. M. Dinh, P. G. Reinhard, and É. Suraud, *Time-resolved fission of metal clusters and nuclei*, *International Journal of Modern Physics E* **17**, 120 (2008).

[INV-103] É. Suraud, *Elements of DFT*, Invited talk at the *Workshop on DFT and Nuclei* (Saclay, France, November 2007).

[INV-104] É. Suraud, *The impact of international collaborations in "heavy physics" for strengthening relations between countries*, Invited talk at the *Humboldt Kolleg Symposium* (Paris, France, November 2007). É. Suraud, *The impact of international collaborations in "heavy physics" for strengthening relations between countries*, *Humboldt Kolleg*, Kluwer (2008).

[INV-105] É. Suraud, *On Time-Dependent DFT with Self Interaction Correction*, Invited talk at the *XXXI International Workshop on "Condensed Matter Theories"* (Bangkok, Thailand, December 2007). J. Messud, P. M. Dinh, É. Suraud, and P. G. Reinhard, *On Time Dependent DFT with SIC*, *International Journal of Modern Physics B* **22**, 4666 (2008).

[INV-106] É. Suraud, *Dynamics of clusters in/on surfaces*, Invited talk at the *International Conference on "Clusters at Surfaces"* (Warnemuende, Germany, May 2008).

[INV-107] É. Suraud, *Dynamical hierarchical method for the irradiation of clusters and molecules in contact with an environment*, Invited talk at the *International Conference on "Radiation Damages in Biomolecular Systems"* (Debrecen, Hungary, June 2008). P. M. Dinh, J. Messud, P. G. Reinhard, É. Suraud, and Z. P. Wang, *Dynamical hierarchical method for the irradiation of clusters and molecules in an environment*, *AIP Conference Proceedings* **1080**, 132 (2008).

[INV-108] É. Suraud, *The Self Interaction Correction revisited*, Invited talk at the *International workshop on "Nuclear Theory" (IWNT27)* (Rila, Bulgaria, June 2008). J. Messud, P. M. Dinh, P. G. Reinhard, and É. Suraud, *The Self Interaction Correction revisited*, *Proceedings IWNT27*, World Scientific, Singapore (2009).

[INV-109] É. Suraud, *Electron emission to analyse cluster dynamics*, Invited talk at the *International Conference on "Nanosystems"* (Dubna, Russia, July 2008). P. M. Dinh, J. Messud, P. G. Reinhard, É. Suraud, S. Vidal, and Z. P. Wang, *Electron emission to analyze cluster dynamics*, *Journal of Physics: Conference Series* **129**, 012018 (2008).

[INV-110] É. Suraud, *On the generalized Slater approximation*, Invited talk at the *XXXII Internal Workshop on "Condensed Matter Theories"* (Leicester, United Kingdom, August 2008). J. Messud, P. M. Dinh, É. Suraud, and P. G. Reinhard, *On the generalized Slater approximation*, *International Journal of Modern Physics B*, in press (2009).

[INV-111] É. Suraud, *Clusters in strong fields*, Invited talk at the *International Conference on "Correlation Effects in Radiation Fields"* (Warnemuende, Germany, September 2008).

[INV-112] É. Suraud, *Dynamics of irradiated clusters and molecules*, Invited talk at the *French-Chinese Workshop on "Intense Lasers and Applications"* (Hangshou, China, November 2008).

[INV-113] É. Suraud, *Sur les limites de l'évaluation par les pairs*, Invited talk at the *Humboldt Kolleg Symposium* (Paris, France, November 2008).

[INV-114] É. Suraud, *Time Dependent Self Interaction Correction*, Invited talk at the *International conference "Nonequilibrium nanostructures"* (Dresden, Germany, December 2008).

[INV-115] É. Suraud, *Metal clusters deposited on surfaces: dynamics of deposit and substrate excitation*, Invited talk at the *DFT Topical Meeting on Nano-objects* (Toulouse, France, December 2008).

9.4 Oral communications leading to a conference proceeding (international conferences)

Fermions Fortement Corrélés

[ACTI-1] L. Levrel, F. Alet, J. Rottler, and A. C. Maggs, *Local simulation algorithms for Coulombic interactions*, in *Proceedings of the 22nd IUPAP International Conference of Statistical Physics – STATPHYS 22* (Bangalore, India, 4-9 July 2004), *Pramana Journal of Physics* **64**, 1001 (2005).

[ACTI-2] F. Alet, B. Lucini, and M. Vettorazzo, *Local simulation algorithms for Coulombic interactions*, in *Proceedings of the Europhysics Conference on Computational Physics 2004* (Genova, Italy, 1-4 September 2004), *Computer Physics Communications* **169**, 370 (2005).

[ACTI-3] S. Wessel, F. Alet, S. Trebst, D. Leumann, M. Troyer, and G. G. Batrouni, *Bosons in optical lattices – From the Mott transition to the Tonks-Girardeau gas*, in *Proceedings of the International conference on Statistical Physics of Quantum Systems "novel orders and dynamics"* (Sendai, Japan, July 2004), *Journal of the Physical Society of Japan Supplements* **74**, 10 (2005).

[ACTI-4] F. Alet, P. Dayal, A. Grzesik, A. Honecker, M. Koerner, A. Laeuchli, S. R. Manmana, I. P. McCulloch, F. Michel, R. M. Noack, G. Schmid, U. Schollwoeck, F. Stoeckli, S. Todo, S. Trebst, M. Troyer, P. Werner, S. Wessel (The ALPS collaboration), *The ALPS project: open source software for strongly correlated systems*, in *Proceedings of the International conference on Statistical Physics of Quantum Systems "novel orders and dynamics"* (Sendai, Japan, July 2004), *Journal of the Physical Society of Japan Supplements* **74**, 30 (2005).

[ACTI-5] A. Honecker, D. C. Cabra, M. D. Grynberg, P. C. W. Holdsworth, P. Pujol, J. Richter, D. Schmalfuss, and J. Schulenbug, *Ground state and low-lying excitations of the spin-1/2 XXZ model on the kagome lattice at magnetization 1/3*, *Proceedings of the International Conference SCES 04*, *Physica B* **359** (2005).

[ACTI-6] S. Capponi, *Effective Hamiltonian approach for strongly correlated systems*, *Proceedings of the Jean-Paul Malrieu symposium* (Lagrasse, France, May 2004), *Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta)*, **116**, 524 (2006).

[ACTI-7] S. Capponi, *Numerical Contractor Renormalization applied to strongly correlated systems*, *Proceedings of the Conference on "Effective models for low-dimensional strongly correlated systems"* (Peyresq, France, Septembre 2005), *AIP Conference Proceedings*, **816**, 16 (2006).

[ACTI-8] T. Sakai and D. Poilblanc, *Polaronic effect in lightly doped High-T_c Cuprates*, *Proceedings of the 24th International Conference on Low Temperature Physics* (LT24, Orlando, Florida, USA, 10-17 August 2005), *AIP Conference Proceedings* **850**, 553 (2006).

[ACTI-9] A. F. Albuquerque, F. Alet, P. Corboz, P. Dayal, A. Feiguin, S. Fuchs, L. Gamper, E. Gull, S. Gürtler, A. Honecker, R. Igarashi, M. Körner, A. Kozhenikov, A. Läuchli, S. R. Manmana, M. Matsumoto, I. P. McCulloch, F. Michel, R. M. Noack, G. Pawlowski, L. Pollet, T. Pruschke, U. Schollwöck, S. Todo, S. Trebst, M. Troyer, P. Werner, and S. Wessel (The ALPS collaboration), *The ALPS project release 1.3: open source software for strongly correlated systems*, in *Proceedings of the 17th International Conference on Magnetism* (Kyoto, Japan, 20-25 August 2006), *Journal of Magnetism and Magnetic Materials* **310**, 1187 (2007).

[ACTI-10] S. Capponi, C. Lacroix, O. Le Bacq, A. Pasturel, and M. D. Núnez-Regueiro, *Valence bond state in the delafossite $YCuO_{2.5}$*, *Proceedings of the International Conference on Highly Frustrated Magnetism* (Osaka, Japan, August 2006), *Journal of Physics: Condensed Matter*, **19**, 145233 (2007).

[ACTI-11] K. Totsuka, P. Lecheminant, and S. Capponi, *A unifying approach to unconventional orders in frustrated spin systems*, *Proceedings of the 17th International Conference on Magnetism ICM2006* (Kyoto, Japan, August 2006), *Journal of Magnetism and Magnetic Materials*, **310**, 1355 (2007).

[ACTI-12] A. Honecker, D. C. Cabra, H.-U. Everts, P. Pujol, and F. Stauffer, *Magnetization plateaux in the classical Shastry-Sutherland lattice*, *Proceedings of the International Conference HFM2006*, *Journal of Physics : Condensed Matter* **19**, 145249, (2007).

[ACTI-13] P. Lecheminant, P. Azaria, E. Boulat, S. Capponi, G. Roux, and S. R. White, *Trionic and quartetting phases in one-dimensional multicomponent ultracold fermions*, *Proceedings of the First Workshop on "State of the Art in Nuclear Cluster Physics"* (Strasbourg, France, May 2008), *International Journal of Modern Physics E*, **17**, 2110 (2008).

[ACTI-14] M. Raczkowski, M. Capello, and D. Poilblanc, *Unidirectional charge instability of the d-wave RVB superconductor*, *Proceedings of the European Conference Physics of Magnetism 2008* (Poznan, Poland, 24-27 June 2008), *Acta Physica Polonica* **115**, 77 (2009).

[ACTI-15] M. Moliner, D.C. Cabra, A. Honecker, P. Pujol, and F. Stauffer, *Finite-temperature ordering in a two-dimensional highly frustrated spin model*, Proceedings of the International Conference *HFM2008*, Journal of Physics: Conference Series **145**, 012053, (2009).

Information et Chaos Quantiques

[ACTI-16] F. Lignières and B. Georgeot, *The asymptotic structure of the p-modes frequency spectrum in rapidly rotating stars*, in *Proceedings of the HELAS Workshop 2008, "Interpretation of Asteroseismic Data"* (2008).

Physique Statistique des Systèmes Complexes

[ACTI-17] S. N. Majumdar, D. S. Dean, and P. L. Krapivsky, *Understanding search trees via statistical physics*, in *Proceedings of the 22nd IUPAP International Conference of Statistical Physics – STATPHYS 22* (Bangalore, India, 4-9 July 2004), *Pramana-Journal of Physics* **64**, 1175 (2005).

[ACTI-18] M. Metaiche and J. Palmeri, *Ion Retention by Nanofiltration: Modelling of Experimental Data by Nanoflux*, in *the Proceedings of the International Forum on Water - Resources, Technologies and Management in the Arab World, Including the 2nd Forum on Water Desalination and Purification Technology Outlook for the Arab World and Non-Governmental Organizations* (Sharjah, United Arab Emirates, 8-10 May 2005), p. 45 (2005).

[ACTI-19] M. Metaiche and J. Palmeri, *Optimisation multi-critères par algorithmes génétiques du design des réseaux d'osmose inverse*, in *Proceedings du Colloque International sur l'optimisation et les systèmes d'information - COSI'07* (Oran, Algeria, 11-13 June 2007), p. 349 (2007).

[ACTI-20] J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Molecular dynamics study of ion partitioning and transport in nanoporous membranes*, in *the Proceedings of Engineering with Membranes 2008* (Algarve, Portugal, 25-28 May 2008), available on CD (2008).

[ACTI-21] J. Palmeri, N. Ben Amar, H. Saidani, and A. Deratani, *Process modeling of brackish and seawater nanofiltration*, in *Proceedings of the MDIW08 Conference (Membranes in Drinking Water Production and Wastewater Treatment)* (Toulouse, France, 20-22 October 2008), paper 277 (available on CD) (2008).

[ACTI-22] M. Metaiche and J. Palmeri, *Development of optimization software of RO systems for water desalination: 'DesaltOp'*, in *the Proceedings of the 3rd International Conference on Water Resources and Arid Environments* (Riyadh, Saudi Arbia, November 2008), p. 31 (2008).

[ACTI-23] M. Metaiche and J. Palmeri, *Optimisation membranaire dans les installations d'osmose inverse sous Desaltop*, in *the Proceedings de la 2ème Journée scientifique sur le traitement et la réutilisation des eaux - JSTRE'08* (Blida, Algeria, 11 March 2008), p. 7 (2008).

[ACTI-24] P. H. Chavanis, G. De Ninno, D. Fanelli, and S. Ruffo, *Out of equilibrium phase transitions in mean-field Hamiltonian dynamics*, in *Proceedings of the Conference on Chaos, Complexity and Transport* (Marseille, France, 5-9 June 2007), p. 3 (2008).

[ACTI-25] P. H. Chavanis, *Generalized Keller-Segel models of chemotaxis. Analogy with nonlinear mean-field Fokker-Planck equations*, in *Proceedings of the Conference on Chaos, Complexity and Transport* (Marseille, France, 5-9 June 2007), p. 256 (2008).

Systèmes de Fermions Finis – Agrégats

[ACTI-26] G. Bousquet, P. M. Dinh, J. Messud, É. Suraud, M. Baer, F. Fehrer, and P. G. Reinhard, *Dynamics of metal clusters in contact with a rare gas substrate: a hierarchical model*, in *Proceedings of Recent Progress in Many-Body Theories – RPMBT14* (Barcelona, Spain, July 2007), *World Scientific, Series on Advances in Quantum Many Body Theories* **11**, Singapore (2008).

[ACTI-27] M. Baer, F. Fehrer, P. G. Reinhard, P. M. Dinh, É. Suraud, L. V. Moskaleva, and N. Roesch, *Dynamics of metal clusters: Free, embedded and deposited*, in *Proceedings of ISACC 2007* (Darmstadt, Germany, 19-23 July 2007), *Latest Advances in Atomic Cluster Collisions*, Imperial College Press (2008).

9.5 Oral communications not leading to a conference proceeding

Fermions Fortement Corrélés

[COM-1] S. Capponi, *Numerical COntractor REnormalization method for quantum spin models*, *meeting of the American Physical Society* (Los Angeles, USA, March 2005).

[COM-2] M. Mambrini, *RVB physics of the $J_1 - J_2 - J_3$ Heisenberg antiferromagnet on the square lattice*, *meeting of the American Physical Society* (Los Angeles, USA, March 2005).

[COM-3] S. Capponi, *Numerical effective Hamiltonian approach for quantum magnets*, *workshop on Highly Frustrated Magnets* (La Londe les Maures, France, November 2005).

[COM-4] D. Poilblanc, *Doped 2D frustrated magnets: spin-charge separation and non-conventional superconductivity*, *workshop on Highly Frustrated Magnets* (La Londe les Maures, France, November 2005).

[COM-5] D. Poilblanc, *On charge ordering in cuprate superconductors and STM experiments*, *French local meeting, "Réunion GDR NEEM"* (Batz-sur-Mer, France, 2005).

[COM-6] D. Poilblanc, *The physics of quantum dimer models*, *International Workshop "Moments and Multiplets in Mott Materials"* (KITP, University of California, Santa Barbara, USA, August-October 2007).

[COM-7] D. Poilblanc, *Pairing glue in correlated electron systems*, *2008 Summer Program of the Aspen Center for Physics* (Aspen, USA, 17 August-7 September 2008).

[COM-8] S. Capponi, *Three-Component Fermi Gas in a one-dimensional Optical Lattice*, *ICAM International Workshop on "Emergent Quantum Phenomena from the Nano- to the Macro- World"* (International Institute for Complex Adaptive Matter (ICAM-I2CAM), Institut d'Études Scientifiques de Cargèse, Corsica, France, 6-19 July 2009).

Information et Chaos Quantiques

[COM-9] D. Braun, *Decoherence in the N–spin boson model GdR Information Quantique* (Palaiseau, France, November 2006)

[COM-10] D. Braun, *QED with a tunneling atom*, *APS March Meeting* (New Orleans, USA, March 2008)

[COM-11] D. Braun, *Decoherence-enhanced measurements*, *DAMOP Meeting of the APS* (Charlottesville, USA, May 2009)

Physique Statistique des Systèmes Complexes

[COM-12] P. H. Chavanis, *Relaxation equations for two-dimensional turbulence*, *Workshop on "Interdisciplinary Aspects of Turbulence"* (Tegernesee, Germany, 18-22 April 2005).

[COM-13] N. Destainville, *Single molecule tracking as a tool to unravel the dynamic membrane organization of the μ opioid receptor*, *CECAM Workshop "Biomembrane Organization and Protein Function – From Computation to Experiment"* (Lyon, France, 4-6 April 2005).

[COM-14] J. Palmeri, N. Ben Amar, H. Saidani, and A. Deratani, *Modeling the membrane nanofiltration (NF) of brackish and sea water*, *EuroMed 2006* (Montpellier, France, 21-25 May 2006).

[COM-15] N. Ben Amar, H. Saidani, J. Palmeri, and A. Deratani, *Temperature dependence of water and neutral solutes transport in nanofiltration membranes*, *Euromembrane 2006* (Taormina, Italy, 24-28 September 2006).

[COM-16] P. H. Chavanis, *Kinetic theory of point vortices in two dimensions*, *Conference "Complex Substances in Turbulence"* (Eilat, Israel, 3-8 November 2007).

[COM-17] N. Destainville, *Phases "cluster" de protéines membranaires : un nouveau mécanisme de confinement ?*, *GDR Microscopie fonctionnelle du vivant* (Marseille, France, 2007).

[COM-18] N. Ben Amar, H. Saidani, A. Deratani, and J. Palmeri, *Temperature effect on rejection of neutral and charged solutes by nanofiltration membrane Desal-5 DK*, *Meda Water International Conference on Sustainable Water Management* (Tunis, Tunisia, 21-24 March 2007).

[COM-19] N. Ben Amar, N. Kechaou, R. Ben Amar, J. Palmeri, and A. Deratani, *Traitements membranaires d'effluents de l'industrie textile et dimensionnement d'une unité de nanofiltration – Cas de la SITEX*, *Technologies de Traitement et de Réutilisation des Eaux Résiduaires Industrielles dans les pays du Bassin Méditerranéen* (Jerba, Tunisia, 24-26 May 2007).

[COM-20] M. Manghi, *Fluctuations govern diffusion in lipid membranes: experimental and theoretical study on controlled stacked membranes*, *GDR Physique de la Cellule au Tissu* (Sète, France, 2008).

[COM-21] N. Kechaou, N. Ben Amar, A. Deratani, and J. Palmeri, *Nanofiltration Tertiary Treatment of a Textile Wastewater in a Denim Facility*, *International Symposium on Biotechnology, ProMembrane International Conference* (Sfax, Tunisia, 4-8 May 2008).

[COM-22] P. H. Chavanis, *Kinetic theory of point vortices in two dimensions*, *Meeting "Turbulence and Statistical Mechanics"* (Les Houches, France, 2-6 March 2009).

Systèmes de Fermions Finis – Agrégats

[COM-23] É. Suraud, *Clusters in matrices*, *Workshop IRSIB* (Caen, France, October 2005).

[COM-24] É. Suraud, *Stochastic TDHF*, *Workshop on Nuclear Mean Field Theories* (Saclay, France, January 2006).

[COM-25] P. M. Dinh, *Time-dependent density functional theory in metal clusters*, *Workshop on Nuclear Mean Field Theories* (Saclay, France, January 2006).

[COM-26] É. Suraud, *Deposition of metal clusters on rare gas surfaces*, *International Conference on Clusters at Surfaces* (Warnemuende, Germany, June 2006).

[COM-27] É. Suraud, *Response of embedded metal clusters to a short laser pulse*, *International Conference on Laser Probing LAP2006* (Vienna, Austria, September 2006).

[COM-28] É. Suraud, *Self Interaction Correction (SIC) in Time Dependent Density Functional Theory for clusters and molecules*, *International Workshop on Many Body Open Quantum Systems* (Trento, Italy, May 2007).

[COM-29] É. Suraud, *Response to a short intense laser pulse of clusters and molecules in contact with an environment*, *French-Chinese Workshop on Lasers, FCILA2007* (Lyon, France, June 2007).

[COM-30] É. Suraud, *Time-dependent microscopic description of the irradiation of clusters and molecules*, *International Workshop on Theoretical Developments for Radiation Damage, COST – P9* (Fréjus, France, September 2007).

[COM-31] P. M. Dinh, *Dynamics of metal clusters in contact with a substrate: A hierarchical approach* *International Workshop on Theoretical Developments for Radiation Damage, COST – P9* (Fréjus, France, September 2007).

[COM-32] J. Messud, *Time Dependent Self Interaction Correction*, *Réunion du GDR Agrégats* (Dourdan, France, February 2009).

9.6 Posters in conferences

Fermions Fortement Corrélés

[AFF-1] G. Roux, S. R. White, D. Poilblanc, S. Capponi, and A. Läuchli, *Role of cyclic four-spin exchange in doped two-leg ladders*, poster presented at the *American Physical Society March meeting* (Los Angeles, USA, March 2005).

[AFF-2] S. Capponi, E. Boulat, P. Lecheminant, and P. Azaria, *Phase diagram of $S = 3/2$ Hubbard model in one-dimension*, poster presented at the *Theory of Quantum Gases and Quantum Coherence* (Cortona, Italy, November 2005).

[AFF-3] F. Alet, J. L. Jacobsen, G. Misguich, V. Pasquier, F. Mila, and M. Troyer, *Interacting classical dimers on the square lattice*, poster presented at the *International Summer School Fundamental Problems in Statistical Physics XII* (Leuven, Belgium, August-September 2005).

[AFF-4] S. Capponi, E. Boulat, P. Lecheminant, and P. Azaria, *Phase diagram of $S = 3/2$ Hubbard model in one-dimension*, poster presented at the conference on *Novel theoretical aspects of frustrated spin systems* (Lyon, France, March 2006).

[AFF-5] M. Indergand, A. Läuchli, S. Capponi, and M. Sigrist, *Correlation induced Peierls instabilities in doped frustrated antiferromagnets: "Valence bond solids" away from half-filling*, poster presented at the conference on *Novel theoretical aspects of frustrated spin systems* (Lyon, France, March 2006).

[AFF-6] S. Capponi and F. F. Assaad, *Spin nematic phases in models of correlated electron systems*, poster presented at the conference on *Mobile Fermions and Bosons on Frustrated Lattices* (Dresden, Germany, January 2007).

[AFF-7] S. Capponi, G. Roux, P. Lecheminant, P. Azaria, E. Boulat, and S. R. White, *Molecular superfluid phase in one-dimensional multicomponent fermionic cold atoms*, poster presented at the *Yukawa International Seminar (YKIS) 2007 "Interaction and Nanostructural Effects in Low-Dimensional Systems"* (Kyoto, Japan, November 2007).

[AFF-8] S. Capponi, G. Roux, P. Lecheminant, P. Azaria, E. Boulat, and S. R. White, *Molecular superfluid phase in one-dimensional multicomponent fermionic cold atoms*, poster presented at the *Latsis Symposium 2008 "Bose Einstein Condensation in dilute atomic gases and in condensed matter"* (Lausanne, Switzerland, January 2008).

[AFF-9] S. Capponi, G. Roux, P. Lecheminant, P. Azaria, E. Boulat, and S. R. White, *Molecular superfluid phase in one-dimensional multicomponent fermionic cold atoms*, poster presented at the *BEC2008 "Theory of Quantum Gases and Quantum Coherence"* conference (Grenoble, France, June 2008).

[AFF-10] S. Capponi, G. Roux, P. Lecheminant, P. Azaria, E. Boulat, and S. R. White, *Molecular superfluid phase in one-dimensional multicomponent fermionic cold atoms*, poster presented at the *Low-temperature physics LT25* conference (Amsterdam, Netherlands, August 2008).

[AFF-11] H. Nonne, P. Lecheminant, S. Capponi, G. Roux, and E. Boulat, *Haldane charge conjecture in one-dimensional multicomponent fermionic cold atoms*, poster presented at the *ICAM International Workshop on "Emergent Quantum Phenomena from the Nano- to the Macro- World"* (International Institute for Complex Adaptive Matter (ICAM-I2CAM), Institut d'Études Scientifiques de Cargèse, Corsica, France, 6-19 July 2009).

Information et Chaos Quantiques

[AFF-12] D. Braun, *Reservoir induced entanglement*, poster presented at the *Quantum Information Workshop* (MPIKS Dresden, Germany, September 2005).

[AFF-13] D. Braun, *On multi-qubit decoherence*, poster presented at the *QIPC06 Conference* (Paris, France, January 2006).

[AFF-14] D. Braun, *On multi-qubit decoherence*, poster presented at the *Conference on "Cold Atoms Meet Condensed Matter"* (Dresden, Germany, March 2006).

[AFF-15] D. Braun, *Decoherence in the N–spin boson model*, poster presented at the *GdR Physique Mésoscopique* (La Grande-Motte, France, October 2006).

[AFF-16] F. Lignières, S. Vidal, B. Georgeot, and D. Reese, *Wave chaos in rapidly rotating stars*, poster presented at the *SF2A-2006: Proceedings of the Annual Meeting of the French Society of Astronomy and Astrophysics*; Eds. D. Barret, F. Casoli, G. Lagache, A. Lecavelier, and L. Pagani, p. 479 (2006).

[AFF-17] D. Braun, B. Georgeot, L. Arnaud, A. O. Lyakhov, and C. Bruder, *Quantifying the role of interference in quantum information processing*, poster presented at the *Asian Conference on Quantum Information Science* (Kyoto, Japan, September 2007).

[AFF-18] O. Giraud, J. Martin, and B. Georgeot, *Bipartite entanglement in random pure states and in localized states*, poster presented at the *Asian Conference on Quantum Information Science* (Kyoto, Japan, September 2007).

[AFF-19] D. Braun, B. Georgeot, L. Arnaud, A. O. Lyakhov, and C. Bruder, *Quantifying the role of interference in quantum information processing*, poster presented at the *QIPC Conference on Quantum Information Processing and Communication* (Barcelona, Spain, October 2007).

[AFF-20] D. Braun, B. Georgeot, L. Arnaud, A. O. Lyakhov, and C. Bruder, *Quantifying the role of interference in quantum information processing*, poster presented at the *APS March Meeting* (New Orleans, USA, March 2008).

[AFF-21] O. Giraud, B. Georgeot and D. L. Shepelyansky, *Delocalization transition for the google matrix*, poster presented at the *Workshop "Anderson Localization in Nonlinear and Many-Body Systems"* (Max Planck Institute for the Physics of Complex Systems, Dresden, 16-20 March 2009).

[AFF-22] K. M. Frahm and D. L. Shepelyansky, *Localization in Chirikov typical map*, poster presented at the *Workshop "Anderson Localization in Nonlinear and Many-Body Systems"* (Max Planck Institute for the Physics of Complex Systems, Dresden, 16-20 March 2009).

Physique Statistique des Systèmes Complexes

[AFF-23] J. Palmeri, X. Lefebvre, P. David, and Z. Twardowski, *L'utilisation du logiciel NanoFlux pour modéliser des procédés de nanofiltration dans l'industrie chimique*, poster presented at the *Conférence CFM (Club Français des Membranes) Applications Industrielles des Procédés Membranaires en Chimie et Production d'Énergie* (Lyon, France, 13-14 June 2005).

[AFF-24] N. Ben Amar, H. Saidani, J. Palmeri, and A. Deratani, *Quels paramètres prendre en compte pour la modélisation de l'effet de la température sur les performances en nanofiltration ? Cas des solutés neutres*, poster presented at the *Conférence MEMPRO 3* (Nancy, France, 5-7 April 2006).

[AFF-25] J. Palmeri, X. Lefebvre, N. Ben Amar, H. Saidani, and A. Deratani, *Brackish and seawater nanofiltration (NF) modeling using NanoFlux software*, poster presented at the *AMTA Biennial Conference, Desalination Comes of Age – The Answer for New Supplies* (Anaheim CA, USA, 30 July-2 August 2006).

[AFF-26] A. Deratani, S. Touil, J. Palmeri, S. Tingry, and S. Bouchtalla, *Pertraction of xylene isomers using cyclodextrin-containing membranes: mass transport mechanism and modeling*, poster presented at the *Euromembrane 2006 Conference* (Taormina, Italy, 24-28 September 2006).

[AFF-27] N. Kechaou, N. Ben Amar, R. Ben Amar, A. Deratani, and J. Palmeri, *Sitex effluent treatment by membrane bioreactor*, poster presented at the *First Maghreb Conference on Desalination and Water Treatment* (Hammamet, Tunisia, 7-10 December 2007).

[AFF-28] C. Mauroy, N. Destainville, C. Lebrun, M. Manghi, E. Haanappel, S. Mazères, and L. Salomé, *Diffusion of lipids in stacked supported bilayers*, poster presented at the *Biophysical Society 52nd Annual Meeting* (Long Beach CA, USA, 2-6 February 2008).

[AFF-29] C. Tardin, P. Rousseau, O. Walisko, N. Destainville, M. Chandler, and L. Salomé, *Insights in the transposition mechanism of the bacterial insertion sequence IS911 revealed by Tethered Particle Motion*, poster presented at the *Biophysical Society 52nd Annual Meeting* (Long Beach CA, 2-6 February 2008).

[AFF-30] J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Ion transport at the water/air and water/nanopore interfaces*, poster presented at the *7th Liquid Matter Conference* (Lund, Sweden, 27 June-1 July 2008).

[AFF-31] N. Kechaou, N. Ben Amar, A. Deratani, J. Palmeri, and A. Sghaier, *Coupling of biological treatment and membrane filtration for the recycling of textile wastewater*, poster presented at the *Fourth International Biennial BioVision Alexandria 2008 Conference* (Alexandria, Egypt, 12-16 April 2008).

Systèmes de Fermions Finis – Agrégats

[AFF-32] M. Baer, G. Bousquet, P. M. Dinh, F. Fehrer, P. G. Reinhard, and É. Suraud, *Dynamics of metal clusters in contact with a substrate: A hierarchical approach*, poster presented at the *Twelfth International Conference on the Applications of Density Functional Theory – DFT 2007* (Amsterdam, Netherlands, 26-30 August 2007).

[AFF-33] J. Messud, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Time-Dependent Self-Interaction Correction*, poster presented at the *Twelfth International Conference on the Applications of Density Functional Theory – DFT 2007* (Amsterdam, Netherlands, 26-30 August 2007).

[AFF-34] J. Messud, P. M. Dinh, P. G. Reinhard, and É. Suraud, *Time-Dependent Self-Interaction Correction*, poster presented at the *Réunion du GDR Agrégats* (Giens, France, 8-11 May 2007).

9.7 Books or book chapters

Fermions Fortement Corrélés

[OS-1] S. Capponi, H. D. Chen, F. Alet, and S. C. Zhang, *Effective Hamiltonian for cuprates: Global phase diagram*, *Condensed Matter Theories*, Vol. **19** (Ed. M. Belkacem and P. M. Sève-Dinh), Nova Science Publishers (2005).

[OS-2] D. Poilblanc, *Modelling and simulating strongly correlated fermions*, in *Lectures on The Physics of Strongly Correlated Electron Systems XI, Eleventh Training Course in the Physics of Strongly Correlated Systems* (Salerno, Italy, 2-13 October 2006), edited by Adolfo Avella and Ferdinando Mancini, *AIP Conference Proceedings* **918**, 82 (2007).

[OS-3] A. Alastuey, M. Magro, and P. Pujol, *Physique et outils mathématiques : mêthodes et exemples (Physics and mathematical tools: methods and examples)*, EDP Sciences, collection *Savoirs Actuels* (2008).

[OS-4] F. Alet, *Numerical simulations of quantum statistical mechanics models*, in *Exact Methods in Low-dimensional Statistical Physics and Quantum Computing*, Lecture Notes of Les Houches Summer School 2008, edited by S. Ouvry, J. L. Jacobsen, D. Serban, V. Pasquier, and L. Cugliandolo, Oxford University Press (2009).

[OS-5] D. Poilblanc, *Mobile holes in frustrated quantum magnets and itinerant fermions on frustrated geometries*, in *Highly Frustrated Magnetism*, Lectures from SISSA International School (Trieste, Italy, August 2007), edited by C. Lacroix, and F. Mila, Springer (2009).

Information et Chaos Quantiques

[OS-6] B. Georgeot, *Quantum algorithms and quantum chaos*, *Lectures Notes of the International School of Physics Enrico Fermi 2005 on Quantum Computers, Algorithms, and Chaos*, IOS Press (ISBN: 1-58603-660-2), Delft, NL (2006).

[OS-7] B. Chirikov and D. L. Shepelyansky, *Chirikov standard map*, *Scholarpedia* **3(3)**, 3550 (2008).

[OS-8] D. L. Shepelyansky, *Boris Valerianovich Chirikov*, *Scholarpedia* **3(10)**, 6628 (2008).

Physique Statistique des Systèmes Complexes

[OS-9] H. Chmiel, X. Lefebvre, V. Mavrov, M. Noronha, and J. Palmeri, *Computer Simulation of Nanofiltration, Membranes and Processes*, in *Handbook of Theoretical and Computational Nanotechnology*, Volume 5, edited by Michael Rieth and Wolfram Schommers, pp. 93-214, American Scientific Publishers (2006).

Systèmes de Fermions Finis – Agrégats

[OS-10] P. G. Reinhard and É. Suraud, *Cluster Dynamics in strong laser fields*, in *Time Dependent Density Functional Theory*, Lecture Notes in Physics **706**, Springer, Berlin (2006).

[OS-11] G. Bousquet, P. M. Dinh, J. Douady, F. Fehrer, B. Gervais, É. Giglio, A. Ipatov, P. G. Reinhard, and É. Suraud, *A hierarchical approach for the dynamics of Na clusters in contact with an Ar substrate*, in *Nova Science publishers*, New York, (2008).

9.8 Vulgarization publications

Fermions Fortement Corrélés

[OV-1] C. Proust and D. Poilblanc, *Des champs magnétiques intenses pour sonder les supraconducteurs*, 6 pages, *Images de la Physique 2009* (in press, CNRS, 2009).

Information et Chaos Quantiques

[OV-2] F. Izrailev, A. Lichtenberg, and D. L. Shepelyansky, *Boris Valerianovich Chirikov (obituary)*, *Physics Today* **6**, 67 (2008).

[OV-3] D. L. Shepelyansky (Ed.), *Website dedicated to Boris Chirikov*.

Physique Statistique des Systèmes Complexes

[OV-4] N. Destainville, *Systèmes complexes, physique et biologique*, *Magazine scientifique de l'UPS* **4**, 9 (2005).

[OV-5] P. H. Chavanis and C. Sire, *Mettre de l'ordre dans le chaos*, *Magazine scientifique de l'UPS* **4**, 11 (2005).

[OV-6] L. Salomé, P.-F. Lenne, and N. Destainville, *Membranes biologiques : vers un modèle physique*, *Images de la Physique 2006*, p. 74 (CNRS, 2006).

[OV-7] C. Sire, *La physique hors des sentiers battus (Physics off the beaten track)*, popular talk presented on many occasions since 2005 (*Ouvertures de l'UPS*, *Fête de la Science*, high-schools, high-school teachers, students, public conferences... download the *pdf* version in French or English).

[OV-8] C. Sire, *Histoire de la cosmologie moderne : 13.7 milliards d'années en 60 minutes (History of modern cosmology: 13.7 billion years in 60 minutes)*, popular talk presented on many occasions since 2005 (*Fête de la Science*, high-schools, high-school teachers, students, public conferences... download the *pdf* version in French).

[OV-9] C. Sire, *Borel et von Neumann : deux grands mathématiciens précurseurs de la théorie du poker (Borel and von Neumann: two famous mathematicians pioneering the theory of poker)*, article published on the poker blog of the French daily *Libération* (2007); see also the entry reviewing Ref. [ACL-197].

[OV-10] N. Destainville, M. Manghi, and J. Palmeri, *Quand les physiciens se penchent sur l'ADN*, *Magazine scientifique de l'UPS* **11**, 12 (2007).

Systèmes de Fermions Finis – Agrégats

[OV-11] P. M. Dinh, J. Navarro, and É. Suraud, *Océans et gouttelettes quantiques*, 159 pages (CNRS Éditions, Paris, 2007).

9.9 Books as Editor

Fermions Fortement Corrélés

[DO-1] G. G. Batrouni and D. Poilblanc (Eds.), *Effective models for strongly correlated systems*, *Proceedings of the ESF Exploratory Workshop* (Peyresq, France, 12-16 September 2005), 302 pages, *AIP Conference Proceedings* **816** (2006).

Information et Chaos Quantiques

[DO-2] G. Casati, D. L. Shepelyansky, P. Zoller, and G. Benenti (Eds.), *Quantum Computers, Algorithms and Chaos*, *Volume 162, International School of Physics Enrico Fermi*, 620 pages, IOS Press, Delft, Netherlands (2006).

Physique Statistique des Systèmes Complexes

[DO-3] C. Sire, coeditor of *Images de la Physique*, a yearly magazine edited by CNRS exposing recent trends in physics for non specialists (2002-2007).

Systèmes de Fermions Finis – Agrégats

[DO-4] M. Belkacem and P. M. Dinh (Eds.), *Condensed Matter Theories*, Vol. **19**, Nova Science Publishers (2005).

9.10 Commercial and Open Source softwares

Fermions Fortement Corrélés

[COD-1] F. Alet, *The ALPS project (Algorithms and Libraries for Physics Simulations)*. The ALPS Project is an open source effort aiming at providing high-end simulation codes for strongly correlated quantum mechanical systems as well as C++ libraries for simplifying the development of such code. F. Alet is actively involved in the libraries and applications development.

Information et Chaos Quantiques

[COD-2] K. M. Frahm and D. L. Shepelyansky (Eds.), *Quantware Software Library*. Quantum Numerical Recipes is an Open Source library which contains several software packages enabling simulations of *quantum computer* evolution on *classical computers*.

Physique Statistique des Systèmes Complexes

[COD-3] J. Palmeri, P. David, and X. Lefebvre, *NanoFlux*, Commercial software developed by the Laboratoire de Physique Théorique (LPT-UMR 5152, Toulouse) and the Institut Européen des Membranes (IEM-UMR 5635, Montpellier) under the NanoFlux Project. *NanoFlux Software* is an advanced tool for the prediction and scaling-up of nanofiltration membrane processes (research and development and industrial filtration and separation applications). Three licences were recently sold to Université de Nantes, CEA, and Aker Kvaerner Chemetics (Vancouver, Canada).

9.11 Habilitation thesis to supervise researches

Fermions Fortement Corrélés

[HDR-1] S. Capponi, *Sans titre/no title*, Thèse d'habilitation à diriger des recherches, Université Paul Sabatier (13/12/2005).

Physique Statistique des Systèmes Complexes

[HDR-2] N. Destainville, *Dynamique de flips dans les pavages aléatoires & Dynamique diffusionnelle de récepteurs membranaires (Flip dynamics in random tilings & Diffusional dynamics of membrane receptors)*, Thèse d'habilitation à diriger des recherches, Université Paul Sabatier (29/11/2005).

9.12 PhD thesis completed or in progress

Fermions Fortement Corrélés

[TH-1] G. Roux, *Échelles de spins dopées sous champ magnétique (Doped spin ladders in strong magnetic field)*, PhD thesis, Université Paul Sabatier (01/09/2004-12/07/2007); supervisors: D. Poilblanc and S. Capponi.

[TH-2] A. Abendschein, *Modèles effectifs pour des systèmes magnétiques sous champ (Effective models for spin systems in magnetic field)*, PhD thesis, Université Paul Sabatier (01/10/2005-23/10/2008); supervisor: S. Capponi.

[TH-3] M. Moliner, *Effects of lattice distortions on low dimensional strongly correlated systems (Effets des distortions du réseau sur les systèmes fortement corrélés de basse dimensionnalité)*, PhD thesis, Université de Strasbourg and Université Paul Sabatier (01/09/2004-03/02/2009); supervisors: D. Cabra and P. Pujol.

[TH-4] F. Trousselet, *Modèles contraints classiques et quantiques à deux dimensions (Constrained classical and quantum models in 2D*, PhD thesis, Université Paul Sabatier (01/10/2005-26/06/2009); supervisors: D. Poilblanc and P. Pujol.

[TH-5] D. Charrier, *Modèles effectifs pour les systèmes magnétiques frutsrés (Effective models for frustrated magnetic systems)*, PhD thesis, Université Paul Sabatier (01/09/2005-18/09/2009); supervisors: P. Pujol and C. Chamon.

[TH-6] D. Schwandt, *Théorie RVB des phases magnétiques exotiques (RVB theory of exotic magnetic phases)*, PhD thesis, Université Paul Sabatier (01/10/2008-$\sim$10/2011); supervisor: F. Alet and M. Mambrini.

[TH-7] Y. Iqbal, *Liquides de spins de Dirac dans des antiferro-aimants quantiques frustrés (Dirac spin liquids in quantum frustrated antiferromagnets)*, PhD thesis, Université Paul Sabatier (01/10/2009-$\sim$10/2012); supervisor: D. Poilblanc.

Information et Chaos Quantiques

[TH-8] L. Arnaud, *Étude de l'interférence et de la décohérence en informatique quantique (Study of interference and decoherence in quantum information)*, PhD thesis, Université Paul Sabatier (01/12/2006-15/10/2009); supervisor: D. Braun.

[TH-9] B. Roubert, *Analyse semiclassique en informatique quantique (Semiclassical analysis in quantum information)*, PhD thesis, Université Paul Sabatier (01/10/2007-$\sim$30/09/2010); supervisor: D. Braun.

[TH-10] M. Pasek, *Application des méthodes du chaos quantique aux oscillations d'étoiles en rotation rapide (Applications of quantum chaos semiclassical methods to the oscillations of rapidly spinning stars)*, PhD thesis, Université Paul Sabatier (01/10/2009-$\sim$30/09/2012); supervisors: B. Georgeot and F. Lignières (LATT-OMP).

Physique Statistique des Systèmes Complexes

[TH-11] V. Desoutter, *Étude de deux systèmes dynamiques dominés par des phénomènes entropiques (Study of two dynamical systems dominated by entropic phenomena)*, PhD thesis, Université Paul Sabatier (01/10/2001-4/10/2005); supervisor: N. Destainville.

[TH-12] M. Metaiche, *Optimization of reverse osmosis desalination systems, operating parameters and numerical simulations (Optimisation des systèmes de désalination, paramètres opératoires, et simulations numériques)*, PhD thesis (co-direction), École Nationale Polytechnique d'Alger (Algeria) and University de Montpellier II, France (01/10/2004-15/12/2007); supervisors: A. Kettab and J. Palmeri.

[TH-13] J. Sopik, *Dynamique de marcheurs aléatoires en interaction (Dynamics of interacting random walkers*, PhD thesis, Université Paul Sabatier (01/10/2003-26/06/2007); supervisor: C. Sire.

[TH-14] J. Dweik, *Molecular modeling of membrane transport (Modélisation moléculaire du transport membranaire)*, PhD thesis, University de Montpellier II (01/09/2005-19/12/2008); supervisor: J. Palmeri.

[TH-15] L. Horvath, *Molecular dynamics studies of water, ions, and macromolecules in nanopores (Étude de dynamique moléculaire de l'eau, des ions, et des macromolécules dans des nanopores)*, PhD thesis (co-direction), Université Paul Sabatier and University Babes-Bolyai (Cluj-Napoca, Romania) (01/10/2006-∼10/2009); supervisors: J. Palmeri and T. Beu.

[TH-16] C. Touya, *Diffusion dans des potentiels aléatoires non gaussiens (Diffusion in non-Gaussian random potentials)*, PhD thesis, Université Paul Sabatier (01/10/2006-∼30/09/2009); supervisor: D. S Dean.

[TH-17] T. Portet, *Étude de l'électroperméablisation de vésicules artificiels (Study of the electropermeabilisation of artificial vesicles)*, PhD thesis, Université Paul Sabatier (01/10/2007-∼10/2010); supervisors: D. S Dean and M.-P. Rols (IPBS).

[TH-18] V. Demery, *Modèles physiques pour l'électroperméabilisation des membranes (Physical models of membrane electropermeabilization)*, PhD thesis, Université Paul Sabatier (01/10/2009-∼30/09/2012); supervisor: D. S Dean.

Systèmes de Fermions Finis – Agrégats

[TH-19] F. Mégi, *Étude théorique d'agrégats soumis à des champs lasers intenses (Theoretical study of clusters in intense laser fields)*, PhD thesis, Université Paul Sabatier (01/09/2001-13/06/2005); supervisor: M. Belkacem and É. Suraud.

[TH-20] G. Bousquet, *Modélisation numérique d'agrégats de sodium en matrice d'argon (Numerical modeling of sodium clusters in argon matrices)*, PhD thesis, Université Paul Sabatier (01/10/2004-14/02/2008); supervisor: É. Suraud.

[TH-21] J. Messud, *Correction d'auto-interaction dépendant du temps (Time-dependent self-interaction correction)*, PhD thesis, Université Paul Sabatier (01/09/2007-∼09/2009); supervisor: É. Suraud.

[TH-22] Z. P. Wang, *Time-dependent description of irradiation of organic molecules (Dynamique de l'irradiation de molécules organiques)*, PhD thesis, Beijing Normal University and Université Paul Sabatier (01/09/2006-∼09/2009); Z. P. Wang spent one year in Toulouse for her PhD from 10/2007 to 10/2008; supervisors: F. S. Zhang and É. Suraud.

[TH-23] S. Vidal, *Méthodes hiérarchiques pour la dynamique des agrégats et molécules en contact avec un environnement (Hierarchical methods for the dynamics of clusters and molecules in contact with an environment)*, PhD thesis, Université Paul Sabatier (01/09/2008-∼09/2011); supervisor: P. M. Dinh.

Laboratoire de Physique Théorique
UMR5152 CNRS/Université Paul Sabatier
IRSAMC
118, route de Narbonne
31062 TOULOUSE
+33 (0)5 61 55 75 72 (tél.)
+33 (0)5 61 55 60 65 (fax)
www.lpt.ups-tlse.fr