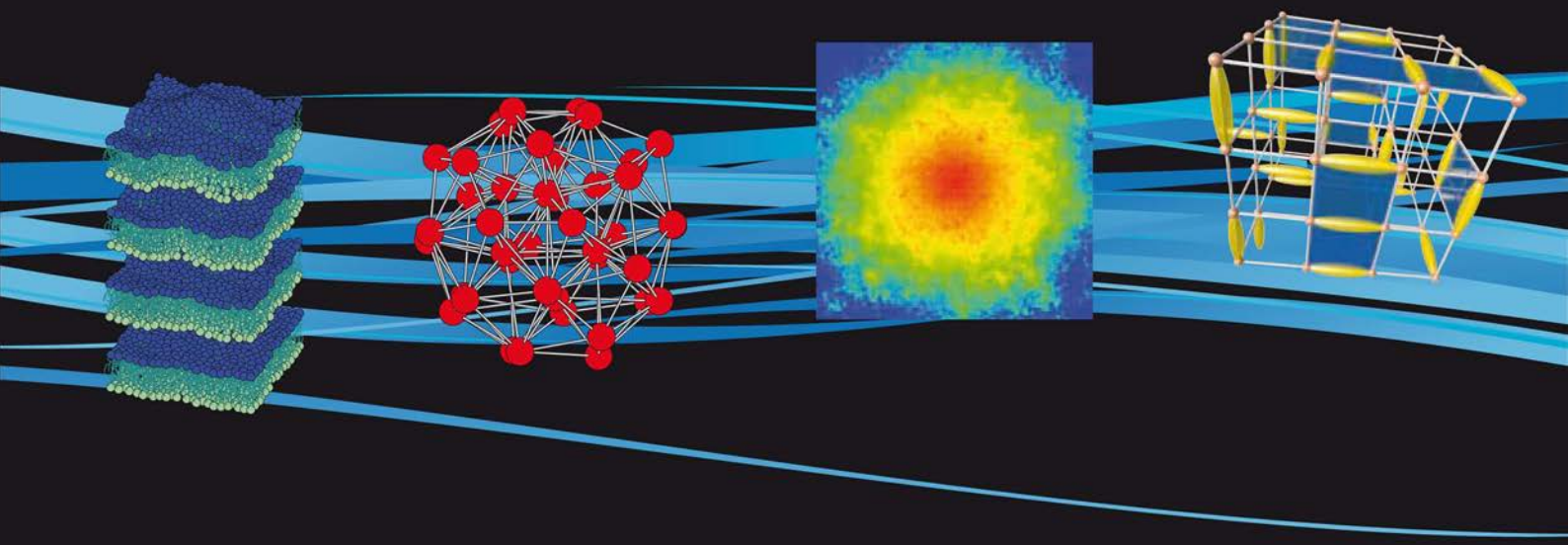
Laboratoire de Physique Théorique



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Scientific Report

Bilan Scientifique

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Contents

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Fermions Fortement Corrélés (FFC)

The treatment of *strong correlations in fermionic systems* is a notoriously difficult task. The current effort undertaken in the FFC group to develop new analytical and numerical tools to tackle these issues adresses 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.

The Strongly Correlated Fermions (FFC) group has a world-wide recognition in numerical techniques thanks to F. Alet, S. Capponi, N. Laflorencie, M. Mambrini and D. Poilblanc. In addition P. Pujol, R. Ramazashvili and A. Petkovic (who has joined the FFC group in 2013) bring a complementary and high-level expertise in analytic techniques. Our scientific activity briefly (and not exhaustively) described below is directly connected to the most active domains of experimental and theoretical research in the field of correlated systems such as frustrated quantum magnets, unconventional and high-T_c superconductors, quantum phase transitions, low-dimensional conductors, topological phases of matter and fractional excitations of novel quantum Hall states, quantum information techniques applied to condensed matter, cold atoms loaded on optical traps, etc.

1.1 Mott insulators, quantum magnets and disordered systems

Key words: *magnetic frustration, valence bond physics, dimer models, magnetization plateaus, impurities and disorder*

Low-dimensional quantum spin materials: effect of dimensionality, frustration and magnetic field

(i) Ladder systems— Ladder materials represent a quite interesting family of systems where low dimensionality can strongly enhance the effect of quantum fluctuations and induce novel states of matter. Part of the activity of the group has focused on clean or doped spin ladders [29, 35, 36, 48, 53, 62, 80], in some cases directly related to real materials, such as $BiCu_2PO_6$ [16, 21, 53, 92] where frustration plays a major role. In particular, a non-trivial competition between frustration-induced incommensurate short range correlations and dimer crystallization, revealed using numerical approaches (exact diagonalization and DMRG) [53], was recently confirmed experimentally [1].

Another non-trivial effect which has been studied concerns the influence of ring-exchange in spin ladder systems [62, 80], relevant for several cuprates materials, such as La_2CuO_4, or $SrCu_2O_3$.

1. K.-Y. Choi, J. W. Hwang, P. Lemmens, D. Wulferding, G. J. Shu, and F. C. Chou, Phys. Rev. Lett. **110**, 117204 (2013).

(ii) Field-induced Bose-Einstein condensation in quantum spin systems— Quite remarkably, gapped antiferromagnets can experience the exact analog of a Bose-Einstein condensation upon the application of an external magnetic field [2]. This has been intensively studied for the frustrated bilayer compound $BaCuSi_2O_6$ [18, 55, 90] where a geometric frustration between adjacent bilayers leads to a frustrated proximity effect which induce a vanishing of the 3D coherence of the condensate. A direct comparison between theoretical calculation and NMR experiments performed at LNCMI has also be done, directly in collaboration with the experimental group [90]. It revealed a more complicated situation where the perfect frustration is slightly broken, thus leading to a strongly reduced, but non zero 3D coherence. The collaboration with the NMR group is still quite active, focusing now on disorder effects leading to a possible intermediate Bose-glass phase in related materials.

Note also that we have studied other aspects of field-induced bosonic physics in spin-gapped antiferromagnets, such as the emergence and the possible stabilisation of a supersolid state [57], as well as a triplon condensate for a spin-$\frac{3}{2}$ AKLT model on the honeycomb lattice studied using PEPS [89].

(iii) Magnetization plateaus— Plateaus in the magnetization curve is an issue that has been the subject of many theoretical and experimental investigations in the last years. Most of the time (although not always), those plateaux are of purely quantum mechanical origin, but one may find some precursor effects in classical systems. These effects are closely related to the well known phenomenon of Order By Disorder (OBD). We have investigated some examples [19, 93] of classical systems in which OBD is responsible not only of the selection of a preferred collinear spin configuration but it also plays the role of the origin of a pseudo-plateau.
Ideal magnetization plateaus are mostly present in quantum systems at zero temperature. One dimension has been for many years the most convincing laboratory to study such phenomena simply because analytical techniques such a bosonization are applicable and some numerical techniques such as DMRG are the most powerful. We have extended this study by showing that the presence of doping shifts and splits the location of the plateau in the magnetization curve [43]. We have also shown in a study of a spin tube that frustration may give rise to a very interesting phenomenology of gapless non-magnetic degrees of freedom in the plateau regime where precisely the magnetic degrees of freedom are gapped [61].

We have also recently addressed the issue of magnetization plateaus in spin-1/2 Heisenberg model on the kagomé lattice which is known to be highly frustrated. Using approximate or exact localized magnon eigenstates, supplemented by large-scale Exact Diagonalizations, we are able to describe in a similar manner the plateau states that occur for magnetization per site $m = 1/3$, 5/9, and 7/9 of the saturation value [81].

Frustration in two-dimensional quantum magnets

It is well-known that magnetic frustration (either geometric or induced by longer-range exchange couplings) can destabilize the standard Néel order and thus give rise to novel phases going from non-magnetic valence-bond crystals (that break some lattice symmetries) to quantum spin liquid (which do not break any symmetry). Our group has a long-standing expertise in this field, including many results as well as the development of new tools, that we will now illustrate.

2. *Bose-Einstein condensation in quantum magnets*, V. Zapf, M. Jaime, and C. D.Batista, Rev. Mod. Phys. **86**, 563 (2014).

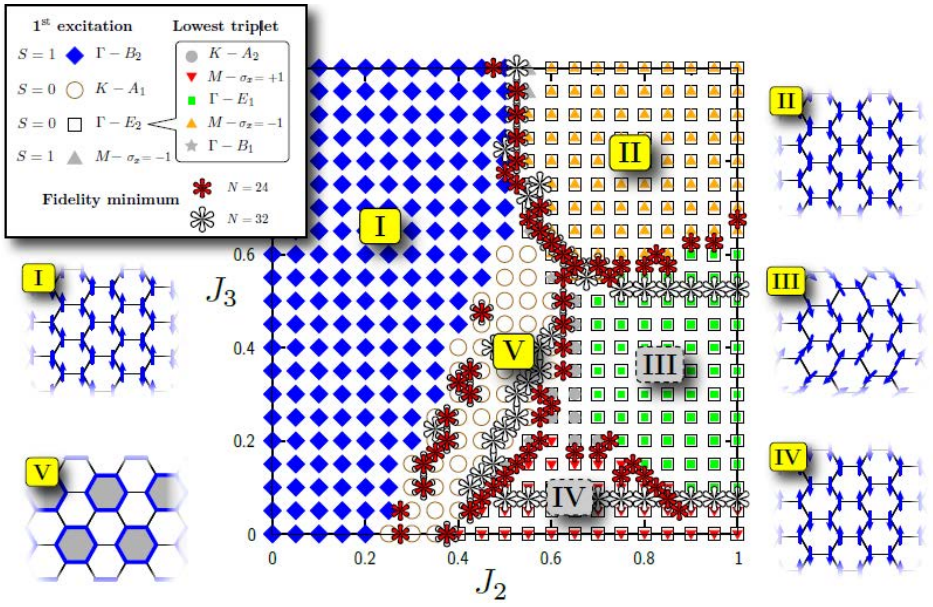

Figure 1.1 : *Phase diagram of the frustrated Heisenberg model on the honeycomb lattice vs J_2 and J_3 which are the next- and next-next-nearest neighbors exchanges. [41]*

Using a variety of numerical techniques (including Exact Diagonalisation in full basis and in the restricted non-orthogonal NNVB basis), supplemented by other analytical approaches allowing to derive effective models [34], we have provided a rather detailed description of the phase diagram of a *frustrated Heisenberg model on the honeycomb lattice* (see Fig. 1.1). While the non-frustrated case displays standard Néel order, we have shown that frustration can lead to the formation of a Valence Bond Crystal which is non-magnetic but breaks some lattice symmetries [41]. The transition between these two states could potentially be second-order as claimed from the deconfined criticality scenario (see next paragraph) and in contradiction with standard Ginzburg-Landau arguments. Moreover, there remains also the possibility to stabilize a real spin liquid state, which does not break any symmetry at all, such as the one proposed for the Hubbard model [3], although more recent numerical work has challenged its stability [4].

Another well-known problem is the *spin-1/2 Heisenberg model on the kagomé lattice* which ground-state is still highly debated. First, using a low-energy effective model, we have proposed a new type of possible ground-state: a chiral spin-liquid (i.e. translation invariant spin singlet state) that breaks point-group symmetry [78]. Alternatively, the spin-1/2 Heisenberg model on the kagomé lattice (possibly with a next-NN interaction) has been studied using Gutzwiller-projected wavefunctions supplemented by variational Monte Carlo (VMC) simulations. The tight competition between Valence Bond Crystals with fairly large unit cells (up to 36 sites) [49, 67], topological $\mathbb{Z}_2$ spin liquids [51] and the algebraic (Dirac) spin liquid [83] has been investigated in great details.

Deconfined quantum criticality

Ten years after the surprising prediction of Senthil *et al.* [5], large-scale quantum Monte Carlo simulations [6] of quantum spin systems with competing interactions have confirmed that a quantum phase transition is possible between two "incompatible" states of magnetic matter in two dimensions: antiferromagnetism and Valence bond

3. Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad, and A. Muramatsu, Nature (London) **464**, 847 (2010).
4. S. Sorella, Y. Otsuka, S. Yunoki, Scientific Reports **2**, 992 (2012); F. F. Assaad and I. Herbut, Phys. Rev. X **3**, 031010 (2013).
5. T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Science **303**, 1490 (2004).
6. see *e.g.* A.W. Sandvik, Phys. Rev. Lett. 104, 177201 (2010)

crystals. Using the magnetic texture induced by non-magnetic impurities as a probe to this physics (in the same vein as NMR experiments, see below), we could indeed determine [27, 39] that such an unusual quantum phase transition takes place on the square lattice. In a more recent development, we showed [76] that the deconfined criticality scenario also applies on the honeycomb lattice: this is even more surprising as the field-theoretical arguments are clueless on the relevance of tripled monopole events, which could render the transition first-order (as the Landau theory of phase transitions would predict). Our simulations indicate that triple-monopole events are also irrelevant, even though they are probably very close to marginality as can be seen in unusual anisotropy effects close to the transition.

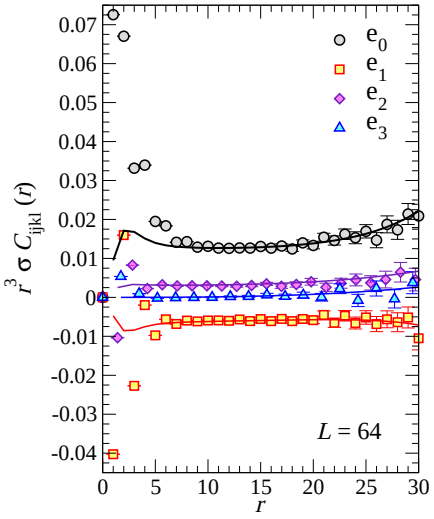

Figure 1.2 : *Singlet-Singlet (four-point) correlation functions of the 3d nearest-neighbor RVB wave-function exhibit a dipolar behavior, as exemplified by the r^3 rescaling (y-axis) and the angular dependence on different lattice directions. [59]*

RVB wave-functions

About 40 years ago, Anderson proposed the appealing Resonating Valence Bond (RVB) picture for describing quantum spin liquids, non-magnetic states that do not break any symmetry down to the lowest temperature. We have revisited this question [31, 59] by showing that short-range valence bond wave-functions on bipartite lattices are far from being featureless gapped spin liquids, as commonly thought up to now. On the square lattice, while the spin sector is indeed gapped, the spinless sector exhibits power-law singlet-singlet correlations [31], a reminiscence of the classical dimer problem on the same lattice. This indicates that the nearest-neighbor RVB wave-functions hosts a *critical U(1) spin liquid* with a spin gap.

The situation is even more surprising in three dimensions. Large-scale Monte Carlo simulations [59] revealed two counter-intuitive behaviors: first and contrary to the naive expectation, the nearest-neighbor RVB wave-function displays long-range antiferromagnetic order on 3d bipartite lattices! Second, the singlet-singlet correlations are dipolar (with an overall r^{-3} decay, see Fig. 1.2), in a surprising analogy with the Coulomb phase physics present *e.g.* in spin ice. This new hybrid state of matter therefore displays aspects of both antiferromagnetism and of emergent magnetostatics: Coulomb meets Néel.

Generalized quantum dimer models

Frustrated bi-dimensional quantum antiferromagnets are characterized by the emergence of very exotic magnetically disordered states at low temperature such as resonating valence-bond (RVB states), VB crystals (VBC), or spin liquids. From a theoretical point of view these systems are particularly hard to treat with traditional approaches. For example the well known route consisting in (i) identifying a well-controlled limit (classical limit, unperturbed limit,...) and (ii) introducing quantum fluctuations and/or corrections to this limit in a putatively perturbative way fails for both steps : because of frustration the classical limit is highly degenerate and often not fully understood, and quantum fluctuations generally do not act as a small perturbation on the classical limit.

On the other hand, many numerical studies suggest that the low energy physics of these systems can be efficiently captured using short range VB states. Once this manifold of state is identified, we built a general framework to project microscopic Hamiltonians, typically the Heisenberg model, into this manifold and use the resulting effective models (Generalized Quantum Dimer Models, GQDM) as a starting point to understand the ground state properties. Such a frame-

work, first initiated by Rokhsar and Kivelson [7] in a different context, has been put [11, 32, 34, 41] on a formal basis and greatly extended, providing a versatile and systematic expansion scheme to deal with frustrated magnets. We used it in conjunction with numerical techniques to characterize ground states and properties of archetypal frustrated models such on the square [11], kagome [32, 34] and honeycomb lattice [41]. An extension was proposed to study the problem of non magnetic impurities on the kagome lattice [37].

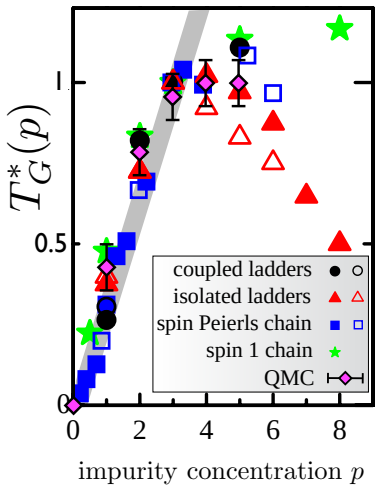

Figure 1.3 : *Universal transition temperatures vs. impurity concentration p for various doped low-d spin-gapped systems: coupled ladders $Bi(Cu_{1-p}(Zn\ ou\ Ni)_p)_2PO_6$; isolated ladders $Sr(Cu_{1-p}(Zn\ ou\ Ni)_p)_2O_3$; Haldane chains $Pb(Ni_{1-p}Mg_p)_2V_2O_8$; spin-Peierls chains $Cu_{1-p}(Zn\ ou\ Ni)_pGeO_3$. Full (open) symbols correspond to nonmagnetic (magnetic) impurities. All data, rescaled by their value at $p = 3\%$, compare well to QMC.*

Impurities and disorder effects in quantum magnets and bosonic systems

Disorder and impurities can deeply modify the physical properties of strongly correlated materials, in particular new localized degrees of freedom are expected to dominate the low energy physics.

(i) Non-magnetic impurities in correlated materials— In constant interaction with experiments, a large variety of effects has been investigated regarding non-magnetic impurities in interacting quantum systems. In particular, Raman spectra of the Shastry-Sutherland antiferromagnet $SrCu_2(BO_3)_2$ doped with nonmagnetic impurities [4]; NMR and μSR responses in doped ladders $BiCu_2PO_6$ [16, 21, 92] (Fig. 1.3); NMR spectra in the spin chain cuprate $Sr2CuO_3$ [17]; Néel ordering mechanism in doped graphene sheets [22].

A precise and quantitative understanding of impurities (either intrinsically present or explicitly added) in such correlated interacting systems is firstly crucial in order to interpret and guide experimental studies. Furthermore it can also lead to new theoretical insights, as shown for instance in Fig. 1.3 where a universal mechanism for impurity-induced long-range ordering is demonstrated, or in the example of deconfined quantum criticality described above.

(ii) Disordered bosonic systems— One of the most spectacular manifestations of the interplay between quantum effects and disorder is provided by Anderson localization. For noninteracting particles, Anderson localization is by now well understood and has been experimentally tested [8]. The situation is considerably more complex when interactions are present. Interacting bosons generically form a superfluid state, but in the presence of disorder it can get converted into an insulating (but still compressible) Bose glass, as studied for interacting bosonic chains [109] and ladders [54] using various analytical (bosonization, two-loop renormalization group) and numerical (DMRG and QMC) tools.

For higher dimension, experimentally relevant for disordered superconducting films [94], superfluidity is more robust against randomness but eventually disappears at large enough disorder, as shown using spin wave theory [91, 105], where spin-wave like excitations gets localized by disorder.

7. D. S. Rokhsar and S. A. Kivelson, Phys. Rev. Lett. **61, 2376 (1988).**
8. *50 years of Anderson localization*, A. Lagendijk, B. van Tiggelen, and D. Wiersma, Physics Today **62**, 24 (2009).

1.2 Quantum Information tools for Condensed Matter systems

Key words: *Entanglement entropies and spectra, fidelity, tensor networks, bipartite fluctuations, participation spectroscopy*

The fields of quantum information theory and of condensed matter have increasingly intertwined over the last few years. On one hand, concepts of quantum information such as entanglement, fidelity or concurrence have shed new light on how to apprehend low-energy states of typical condensed matter systems. One very clear outcome in that direction is the creation of new algorithms (or better understanding of existing ones) to simulate condensed matter systems: we can for instance mention the efficient algorithms based on Tensor Networks (TN) including Matrix Product States (MPS) in 1D, Time Evolving Block Decimation techniques, not to forget DMRG. On the other hand, typical condensed matter methods (such as Monte Carlo methods) have also been adapted to compute entanglement properties of such low-lying states, allowing to scrutinize new physical concepts (such as area law or topological entanglement properties). We have used such techniques (in particular QMC and TN methods) to study entanglement or fidelity properties of quantum antiferromagnets and other condensed matter systems.

Fidelity susceptibility

Fidelity is a fundamental notion in quantum information theory, which quantifies how a message encoded in a wave function $|\Psi_{\rm ini}\rangle$ is well transmitted into another wave-function $|\Psi_{\rm out}\rangle$ through a quantum communication procedure: it is simply the overlap $F = |\langle\Psi_{\rm ini}|\Psi_{\rm out}\rangle|$. The overlap is a frequent tool in condensed matter to measure the quality of a variational wave-function or even more simply in Anderson's orthogonality catastrophe. Since a few years, this concept was adapted to quantum phase transitions controlled by an external parameter. The idea is to simply compute the overlap between ground-states wave-functions for two (close) values of the control parameter. Close to the critical point, we expect a sudden drop of fidelity as the two ground-states on both sides of the transitions are physically different.

This original way of detecting a quantum phase transition is unfortunately difficult to operate from a practical point of view, as we do not know the ground-states in general. We have shown how to compute fidelity and its susceptibility χ_F efficiently with QMC and applied it to lattice quantum models [23, 34]. For instance, a very clear divergence of χ_F signals the quantum phase transition occurring at $h_c \simeq 3.04$ for the 2d Ising model in transverse field, and also allows to determine some critical exponents.

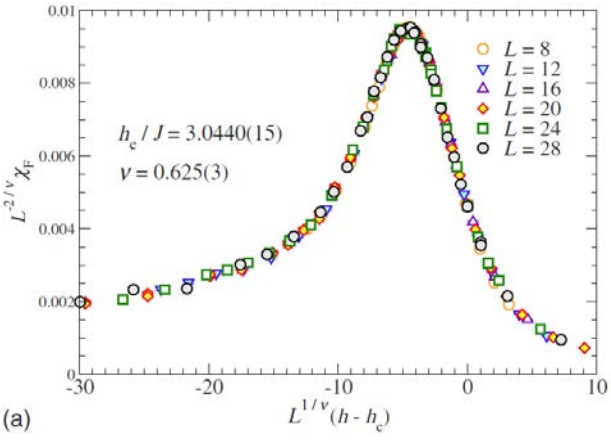

Figure 1.4 : *Data collapse of the fidelity susceptibility χ_F close to the critical point for the 2d transverse field Ising model for different system sizes.*

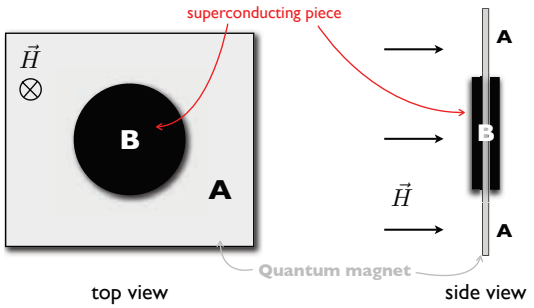

Figure 1.5 : *Meissner screen proposed to extract the fluctuation of the magnetization within a subregion A. The superconducting device is placed on top of the quantum antiferromagnet (on region B) so that the Meissner effect will induce $h_B = 0$ in the antiferromagnet whereas $h_A = H$.*

Contrary to approaches based on symmetry breaking, here *we do not need to provide the order parameter or the relevant correlation function* to detect the transition: fidelity directly detect the phase transition at the wave-function level. This approach is of course superfluous for the transverse field Ising model (which physics is well understood) but is particularly interesting for phase transitions without order parameter or symmetry breaking (such as spin liquids or topological phase transitions). Moreover, as we discussed, the finite-size scaling of χ_F directly provide ν, even though we did not specify the corresponding correlation length!

Entanglement and bipartite fluctuations

For quantum systems where globally conserved quantities, such as particle number $\hat{N}$ or spin $\hat{S}^z$, fluctuate within subsystems, the bipartite fluctuations of such U(1) charges can be nicely related to the bipartite entanglement entropy [56, 73, 72, 111]. In particular, for free fermions an exact correspondence has been found [73], thus opening very nice perspectives to directly measure the entanglement entropy in mesoscopic systems such as quantum point contacts. The direct measurement of subsystems fluctuations of magnetization for quantum antiferromagnets is also a very promising perspective, as proposed in Refs. [56, 73] where a Meissner screen device was suggested, see Fig. 1.5

Several other developments have then been made, first regarding the improved estimate of the Luttinger parameter for interacting quantum liquids, leading to a very precise way to numerically detect quantum critical points in 1D (and also in 2D) [72]. More recently, these ideas have also been applied to quantum Hall states [111].

Entanglement spectra and Tensor Network techniques: application to topological liquids

In many physical scenarios, close relations between the bulk properties of quantum systems and theories associated with their boundaries have been observed. In a pioneering work[9], it was suggested that the *"entanglement spectrum"* (a presentation of the Schmidt decomposition coefficient of a sub-system analogous to a set of "energy levels") of a $\nu = 5/2$ Fractional Quantum Hall State share many common features with the exact (edge) excitations. More recently, the entanglement spectrum (ES) of gapped two-leg quantum Heisenberg ladders on a periodic ribbon (partitioned into two identical periodic chains) was shown to closely reflects the low-energy gapless spectrum of each individual edge [36] (see also [47]), extending the existence of a direct correspondence between the low-energy ES and the true (edge) spectrum to the field of quantum magnetism.

In fact, duality mapping between the bulk of a quantum spin (or correlated electron) system and its boundary can be made much more precise using Projected Entangled-Pair States (PEPS), a form of 2D TN represented in Fig. 1.6, providing a full "holographic framework" for the study of quantum many-body systems via their boundary. This duality associates to every region a Hamiltonian on its boundary, in such a way that the ES of the bulk corresponds to the excitation spectrum of the boundary Hamiltonian [50]. We find that a gapped bulk phase with local order corresponds to a boundary Hamiltonian with local interactions, whereas critical behavior in the bulk is reflected on a diverging interaction length of the boundary Hamiltonian.

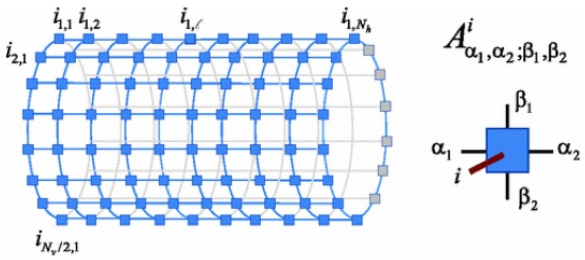

Figure 1.6 : *Typical cylindrical geometry used to investigate quantum magnets and topological phases of matter. The corresponding PEPS ansatz is obtained by replacing each lattice site with a tensor A and contracting the virtual indices α and β along the horizontal and vertical directions. Taken from Ref. [50].*

We applied the PEPS techniques to investigate many-body states with long-range topolog-

9. Hui Li and F. D. M. Haldane, Phys. Rev. Lett. **101**, 010504 (2008).

ical order. We established relations between different gapped $\mathbb{Z}_2$ liquids, the toric code state, the orthogonal dimer state, and the $SU(2)$ singlet RVB state on the kagome lattice [68]. By making use of disconnected topological sectors in the space of dimer lattice coverings, we explicitly derived (orthogonal) "minimally entangled" PEPS RVB states [66] (see also [87] for gapless spin liquids) and extracted the correlation lengths of the elementary topological excitations – the spinon and the "vison" [88]. We also showed how topological order in a system can be identified from the structure of the PEPS transfer operator [84] and subsequently used these findings to analyze the structure of the boundary Hamiltonian: We found that in a topological phase, the boundary Hamiltonian consists of two parts: A universal *nonlocal* part which encodes the nature of the topological phase and a non universal part which is local and inherits the symmetries of the topological model.

Lastly, we constructed 2D PEPS breaking a continuous $U(1)$ symmetry in order to describe magnetic "superfluids" [89] or charged RVB superconductors [107].

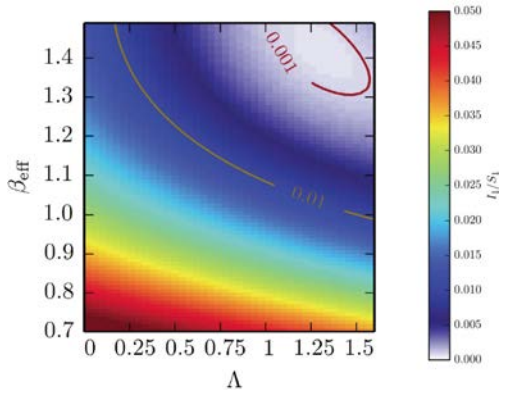

Figure 1.7 : *Location of minima in the difference between participation spectra of the true system and a potential entanglement boundary Hamiltonian. It provides optimal entanglement temperature ($\beta_{\rm eff}$) and parameter (here Λ) of the boundary Hamiltonian. Taken from Ref. [106].*

Shannon-Réyni entropies and participation spectra

The study of the statistics of the coefficients of a wave-function expanded in a given basis has a long history in physics, notably to understand localization phenomena in disordered systems. Recently, this approach has received a second breath by considering the so-called Shannon-Rényi (or "participation") entropies of ground-states of *pure* condensed-matter systems. Consider the expansion in a basis $\{|i\rangle\}$ of the ground-state wave-function $|\Psi_0\rangle = \sum_i a_i|i\rangle$, and define the "participation" of basis state $|i\rangle$ by $p_i \equiv |a_i|^2$. Recent work (review in Ref. [106]) had shown that universal information on the ground-state is contained in the scaling of participation entropies $S_q = \frac{1}{1-q}\ln\sum_i p_i^q$ with the number of particles (or spins etc) N in the system.

We have developed new quantum Monte Carlo techniques [96] that allows to compute participation entropies S_q as well as the spectrum $\{\epsilon_i = -\ln p_i\}$, on much larger systems than previously possible. Using these techniques on a variety of quantum spin models, we found that quantum critical points, discrete and continuous symmetry breaking can be detected and characterized in a universal fashion by subleading terms in the scaling of participations entropies [96, 98], as well as the form of the participation spectrum [98].

While similar looking, participation and entanglement entropies are clearly different quantities: the participation entropies quantify localization in a given Hilbert space basis while von Neumann-Rényi entropies quantify entanglement between parts of a system. We could establish nonetheless [106] that a precise study of participation spectra allows to discriminate entanglement boundary Hamiltonians (see before and Fig. 1.7). Moreover, we also showed that the measurement of entanglement entropies in quantum Monte Carlo can be greatly improved by considering the behavior of participation entropies [110].

Overall, this set of studies provides first steps to establish *participation spectroscopy* [106] as a new type of theoretical spectroscopy to identify and characterize condensed-matter ground-states.

1.3 Correlated electrons, ultra-cold atoms and topological matter

Key words: *unconventional superconductors, , spin-orbit coupling, symmetry-protected topological phases, non-Abelian anyons, cold atom simulators*

Antiferromagnetic conductors

Antiferromagnetism is widespread in materials with interesting electron properties. Chromium and its alloys, numerous borocarbides, electron- and hole-doped cuprates, iron pnictides, and various organic and heavy fermions compounds all have an antiferromagnetic state present in their phase diagram. The physics of these antiferromagnetic phases has been a subject of active research.

In a series of papers [12, 13, 14, 38], we developed the theory of a fundamental yet largely overlooked phenomenon in the electron magnetism of antiferromagnetic conductors: a conspiracy between antiferromagnetic ordering and the crystal symmetry turns the Zeeman coupling into a spin-orbit interaction. This phenomenon leads to a number of spectacular effects such as peculiar structure of Landau levels, electric excitation of spin resonance and more. Precise predictions have been made, and are awaiting experimental verification.

Another part of this work touches upon high-temperature superconductivity in copper oxides, where recent experiments appear to have detected signs of a "hidden" order in the mysterious underdoped region of the phase diagram. This region is adjacent to the parent (undoped) antiferromagnetic state of cuprates, and thus antiferromagnetic correlations are likely to play a role in the "hidden" ordering. In the Ref. [69], we showed how peculiarities of the Zeeman spin-orbit coupling in an antiferromagnetic state may allow, through magnetic quantum oscillations experiments, to draw precise conclusions concerning the electron structure of the underdoped state, including the location of the carrier pockets in the Brillouin zone.

We continue to investigate "hidden" order in the cuprates in collaboration with Dr. Imam Makhfudz, who has been a post-doctoral researcher at the LPT since late 2013. This work is carried out in close interaction with Dr. Cyril Proust and his coworkers at LNCMI Toulouse and with Dr. David Le Boeuf at LNCMI Grenoble.

Doped dimer models

A very important question in the field of frustrated magnetism and some of the low-energy effective theories like the quantum dimer model is the role of doping. Doping can be achieved in some Mott insulator materials, for instance, by chemical substitution (or by applying a magnetic field, in which case "hole" mimic spinons polarized along the field). When holes are electric charge carriers, an important issue is the conducting properties of the doped state. To answer this question, it is essential to know the statistical nature of the holes. Indeed, if holes are bosons, they could Bose-condense (unless a "gauge" interaction prevents it) and give rise to a superconducting phase without invoking Cooper pairs. We have shown that basically any 2D doped quantum dimer model (DQDM) in which holes behave as fermions is equivalent to another dual dimer model, in which hole are bosons [65]. This rigorous result establishing equivalence classes between models helped to classify the phase diagrams of DQDM on non-frustrated and frustrated lattices [82].

Superconductivity in the t–J model and beyond

The search for superconductivity in the 2D Hubbard model – or its strong-coupling t–J model analog – is a long-standing (unresolved) issue originally triggered by the famous discovery of high-temperature superconductivity in cuprate perovskites (Bednorz and Müller 1987 Nobel Prize in Physics). This investigation is complicated by the emergence of several competing phases close in energy such as the stripe phase (involving charge ordering) seen both experimentally and in the above-mentioned theoretical models. We have tackled this hard problem by following several routes, making significant progress.

First, using projected BCS Gutzwiller wave function (using Renormalized Mean-Field or Monte Carlo sampling to evaluate observables),

we found the emergence of spontaneous modulations in the d-wave superconducting RVB phase at 1/8-doping. Half-filled charge domains separated by four lattice spacings are found to form along one of the crystal axis leading to modulated superconductivity with out-of-phase d-wave order parameters in neighboring domains [9], consistently with observed patterns of unidirectional domains in some high-T_c superconductors. Using similar numerical techniques, the spatial extent of the wave-function of a non-magnetic impurity in a d-wave high-temperature superconductor was accurately determined [8]. In the presence of magnetic frustration stabilizing a valence-bond solid at half-filling, we showed the system evolves under doping into novel phases characterized by superconductivity coexisting with the underlying valence-bond solid order [10].

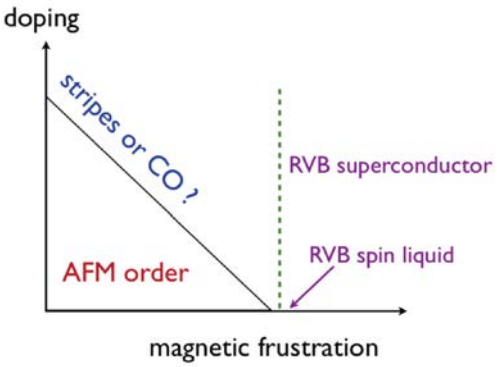

Figure 1.8 : *Schematic phase diagram of an antiferromagnetic Mott insulator as a function of doping and magnetic frustration. Taken from Ref. [107].*

More recently, we are re-visiting this topic using more powerful Tensor Network techniques (see above). We construct a family of simple fermionic projected entangled pair states (fPEPS) on the square lattice which are exactly hole-doped resonating valence bond (RVB) wavefunctions with short-range singlet bonds. Under doping the insulating RVB spin liquid evolves immediately into a *RVB superconductor* [107]. We provide evidence that this scenario is relevant to the frustrated t-J_1-J_2 model (including both nearest and next-nearest neighbor antiferromagnetic interactions J_1 and J_2, respectively) for $J_2 \simeq J_1/2$ (see Fig. 1.8). The orbital symmetry of the optimized RVB superconductor has predominant d-wave character, although we argue a residual (complex s-wave) time reversal symmetry breaking component should always be present in connection with some experimental claims in superconducting cuprates.

Chains of ultracold fermionic atoms

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. It is possible to realize ideal strongly correlated systems thanks to 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, 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.

Ultracold atomic gases also 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.

For a one-dimensional lattice, thanks to powerful analytical and numerical techniques, we have already made several important contributions in this field [3, 20, 28, 42, 45]. For instance, we have considered the general case of half-filled multicomponent fermionic cold atoms and we have exhibited an exact SU(2) symmetry in the charge sector for some parameters [20, 42], which leads to an analogous of the famous Haldane conjecture (that states that half-integer and integer spin chains behave quite differently).

Our latest work on this topic has shown the existence of symmetry-protected topological phases in one-dimensional alkaline-earth cold fermionic atoms with general half-integer nuclear spin I at half filling [79]. Such an en-

larged SU(2I+1) symmetry which depend only on the nuclear spins degrees of freedom has in fact been established *experimentally* with Ytterbium [10]. The main advantage of these systems is the existence of a metastable state close to the ground-state, thus leading to a two-orbital SU(N) Hubbard model with a very rich phase diagram. Clearly, more work should be done along these directions in the near future.

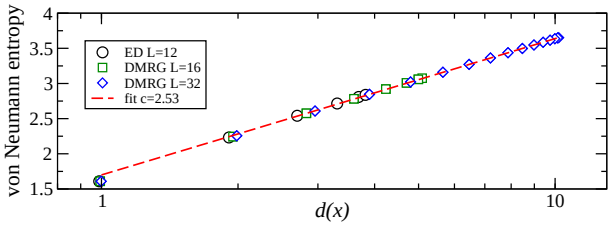

Figure 1.9 : *von Neumann entropy of a SO(5) spin chain as a function of conformal distance $d(x) = L/\pi \sin(\pi x/L)$. The logarithmic increase allows a determination of the central charge $c = 2.5$. [40].*

Finally, let us mention a related project: for spin 3/2 model with only local SU(2) interactions, the Hubbard model has an extended SO(5) symmetry [11] so that in one dimension, its low energy properties can be described in some region by the Heisenberg SO(5) chain. We have mapped out the phase diagram of the bilinear-biquadratic SO(5) chain [40], similar to what has been done for the spin-1 (equivalent to SO(3)) chain, and thus confirming recent conjectures. Most particularly, the Heisenberg point turns out *not* to be in the same phase as the AKLT point, contrary to the spin-1 case, and they are separated by a phase transition characterized by an unusual central charge $c = 5/2$ (see Fig. 1.9).

Excitations with non-Abelian statistics

Anyons are pseudo-particles whose statistics interpolate between the Bose-Einstein and Fermi-Dirac statistics. First studied in the nineties [12], anyons are common features of 2D topological quantum liquids such as the Fractional Quantum Hall state [13]. Statistics is characterized by the representation, often non-Abelian, of the braid group [14] (defining how particle world lines braid around each other - see Fig. 1.10).

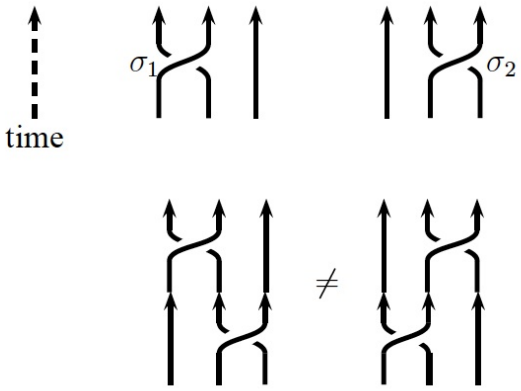

Figure 1.10 : *Elementary braid operations operating on three particle world-lines (top) which do not commute (bottom).*

Following pioneering work by M. Freedman (1986 Fields Medallist) we have constructed effective (low-energy) lattice models of *interacting* non-Abelian anyons and investigated, in anyon chains of unusual central charges ($c = 1/2,\ 4/5\,, 7/10 \cdots$) coupled into "ladders", possible condensations into new topological liquids [46, 48]. Also, we found a fractionalization of the anyons [64, 86] into charge and (neutral) anyonic degrees of freedom – a generalization of spin-charge separation of electrons in Luttinger liquids. An extension of fractionalization of anyons to two-dimensions (very exotic since it does not occur with electrons) is currently investigated by M. Soni (PhD student).

10. S. Taie *et al.* Phys. Rev. Lett. **105**, 190401 (2010).
11. C. Wu, J.-P. Hu, and S.-C. Zhang, Phys. Rev. Lett. **91**, 186402(2003).
12. F. Wilczek, *Fractional Statistics and Anyon Superconductivity*, World Scientific Singapore (1990).
13. G. Moore and N. Read, Nucl. Phys. B **360**, 362 (1991); N. Read and E. Rezayi, Phys. Rev. B **59**, 8084 (1999); For experimental search of non-Abelian statistics see e.g. J.B. Miller, et al., Nature Physics **3**, 561 (2007).
14. C. Nayak et al., Rev. Mod. Phys. **80**, 1083 (2008).

2

Cohérence Quantique (Quantware)

The Quantware team regroups researchers having an expertise in classical and quantum chaos, mesoscopic, many-body physics and complex networks. The group has applied these methods and concepts to different branches of physics with experimental relevance, including in particular quantum information, electron transport at nanoscale, cold atoms, networks of Web, Wikipedia, world trade, games... The group has also been investigating chaos-related problems in quantum optics, atomic physics, condensed matter, and astrophysics.

At present permanent researchers of the Quantware include Klaus Frahm (PR2), Bertrand Georgeot (DR2 CNRS), Gabriel Lemarié (CR2 CNRS) (arrived in February 2012), Ion Nechita (CR2 CNRS) (arrived in October 2010) and Dima L. Shepelyansky (DR1 CNRS, head of the group). During the report period the following group members left the group: Daniel Braun (PR2-PR1) (left in Jan 2014 becoming Prof. at Univ. of Tübingen), Olivier Giraud (CR1 CNRS) (moved in January 2010 to LPTMS Orsay), Robert Fleckinger (PR Emeritus) (complete retirement in 2010). Non permanent staff have included post-docs: L. Ermann (post-doc ANR-CNRS, from Aug 2009 to July 2011), R. Dubertrand (post-doc NEXT-CNRS, from Sept 2012 till present), Y.-H. Eom (post-doc EC FET Open NADINE Oct 2012 - till present) and PhD students: L. Arnaud (UPS Nov 2006 - Dec 2009), B. Roubert (DGA Oct 2007 - Sept 2011), M. Pasek (UPS Oct 2009 - Dec 2012), V. Kandiah (CNRS-Region Midi-Pyrénées Sept 2011 - till present), F. Damon (UPS Oct 2012 - till present).

Since 2009, the Quantware group has been funded by: ANR contracts (ANR-NANO contract *MICONANO* (Dec 2005 - April 2009; partner) and *NANOTERRA* (Jan 2009 - Dec 2012, partner); ANR contracts *RMTQIT* (partner) and *K-BEC Kick Rotor* (2013-2016, partner), grant *OMASYC* from University Paul Sabatier (2011-2013, partner), Labex NEXT grant *ENCOQUAM* (2012-2015, partner), European contracts *EuroSQIP* (Nov 2005 - Oct 2009, partner) and FET Open *NADINE* (May 2012 - April 2015, coordinator), and also smaller contracts (PEPS,PICS...). The Quantware group had two postdoctoral fellowships funded by ANR and Labex NEXT, and one by Europe.

Foreign scientists who have visited the Quantware group for a period of at least one month since Jan 2009 include O. Zhirov (Russian Academy, Novosibirsk), A. Pikovsky (U. of Potsdam), L. Ermann (CNEA Tandar Lab, Buenos Aires), I. Garcia-Mata, (CONICET Tandar Lab, Buenos Aires), R. Belosludov (Inst. for Material Research, Sendai, Japan), J. Martin (Univ. of Liège, Belgium), P. Braun

(Univ. of Essen, Germany), U. MARZOLINO (Univ. of Freiburg, Germany).

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

During the last five years, the QUANTWARE group has published 128 articles in refereed journals and has contributed 72 invited conference talks. The main aspects of the scientific activity of the QUANTWARE group during the 2009-2014 period are highlighted below. Five Quantware highlights are:

- synchronization theory of microwave stabilization of edge transport and zero-resistance states [8];
- spectral properties and emergence of PageRank for web networks of British universities [53];
- determination of entanglement of cultures from top ranked historical figures of multilingual Wikipedia [97];
- results regarding the behavior of the collective spectra of a subspace of random matrices [79];
- quantum chaos with matter waves [63, 85].

For more details, see the personal web pages of the members of the QUANTWARE group.

2.1 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.

Probabilistic techniques in Quantum Information Theory

I. Nechita

The theory of random matrices provides important tools for QIT. It is thus natural that (quantum) probability has applications to the latter field. A longstanding group of conjectures known as "additivity problems" have been central to QIT in the last decade. One of the most spectacular recent results on the additivity problems was Hastings' work showing that the minimal output von Neumann entropy of a quantum channel is not additive, thereby disproving what was the biggest conjecture of the field. Hastings was motivated by the previous work of Hayden and Winter who proved the non-additivity of the minimal output p-Rényi entropy for any $p > 1$. The arguments of these authors are based on random matrices. It is remarkable that even now, there are no *explicit* examples of quantum channels violating these "additivity problems", all known constructions being based on random techniques.

Inspired by Hastings' work, we took a completely different direction in the investigation of the additivity problems [31, 33, 56, 57, 78, 79, 106, 125]. Working in the framework of free probability, we have developed powerful new tools for analyzing spectral behavior of random quantum channels and of their output. Our approach is able to provide much better bounds on both the size of additivity violations, and the dimensions at which violations appear, than other approaches.

The methods we have developed rely on norm estimates that have been obtained by Haagerup and Thorbjornsen, and on graphical calculus for computing average values. The graphical method we use for computing probabilistic quantities, such as entropies of quantum states allows for a better understanding of the abstract representation-theoretical computations. For instance, the Hayden-Winter example is presented in Figure 2.1, where the diagram for the second moment of the output $\mathrm{Tr}(Z^2)$ is drawn. The techniques developed by Collins and Nechita in [33] allow to compute all moments of such random matrices in a graphical way, by expanding the diagrams as sums of permutations, when one takes the expectation value over the random, Haar-distributed, unitary matrix U. This method is a graphical implementation of the Schur-Weyl duality and can be very useful in applications.

Moreover, using different techniques, Nechita

together with Collins and Belinschi [79] obtained results on the "singular value sets" of matrices from subspaces of tensor products which provide the first examples of macroscopic violations for the additivity of the minimum output entropy. This work was a breakthrough in the field, because it allowed, for the first time, to obtain precise results instead of bounds.

We also investigated the set of quantum channels acting on a single qubit [122]. We have provided universal sets of quantum channels for all unital qubit channels as well as for all extremal (not necessarily unital) qubit channels, in the sense that all qubit channels in these sets can be obtained by concatenation of channels in the corresponding universal set. We have also shown that our universal sets are essentially minimal.

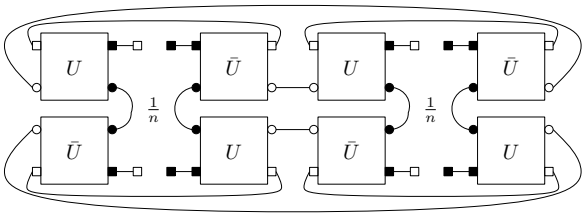

Figure 2.1 : *The graphical representation of the second moment of the output of a product between a random quantum channel Φ^U and its complex conjugate, when presented with a maximally entangled input.*

Besides work in the theory of quantum channels, some very recent results in entanglement theory are revealing free probability as a powerful tool in QIT. The group in Toulouse built on Aubrun's study of the *positive partial transpose* (PPT) property for random quantum states, which showed that the PPT criterion for detecting entanglement is related to a new instance of the famous Semicircle Law from Random Matrix Theory (the analogue of the classical Gaussian distribution in free probability). Nechita, together with Aubrun and Banica [76, 102, 124] showed that there is a deeper connection between the partially transposed random quantum states and freeness, expressing limiting spectral densities of such matrices in terms of free probabilistic objects and operations.

These very recent developments open new routes of inquiry, and one of the future directions of research on the group will be to further investigate connections between random matrices, free probability and quantum information theory.

Entanglement, algorithms

B. Georgeot, D. Braun

Several applications of quantum algorithms have been investigated, in particular optimal quantum circuits for small number of qubits accessible to experimentalists have been constructed [20]. In parallel, in collaboration with Nicolas Destainville of the PhysStat team of the LPT we have built a new algorithm for an exact Monte Carlo sampling, which is faster than classical algorithms, albeit only quadratically [41]. We have also proposed a new implementation of quantum computers using atoms deposited on surfaces and manipulated through Scanning Tunneling Microscopes. The atoms are deposited in such a way as to minimize certain sources of decoherence [39].

The group has also investigated the transfer of quantum information through a spin chain and demonstrated the extreme sensitivity of this transfer on the boundary conditions [38]. We also adapted the concept of classicality of a quantum state from quantum optics to quantum systems with a finite dimensional Hilbert space. We then introduced a measure of non-classicality, based on the distance to the convex set of classical states, which allowed us to identify maximally quantum states. For a large number of particles, these states have much larger geometric entanglement than any other known state before [36, 37, 81]. It is likely that these "Queens of Quantum" will be important for future applications in quantum computing. This approach to measuring the "quantumness" of a state has also clarified the nature of exciton transfer in the Fenna-Matthews-Olson complex during photosynthesis in certain bacteria. In collaboration with researchers in Hamburg (Germany) we showed for the first time clearly that the energy flow is drastically quantum on a biologically relevant timescale [62].

In joint work with Nathan Wiebe from the Institute of Quantum Computing (University Waterloo, Canada) and Seth Lloyd MIT (Cambridge, USA) we have developed a quantum algorithm for a future quantum computer with a

high potential for applications in all of science. The algorithm accelerates exponentially fitting a model to a very large amount of data, in the sense that the quality of the fit for a given model can be assessed exponentially faster than with the best classical algorithm. Once the best model is found, the parameters of the fit can be obtained. This work, published in Physical Review Letters accompanied by a synopsis of the Publishers in "*Physics — spotlighting exceptional research*", saw a very strong interest, and presents one of very few known algorithms with a demonstrated exponential speed-up (under weak assumptions), and follows a very different approach than the famous Shor algorithm for factoring a large integer [82].

Quantum-enhanced measurements:

D. Braun

The idea of "quantum-enhanced measurements" is to use quantum coherence to render conventional measures more sensitive to parameters. For example, with highly entangled quantum states one can in principle reach the Heisenberg limit of accuracy. Unfortunately, these states are almost impossible to produce because of decoherence. But in 2010, it was demonstrated in the group that decoherence itself can be exploited for precision measurements. In a decoherence subspace, decoherence is suppressed due to destructive interference. This interference can be very sensitive to the parameters of the system and therefore allow very precise measurements. Having understood this, we developed a more general scheme using a "quantum bus" for coherent averaging that achieves the Heisenberg limit without using entangled states. The paper was published in Nature Communications [60], led to an article in the CNRS "News", a large number of invited lectures, and substantial interest from experimentalists.

The group also used the formalism of the "quantum Cramer-Rao" bound to calculate the optimal quantum state and the minimum mass that can be measured with nano-mechanical oscillators which have a strong potential as a gas chromatograph or ultra sensitive èèartificial nose" [61].

In another study, the optimal sensitivity for parameter estimation using Gaussian states of light was calculated. These results marked the beginning of a collaboration with Claude Fabre and Nicolas Treps at the Laboratoire Kastler Brossel, in which we found the optimal procedure (in terms of sensitivity) to measure any parameter encoded in multimode Gaussian states of light (including light produced by a laser, but also squeezed states), with the prospect of significant technological impact [111].

With Fabio Benatti (Trieste, Italy) we clarified the role of entanglement for precision measurements using non-distinguishable particles. We demonstrated that one can surpass the standard quantum limit without entanglement in this case [110]. This work continued with a collaboration with Ugo Marzolino who spent three months as an invited CNRS researcher at the LPT and with whom we examined how precisely one can measure in principle temperature and chemical potential of cold bosonic and fermionic gases [112]

2.2 Electron transport at nanoscale

D. L. Shepelyansky

Ratchet transport

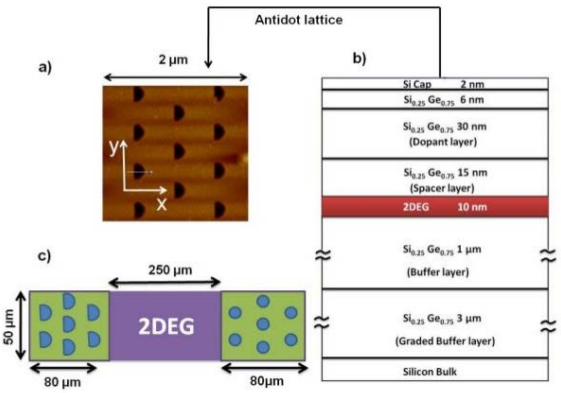

Figure 2.2 : *Semidisk Galton board of antidots experimentally realized by the group of J.-C.Portal, LNCMI, Grenoble (Nanotechnology* **22**, *245401 (2011)) to study the ratchet effect theoretically predicted by Quantware group.*

For systems without spatial inversion symmetry, the appearance of directed flow of parti-

cles 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. 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. 2.2). The theoretical studies predict that the directionality of ratchet flow in such systems can be controlled by the polarization of radiation, which has been confirmed by recent experiments with a semi-disk Galton board for 2DEG in Si/SiGe heterojunctions by the group of Portal.

The theory of ratchet transport of interacting and non-interacting electrons has been developed in [25, 48, 65]. This research is supported by the ANR projects *MICONANO* and *NANOTERRA* coordinated by the group of J.-C. Portal.

Microwave induced zero-resistance states in 2DEG

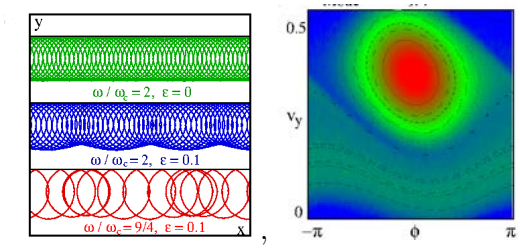

Figure 2.3 : *Left: electron orbits moving along edge in a microwave field, Right: density of orbits trapped in a microwave resonance at $j = 2.25$ (from [8]).*

In 2002-2003, in the experiments of R. Mani and M. Zudov, it was discovered that a weak microwave radiation generates a striking change of resistance of tow-dimensional electron gas in high mobility samples. The microwave field creates almost zero-resistance states when the ratio of microwave frequency to synchrotron frequency takes values $j = 1.25, 2.25, 3.25, ...$ Since that time a large number of theoretical explanations has been proposed. A recent review of experimental and theoretical works is given by *I. A. Dmitriev et al.* Rev. Mod. Phys. **84**, 1709 (2012). Similar effects have been observed for electrons on surface of liquid helium in presence of microwave field at RIKEN, Tokyo by (*D.Konstantinov et al.* Jour. Phys. Soc. Japan **81**, p.093601 (2012).

In [8, 94], we develop a synchronization theory for the dynamics of two dimensional electrons under a perpendicular magnetic field and microwave irradiation showing that dissipative effects can lead to the synchronization of the cyclotron phase with the driving microwave phase at certain resonant ratios between microwave and cyclotron frequencies. We demonstrate two important consequences of this effect: the stabilization of skipping orbits along the sample edges and the trapping of the electrons on localized short ranged impurities. We then discuss how these effects influence the transport properties of ultra high mobility two-dimensional electron gas and propose mechanisms by which they lead to microwave induced zero resistance states. Our theoretical analysis shows that the classical electron dynamics along edge and around circular disk impurities is well described by the Chirikov standard map providing an unified formalism for those two rather different cases. We argue that this work will provide the foundations for a full quantum synchronization theory of zero-resistance states for which a fully microscopic detailed theory still should be developed.

Thermoelectricity of Wigner crystal in a periodic potential

The properties of Wigner crystal in a periodic potential have been studied in [50, 68]. For a case of snaked nanochannels it is shown that conductivity is characterized by a conducting sliding phase at low charge densities and an insulating pinned phase above a critical charge density. The transition between these phases has a devil's staircase structure typical for the Aubry transition in dynamical maps and the Frenkel-Kontorova model.

In [99] we study numerically the thermoelectricity of Wigner crystal placed in a periodic potential and being in contact with a thermal

bath modeled by the Langevin dynamics. At low temperatures the system has sliding and pinned phases with the Aubry transition between them. We show that in the Aubry pinned phase the dimensionless Seebeck coefficient can reach very high values of several hundreds. At the same time the charge and thermal conductivity of crystal drop significantly inside this phase. Still we find that the largest values of ZT factor are reached in the Aubry phase and for the studied parameter range we obtain $ZT \leq 4.5$ (see Fig. 2.4). We argue that this system can provide an optimal regime for reaching high ZT factors and realistic modeling of thermoelectricity.

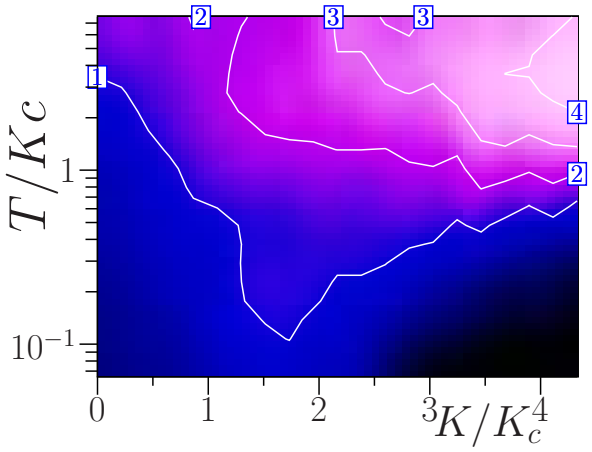

Figure 2.4 : *Dependence of figure of merit of thermoelectricity ZT on rescaled amplitude of potential K/K_c and temperature T/K_c, shown by color changing from $ZT = 0$ (black) to maximal $ZT = 4.5$ (light rose) (from [99]).*

2.3 Anderson localization, interactions and nonlinearity

D. L. Shepelyansky

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 asymptotically large times appear in the literature. The active interest for the interplay of nonlinearity and localization has been much fostered by recent experimental studies with Bose-Einstein condensates (BEC) in optical lattices and nonlinear photonic lattices.

In [1, 4, 5, 51, 69, 98, 119], 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 $\Delta n^2 \propto t^\nu$. The numerical values of ν are found to be approximately $0.3 - 0.4$ for the dimension $d = 1$ in satisfactory agreement with the theoretical estimate $\nu = d/(3d + 2)$ for dimension d. The emergence of dynamical thermalization, characterized as an ergodic chaotic dynamical state with a Gibbs distribution over the modes [5, 98]. The exponent ν has been measured in BEC experiments in optical lattice which found approximate value of $\nu \sim 0.4$ (LENS group at Florence *E. Lucioni et al.* Phys. Rev. Lett. **106**, 230403 (2011)). Certain links with the Kolmogorov turbulence flow in finite systems are discussed in [69].

2.4 Quantum multifractality

B. Georgeot

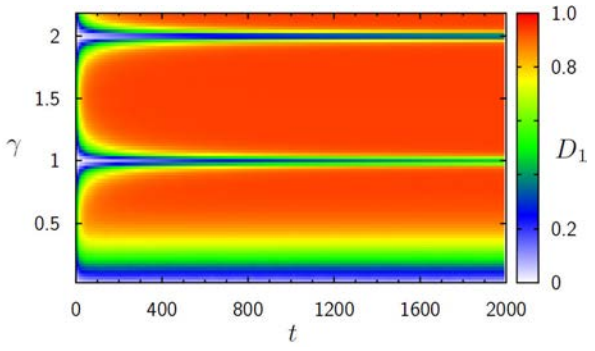

Figure 2.5 : *Multifractality as a function of parameter and time t for a wavepacket of a quantum map. Colors denote multifractality strength from white (strong) to red (weak). (from [87]).*

Several models where quantum wave functions display multifractal properties have been recently identified. In the quantum chaos field, they correspond to pseudo integrable systems. In condensed matter, they include electrons in

a disordered potential at the Anderson metal-insulator transition. These multifractality properties lead to particular transport properties and appear in conjunction with specific types of spectral statistics. In parallel, progress in experimental techniques allow to observe finer and finer properties of the wavefunctions of quantum or wave systems, as well as to perform experiments with unprecedented control on the dynamics of the systems studied.

The group has studied these multifractal states in great details, through a combination of extensive numerical studies on paradigmatic models and analytical techniques, within a long-standing collaboration with colleagues in Argentina, Belgium and Orsay (O. Giraud, formerly at LPT, and former LPT postdocs having obtained permanent positions abroad). It has been possible to characterize the entanglement present in such states [17] and to build efficient quantum algorithms enabling to compute the multifractality of quantum states [18]. More recently, we have studied systematically the difference between the multifractality of dynamical models and disordered systems, and shown that differences did exist between these two types of multifractal systems [42]. We also concentrated on the possibility to observe experimentally this multifractality. Indeed, although many theoretical studies have been devoted to quantum multifractality, it has been difficult to observe it in a real setting. There are technical questions related to the high resolution needed to explore different scales in the wave function, but fundamentally it is of critical importance to assess to what extent multifractality survives in a real experimental setting. To explore this question, we have studied the dynamics of wave packets, much more common in experiments than eigenfunctions studied by most theoretical works, and shown that they display a form of multifractality weaker than for the eigenfunctions, but clearly related [87] (see Fig. 2.5). We have also investigated the destruction of multifractality by a perturbation, and shown that this process is universal, following two separate scenarios with different experimental consequences [126].

2.5 Chaos and cold atoms

Theoretical proposal of time reversal of Bose-Einstein condensates in kicked optical lattices has been realized experimentally by *A. Ullah and M. D. Hoogerland* Phys. Rev. E **83**, 046218 (2011).

B. Georgeot, D. L. Shepelyansky

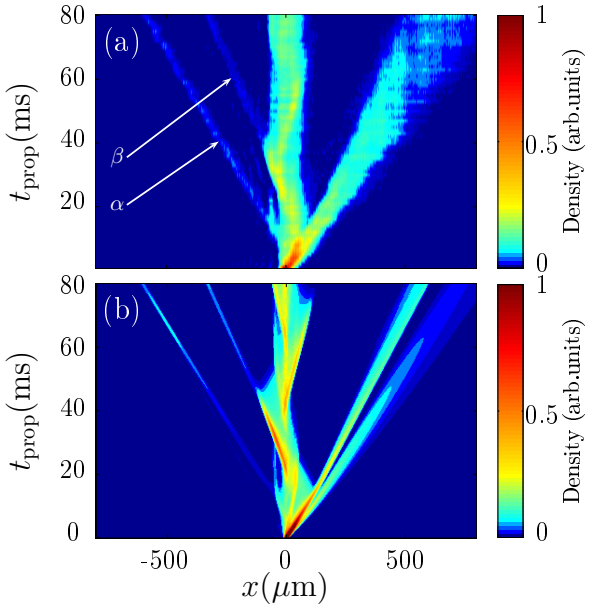

Figure 2.6 : *a) Measured density distribution of the wavepacket for different propagation times, showing the tunable tunnel barriers from where parts of the wave function (α and β) can leak. b) Theoretical prediction for a wavepacket whose velocity distribution matches the experimental one. (from [113]).*

We are collaborating with the experimental group of David Guéry-Odelin in the LCAR in Toulouse on studying atom lasers in presence of defects. Such systems are very versatile, since the defect potential, created by a laser beam crossing the guiding beam of the atoms, can be engineered very precisely. The scattering theory for such systems was developed in [40]. In [64], it was demonstrated that quantum chaos effects can be observed with atom lasers, opening new possibilities for the simulation of quantum systems. In [85], it was shown that chaotic effects can be harnessed in order to realize a beam-splitter for atoms, opening new technological possibilities to

atomic optics, an achievement which gave rise to research highlights in *Physics*, *Nature Physics*, and *Nature Photonics*. At last, in [113], we have shown that it is possible to use optical lattices of varying depth to construct spatial gaps which act as tunable tunnel barriers which can reach regimes out of reach for conventional setups. All these works mix theoretical studies with direct experimental implementations (see an example in Fig. 2.6).

2.6 Google matrix of complex networks

K.M. Frahm, B. Georgeot, D.L. Shepelyansky

On the scale of the past ten years, modern societies have developed enormous communication and social networks. Their classification and information retrieval becomes a formidable task for the society. Various search engines have been developed by private companies which are actively used by Internet users. Due to the recent enormous development of World Wide Web and communication networks, new tools and algorithms should be invented to characterize the properties of these networks on a more detailed and precise level. It is also highly important to have new tools to classify and rank enormous amount of network information in a way adapted to internal network structures and characteristics. The NADINE project develops new algorithms to facilitate classification and information retrieval from large directed networks, including PageRank and CheiRank with two-dimensional ranking proposed by partners. The Google matrix formed by the links of the network is analyzed by analytical tools of Random Matrix Theory and quantum chaos and by efficient numerical methods for large matrix diagonalization including the Arnoldi method. New tools and algorithms produced by the project will create fundamental basis for developers of new types of search and social media services, which will put Europe on leading positions in this important area. The publications in this research line are [6, 22, 23, 24, 26, 27, 28, 29], [46, 47, 52, 53], [65, 66, 70, 71, 72], [88, 91, 92, 93, 95, 96, 97, 115, 116, 117]. Below we described selected results of this research.

Short definitions for the Google matrix which describes directed networks are given below. A directed link is formed from a node j to a node i when j points to i and an element A_{ij} of the adjacency matrix is taken to be unity when there is such a link and zero in absence of link/ The matrix S_{ij} of Markov transitions on a directed network is constructed from the adjacency matrix $A_{ij} \to S_{ij}$ by normalizing elements of each column so that their sum is equal to unity ($\sum_i S_{ij} = 1$) and replacing columns with only zero elements (*dangling nodes*) by $1/N$, with N being the matrix size. Then, following the work of Brin and Page (1998), the Google matrix of the network takes the form

$$G_{ij} = \alpha S_{ij} + (1-\alpha)/N \ . \qquad (2.1)$$

The damping parameter α in the WWW context describes the probability $(1-\alpha)$ to jump to any node for a random surfer. For WWW the Google search engine uses $\alpha \approx 0.85$. The matrix G belongs to the class of Perron-Frobenius operators, its largest eigenvalue is $\lambda = 1$ and other eigenvalues have $|\lambda| \leq \alpha$. The right eigenvector at $\lambda = 1$, which is called the PageRank, has real nonnegative elements $P(i)$ and gives a probability $P(i)$ to find a random surfer at site i. Due to the gap $1-\alpha \approx 0.15$ between the largest eigenvalue and other eigenvalues the PageRank algorithm permits an efficient and simple determination of the PageRank by the power iteration method which multiplies a random initial vector by G. Due to the spectral gap the process converges to the PageRank after several tens of iterations. A multiplication of a vector by G requires only $O(N)$ multiplications since an average number of links per node is of the order of a few tens for WWW and many other networks. We have seen that at $\alpha = 1$ the largest eigenvalue $\lambda = 1$ is usually highly degenerate due to many invariant subspaces which define many independent Perron-Frobenius operators which provide (at least) one eigenvalue $\lambda = 1$ [53].

Once the PageRank is found, all nodes can be sorted by decreasing probabilities $P(i)$. The node rank is then given by index $K(i)$ which reflects the relevance of the node i. The top PageRank nodes are located at small values of $K(i) = 1, 2, ...$ It is known that the PageRank probability is related to the number of ingoing links, characterizing how popular or known is a

given node. Assuming that the PageRank probability decays algebraically as $P_i \sim 1/K_i^{\beta}$ we obtain that the number of nodes N_P with PageRank probability P scales as $N_P \sim 1/P^{\mu_{in}}$ with $\mu_{in} = 1 + 1/\beta$ so that $\beta \approx 0.9$ for $\mu_{in} \approx 2.1$, in agreement with the numerical data for WWW.

In addition to a given directed network A_{ij}, it is useful to analyze an inverse network with inverted direction of links with elements of adjacency matrix $A_{ij} \to A_{ji}$. The Google matrix G^* of the inverse network is then constructed via corresponding matrix S^* according to the relations for G using the same value of α. The right eigenvector of G^* at eigenvalue $\lambda = 1$ is called the CheiRank giving a complementary rank index K^* of network nodes. The CheiRank probability $P^*(K^*)$ is related to the number of outgoing links highlighting the node communicativity.

Wikipedia network

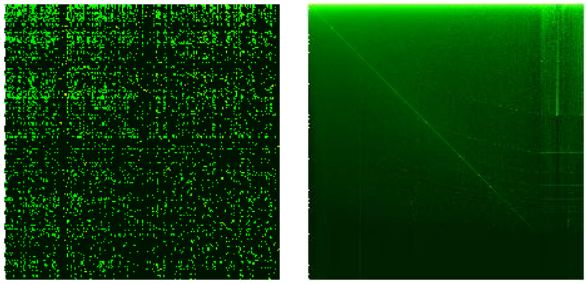

Figure 2.7 : *Google matrix of the network Wikipedia English articles for 2009 in the basis of PageRank index K (and K'): left: top 200×200 elements are shown, right the whole matrix of size $N = 3282257$ is shown in coarse-grained cells 500, color shows the matrix elements from zero (black) to maximum (white) (from [65]).*

In [29] we study network of English Wikipedia. Information retrieval and ranking of Wikipedia articles become the challenge of modern society. While PageRank highlights very well known nodes with many ingoing links, CheiRank highlights very communicative nodes with many outgoing links. In this way the ranking becomes two-dimensional.

Using CheiRank and PageRank we analyze the properties of two-dimensional ranking of all Wikipedia English articles and show that it gives their reliable classification with rich and nontrivial features. Detailed studies are done for countries, universities, personalities, physicists, chess players, Dow-Jones companies and other categories. The matrix elements $G_{K,K'}$ of Wikipedia are shown in Fig. 2.7. The distribution of articles (nodes) over PageRank-CheiRank plane is shown in Fig. 2.8 (for comparison we show this distribution for Linux Kernel network which has qualitatively different structure).

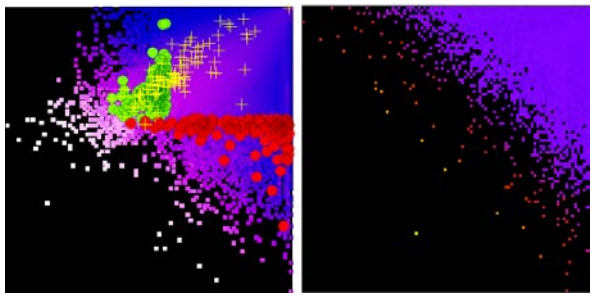

Figure 2.8 : *Density distribution of network nodes shown on the plane of PageRank and CheiRank indexes in log scale for all $1 \le K, K^* \le N$. Left: data for Wikipedia Aug (2009), green/red points show top 100 persons from PageRank/CheiRank, yellow pluses show top 100 persons from Hart's book (from [29]); Right: distribution for Linux Kernel V2.4 (from [65]).*

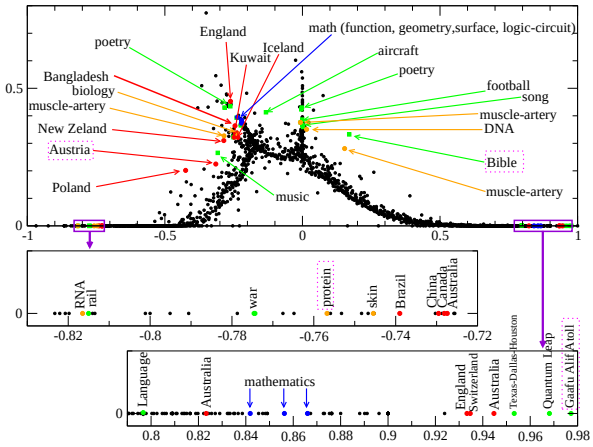

Figure 2.9 : *Complex eigenvalue spectrum of the matrices S for Wikipedia. Highlighted eigenvalues represent different communities of Wikipedia and are labeled by the most repeated and important words following word counting of first 1000 nodes (from [91]).*

In [94] we study the properties of eigenvalues and eigenvectors of the Google matrix of the Wikipedia articles hyperlink network and other real networks. With the help of the Arnoldi method we analyze the distribution of eigenvalues in the complex plane and show that eigenstates with significant eigenvalue modulus are located on well defined network communities. We also show that the correlator between PageRank and CheiRank vectors distinguishes different organizations of information flow on BBC and Le Monde web sites. The spectrum of Google matrix of Wikipedia is shown in Fig. 2.9.

The top historical figures classified from multilingual Wikipedia editions are obtained in [95, 97]. Such an approach allows to understand How different cultures evaluate a person. Is an important person in one culture also important in some other culture? We address these questions via ranking of multilingual Wikipedia articles. With three ranking algorithms based on network structure of Wikipedia, we assign ranking to all articles in 9 (and recently 24, a work for which the preprint has already received an important international media coverage) multilingual editions of Wikipedia and investigate general ranking structure of PageRank, CheiRank and 2DRank. In particular, we focus on articles related to persons, identify top 30 persons for each rank among different editions and analyze distinctions of their distributions over activity fields such as politics, art, science, religion, sport for each edition. We find that local heroes are dominant but also global heroes exist and create an effective network representing entanglement of cultures. The Google matrix analysis of network of cultures shows signs of the Zipf's law distribution. This approach allows to examine diversity and shared characteristics of knowledge organization between cultures. The developed computational, data driven approach highlights cultural interconnections in a new perspective.

Ulam networks and fractal Weyl law

In [22, 24] using the Ulam method proposed in 1960, we show that the fractal Weyl law is valid for the Perron-Frobenius operators of dynamical maps with dissipation or absorption. Such operators effectively generate the Ulam networks which properties are similar to those of Google matrices of various directed networks. According to this law the number of states with eigenvalue modulus $|\lambda|$ in a certain ring (e.g. $0.2 < |\lambda| \leq 1$) scales as $N^{d/2}$ where $d < 2$ is a fractal dimension of underlying set.

The application of this result to the Linux Kernel network [46], generated by procedure calls in the code, shows that the fractal dimension of Linux is approximately 1.3 and is also described by the fractal Weyl law. For the citation network of Physical Review for all years we find $d \approx 1$ [115].

The spectrum of Ulam networks of symplectic and intermittency maps is studied in [23, 28, 66, 93].

Google matrix of the world trade

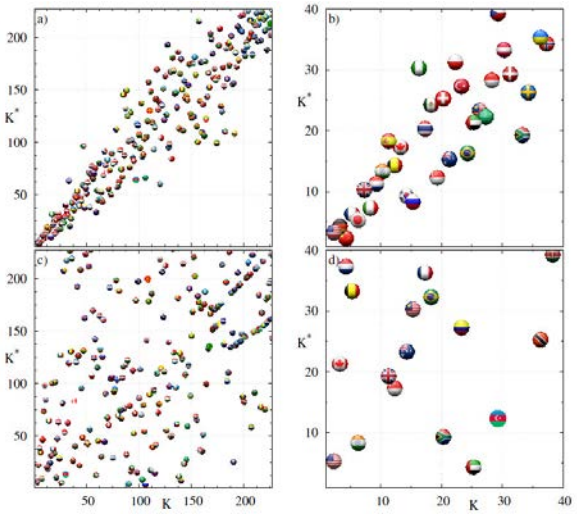

Figure 2.10 : *Country positions in PageRank-CheiRank plane (K, K^*) for world trade in various commodities in 2008. Each country is shown by circle with its own flag. The panels show the ranking for trade in the following commodities:* all commodities (a, b)*; and* crude petroleum (c, d)*. Left panels show a global scale with all 227 countries, while right panels give a zoom in the region of* 40×40 *top ranks. (from [52]).*

In [52], using the United Nations Commodity Trade Statistics Database, we construct the Google matrix of the world trade network and analyze its properties for various trade commodities for all countries and all available years from 1962

to 2009. The trade flows on this network are classified with the help of PageRank and CheiRank algorithms developed for the World Wide Web and other large scale directed networks. For the world trade this ranking treats all countries on equal democratic grounds independent of country richness. Still this method puts at the top a group of industrially developed countries for trade in *all commodities*. Our study establishes the existence of two solid state like domains of rich and poor countries which remain stable in time, while the majority of countries are shown to be in a gas like phase with strong rank fluctuations. A simple random matrix model provides a good description of statistical distribution of countries in two-dimensional rank plane. The comparison with usual ranking by export and import highlights new features and possibilities of our approach. This research is continued in [88].

An example of distribution of world countries on PageRank-CheiRank plane is shown in Fig. 2.10.

Google matrix of DNA sequences

In [92], for DNA sequences of various species we construct the Google matrix G of Markov transitions between nearby words composed of several letters. The statistical distribution of matrix elements of this matrix is shown to be described by a power law with the exponent being close to those of outgoing links in such scale-free networks as the World Wide Web (WWW). At the same time the sum of ingoing matrix elements is characterized by the exponent being significantly larger than those typical for WWW networks. This results in a slow algebraic decay of the PageRank probability determined by the distribution of ingoing elements. The spectrum of G is characterized by a large gap leading to a rapid relaxation process on the DNA sequence networks. We introduce the PageRank proximity correlator between different species which determines their statistical similarity from the view point of Markov chains. The properties of other eigenstates of the Google matrix are also discussed. Our results establish scale-free features of DNA sequence networks showing their similarities and distinctions with the WWW and linguistic networks.

The properties of Poincaré recurrences of DNA sequences are analyzed in [67] (see also related [30]).

Google matrix of the game of go

In [84], a new application of complex networks was constructed. Indeed, the tools of complex networks were never applied to the study of human games. Nevertheless, games represent one of the oldest human activity, and may give insight into the human decision-making processes. In [84, 127], a network was built that describes the game of go, one of the oldest and most famous board games. The complexity of the game is such that no computer program is yet able to beat a good player, in contrast with chess where world champions have been bested by game simulators. We have constructed directed networks of increasing complexity, defining nodes as local patterns on plaquettes of increasing sizes, and links as actual successions of these patterns in databases of real games. We have identified the peculiarities of these networks compared to other types of networks. We have explored the ranking vectors and community structure of the networks and shown that this approach enables to extract groups of moves with common strategic properties. These works led to a press release of the CNRS translated in English, Spanish and Italian, and to several interviews in the media [51, 52, 53]. These studies should help to improve the computer simulations of the game.

2.7 Applications to astrophysics

B. Georgeot, D.L. Shepelyansky

Dark matter chaos in the Solar System and binary systems

In [10, 89] we study the capture of galactic dark matter particles (DMP) in the Solar System produced by rotation of Jupiter. It is shown that the capture cross-section is much larger than the area of Jupiter orbit being inversely diverging at small particle energy. We show that the dynamics of captured particles is chaotic and is well described by a simple symplectic dark map. This dark map description allows to simulate the scattering and dynamics of 10^{14} dark matter particles during the life time of the Solar System and to determine dark matter density profile as a function of distance from the Sun. The mass

of captured dark matter in the radius of Neptune orbit is estimated to be $2 \cdot 10^{15} g$. The radial density of captured dark matter is found to be approximately constant behind Jupiter orbit being similar to the density profile found in galaxies. Example of distribution of DMP density in the Solar System is shown in Fig. 2.11).

In [118], using symplectic map description, we study the capture of galactic DMP in two-body and few-body systems. This approach allows to model scattering of 10^{16} DMP following time evolution of captured particle on about 10^9 orbital periods. We obtain DMP density distribution inside such systems and determine the enhancement factor of their density in a center vicinity compared to its galactic value as a function of mass ratio of bodies and a ratio of body velocity to velocity of galactic DMP wind. We find that the enhancement factor can be of the order of ten thousands.

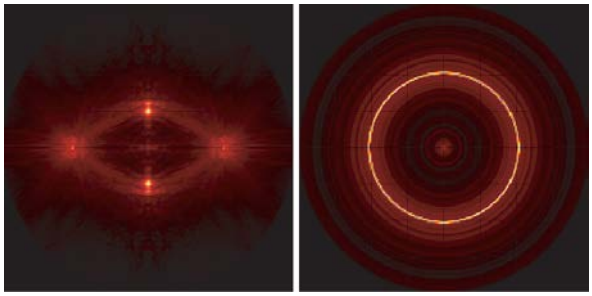

Figure 2.11 : *Density of captured DMP in the Solar System at present time $t_S = 4.5 \times 10^9$ years, shown in the plane perpendicular to Jupiter orbit (left) an in the Jupiter orbit (right) (area of 4×4 Jupiter radius is shown; black is for zero, white is for maximal density) (from [89]).*

This research is done in collaboration with J. Lages and PhD student G. Rollin from the University of Besançon.

Wave chaos in rapidly rotating stars

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.

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.

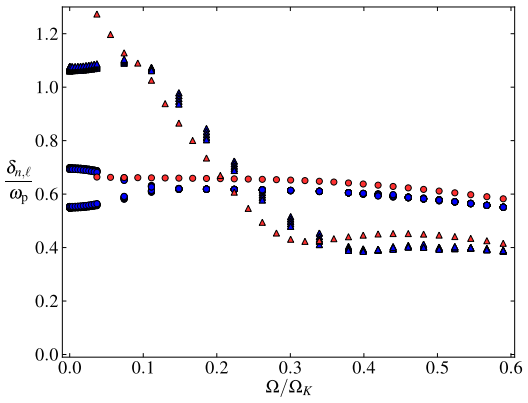

Figure 2.12 : *Comparison of semiclassical theory (red) and numerical simulations of a realistic star model (blue) for two sets of frequency differences in rapidly rotating stars at different rotations Ω (from [86]).*

In [19] we have shown that the tools of quantum chaos enable to shed light on this problem. Indeed, the centrifugal distortion introduces chaotic dynamics on part of the phase space and specific tools are needed to cope with such effects. In particular, it is possible to construct asymptotic theories describing regularities for subsets of modes, those which are localized in stable

phase space regions. Our studies [64, 86] realized in collaboration with astrophysicists from the IRAP in Toulouse have shown that a semi-classical theory enables to predict the frequency distribution of such modes for realistic star models (see Fig. 2.12). In [43], we have tried to extract relevant quantities from synthetic spectra constructed from star models, in order to guide astrophysicists in the understanding of real stellar spectra.

2.8 Experiments based on Quantware theory

The theoretical results obtained by Quantware group initiated a number of experiments listed below:

❍ The theory of chaotic but deterministic ratchet transport in a microwave field [*A. D. Chepelianskii et al.*, Phys. Rev. E **78**, 041127 (2008)] has been investigated and confirmed in experiments of J.-C. Portal group [Nanotechnology **22**, 245401 (2011); Appl. Phys. Lett. **98**, 193505 (2011)].

❍ The theory of microwave induced magnetic moment [*A. D. Chepelianskii and D. L. Shepelyansky* Eur, Phys. J. B **55**, 261 (2007)] has been confirmed in 2DEG experiments *A. D. Chepelianskii and H. Bouchiat*, Phys. Rev. Lett. **102**, 086810 (2009).

❍ The stabilization theory of edge electron transport in a microwave field [8, 94] has been partially confirmed in experiments of Gusev group [*A. D. Levin et al.*, Phys. Rev. B **89**, 161304(R) (2014)].

❍ Loschmidt cooling by time reversal of atomic matter waves proposed by *J.Martin et al.*, Phys. Rev. Lett. **101**, 074102 (2008) has been realized with BEC in kicked optical lattices by *A. Ullah and M. D. Hoogerland*, Phys. Rev. E **83**, 046218 (2011).

❍ The theory of destruction of Anderson localization by nonlinearity [*D. L. Shepelyansky et al.*, Phys. Rev. Lett. **70**, 1787 (1993); **100**, 094101 (2008) has been partially confirmed in BEC experiments of LENS group from Florence [*E. Lucioni et al.*, Phys. Rev. Lett. **106**, 230403 (2011)].

❍ The developed theory of 3d Anderson transition in frequency modulated field [*F. Borgonovi and D. L. Shepelyansky,*, J. de Physique I France **6**, 287 (1996); [119]] has been confirmed in experiments of Garreau's group in Lille [*M.Lopez et al.* New J. Phys. **15**, 065013 (2013)].

❍ The theory of quantum chaotic scattering of cold atoms [40, 64] has been experimentally studied and confirmed in [64, 85, 113].

❍ The ranking of people via network of Wikipedia articles started in [29, 95, 97] (see also this link) is now followed by similar projects *Who is bigger?* at Stony-Brook and *Pantheon* at MIT.

3

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. 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 and proteins, 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 (reaction-diffusion models, 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...).

3.1 Long-range interactions

P.-H. Chavanis

The statistical mechanics of self-gravitating systems is of broad conceptual interest and has applications in different branches of astrophysics and cosmology. It shares numerous analogies with other systems with long-range interactions such as two-dimensional and geophysical turbulence, the chemotaxis of bacterial populations in biology, and toy models introduced in statistical mechanics such as the Hamiltonian Mean Field (HMF) model. We illustrate below this rich topic with a few examples, namely the still mysterious nature of quasi stationary states in systems with long-range interactions (using the HMF model as a prototype), the loss of stability of supernovae in astrophysics, and in the context of self-gravitating canonical gas and two-dimensional turbulence.

Quasi stationary states in the Hamiltonian Mean Field (HMF) model described by polytropic distributions

The HMF model [1] describes the evolution of N rotators coupled through an attractive cosine interaction. The Hamiltonian reads

$$H = \frac{1}{2}\sum_{i=1}^{N} p_j^2 + \frac{1}{2}\sum_{i,j=1}^{N}[1-\cos(\theta_i-\theta_j)], \quad (3.1)$$

where θ_i represents the orientation of the i-th rotator and p_i stands for the conjugated momentum. The HMF model is the simplest system with long-range interactions that one can imagine. Interestingly, it displays many common features with more realistic systems with long-range interactions such as self-gravitating systems and two-dimensional vortices.

For $t \to +\infty$, the distribution function $f(\theta, p, t)$ reaches a statistical equilibrium state described by the Boltzmann distribution. However, at intermediate times, the system gets stuck in a quasi stationary state (QSS) that differs from the Boltzmann distribution. The lifetime of this QSS increases algebraically with the number

1. M. Antoni & S. Ruffo, Phys. Rev. E **52**, 2361 (1995).

of particles, and diverges in the thermodynamic limit. Therefore, the importance of this QSS is considerable since it corresponds to what is observed in practice. For example, in astrophysics, elliptical galaxies are in such non-Boltzmannian QSSs. The prediction of the QSS reached by the system from a given initial condition remains an open problem. It is now well-understood that the evolution of the system towards the QSS is governed by the Vlasov equation which describes a collisionless dynamics. As a result, the QSS is expected to be a stable steady state of the Vlasov equation on a coarse-grained scale. The difficulty is that the Vlasov equation admits an infinite number of steady states so it is difficult to predict the one that is actually selected by the system.

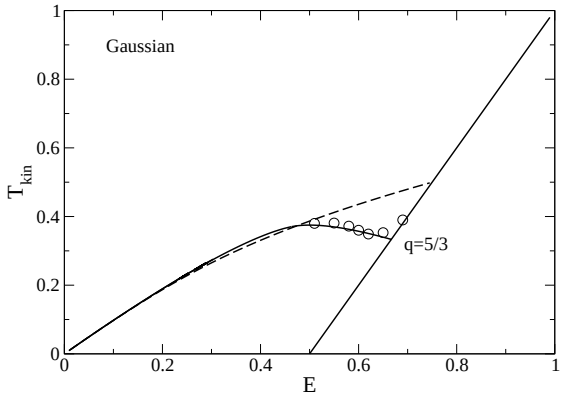

Figure 3.1 : *The numerical caloric curve (bullets) corresponding to Gaussian initial conditions displays a region of negative kinetic specific heat $C_{kin} = dE/dT_{kin} < 0$. It is compared to the theoretical caloric curve of polytropic distributions with index $q = 5/3$ (solid line). The caloric curve corresponding to the Boltzmann or to the Lynden-Bell prediction has a positive specific heat (dashed line) and cannot account for the observations.*

The QSS results from a mixing process in phase space due to purely mean field effects. This corresponds to the phenomenon of nonlinear Landau damping. If mixing is efficient, the QSS can be predicted by Lynden-Bell's theory of violent relaxation [2]. In the context of the HMF model, we have found that this theory provides a good prediction of the QSS in many cases. However, there exist situations in which the system does not mix well (the mixing is not ergodic) so that deviations to the prediction of Lynden-Bell are observed.

In a recent work [104], we have performed a systematic numerical study of the QSS as a function of the initial condition. We have considered different classes of initial conditions, for exemple the case of spatially homogeneous systems with a Gaussian velocity distribution. We have observed numerically that, in many cases, the QSS could be fitted by a polytropic distribution of the form

$$f(\epsilon) = [1 - (q-1)(\beta\epsilon + \alpha)]^{1/(q-1)}, \qquad (3.2)$$

where ϵ is the individual energy of the particles, β a generalized (out-of-equilibrium) inverse temperature, and α a chemical potential. Such distributions are also called q-Gaussians or Tsallis distributions in statistical physics. The index q depends on the class of initial conditions but, for a given class, it takes the same value whatever the total energy E of the system. For exemple, the index corresponding to a Gaussian initial distribution is $q = 5/3$. Using the theory of polytropes developed in [39] it is possible to determine the theoretical caloric curve giving the kinetic temperature T_{kin} as a function of the energy E and to compare this curve with the numerical one. A good agreement is found with the numerical simulations (see Fig. 3.1). **In particular, the theory of polytropes explains the region of negative kinetic specific heats observed numerically**. The observation of this negative specific heat region was the initial motivation to study the HMF model in 1995, and it remained unexplained for a long time.

We have also studied the collisional evolution of the HMF model (beyond the Vlasov regime) due to finite N effets, and we have found numerically that **the system evolves through a sequence of polytropic distributions with a time-dependent index $q(t)$** [104]. This property (that remains mysterious) is valid not only in the homogeneous phase but also in the inhomogeneous phase. Therefore, for specific initial conditions, the whole evolution of the system,

2. D. Lynden-Bell, MNRAS **136**, 101 (1967).

from $t = 0$ to $+\infty$, can be fitted by polytropic distributions with a time dependent index $q(t)$ reaching ultimately $q = 1$ (Boltzmann).

Loss of stability of supernovae and Painlevé I equation

P.-H. Chavanis

Exploding supernovae are not fully elucidated phenomena. The trouble is that the condition of nuclear matter in stars cannot be reproduced on Earth. In a recent study [120] we have provided a new model of supernovae represented as dynamical systems subjected to a loss of stability, just before they explode. This is an original description of supernovae based on the theory of catastrophes. We showed that just before the explosion, the equilibrium state no more exists. Because similar stability loss also occurs in dynamical systems in Nature, this model could be used for predicting natural catastrophes such as earthquakes before they happen.

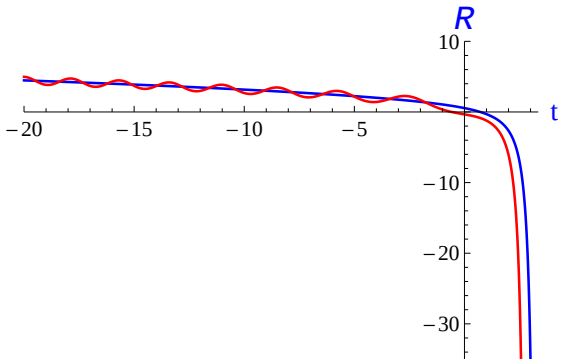

Figure 3.2 : *Evolution of the radius R of the star (according to the Painlevé I equation) showing the slow time scale and the fast time scale following the loss of dynamical stability. Note that the collapse is preceded by growing oscillations.*

We have shown that the star's loss of stability can be described in mathematical terms as a so-called dynamical saddle-node bifurcation. This approach enables one to devise a universal equation describing supernovae dynamics at its onset, taking into account the initial physical conditions of stability. This equation, which is of the Painlevé I form

$$\ddot{R} = -ct - bR^2, \tag{3.3}$$

corresponds to the normal form of the Euler-Poisson system at the saddle node. Here, R represents the deviation of the radius of the star to its critical value and t is the time (c and b are numerical coefficients that can be determined from the hydrodynamic equations). **Unlike previous studies, this one explains why the time scale of supernovae explosion, lasting between ten and thirty seconds, is considerably shorter than the overall pace of the evolution of the star, in the billion years range.**

Another important challenge in supernovae concerns the fact that their explosions show a violent outward flow. However, an initial inward flow causes the star core to collapse into a neutron star or a black hole. It is still unclear how this inward flow is superseded by the outward flow of the explosion. We have developed a detailed model displaying a global free fall after following the loss of stability of the star. The next step is to find specific circumstances where there is both an inward and a partly outward motion just after the bifurcation, which could explain that the explosion is possibly genuine and not the result of a reversed implosion.

Other long-range interacting systems

P.-H. Chavanis, C. Sire

Self-gravitating gas

For the past ten years, the dynamics of self-gravitating Brownian (or Lévy) particles has been extensively studied in the group. This model can be derived from the usual Newtonian equations of a self-gravitating gas, but in the presence of viscous dissipative forces and external forcing, and in the limit of very strong dissipation. Although its relevance for astrophysics is limited, this model shares several qualitative common features (equilibria, gravitational collapse...) with the original system, and allows for a **full analytical analysis** (contrary to the original problem). It describes the dynamics of a self-gravitating gas in the **canonical** ensemble (constant temperature T), whereas the original Hamiltonian problem strictly conserves the energy (**microcanonical** ensemble), illustrating again the non inequivalence of thermodynamical ensembles for long-range interacting systems. In

addition, this model also applies to the chemotaxis of bacteria (the role of the gravitational potential is played by chemicals released by the bacteria resulting in an effective long-range force between them). In [95], the different possible behaviors of the system have been classified as a function of the temperature T (including the case $T = 0$ [62]), the polytropic index n (the local diffusion coefficient of the particles is defined as $D(\mathbf{r}, t) = T\rho^{1/n}(\mathbf{r}, t)$, where $\rho(\mathbf{r}, t)$ is the local density of the gas), the space dimensionality, and depending on the presence or not of a bounding box: equilibrium density profiles, (self-similar) gravitational collapse and post-collapse, evaporation phase...

Two-dimensional decaying turbulence

In a two-dimensional fluid, coherent vortices are subjected to their mutual advection which derives from an effective Hamiltonien formally identical to the long-range one of $2D$ electrostatics $\mathcal{H} = \sum_{i \neq j} \Gamma_i \Gamma_j \log(r_{ij})$. The effective charges are the circulation Γ_i of the vortices, while the conjugate variables are the coordinates x_i and y_i of the vortices (instead of the usual couple impulsion/position). In decaying turbulence, an initially turbulent flow is left to decay by a process of vortex mergings which can be described by an effective aggregation model of vortices evolving according to this Hamiltonian dynamics. By studying analytically and numerically such a model describing the motion of two or three vortices in the effective noise caused by the other vortices of the fluid, it has been shown in [73] that the slow power-law decay of the number of vortices observed numerically and experimentally can be attributed to the fact that at low vortex density, two-body mergings become inefficient. The relevant process then involves three vortices, and more precisely, a dipole (a quasi ballistic vortex-antivortex pair) colliding with an isolated (anti)vortex, followed by the merging of this (anti)vortex with the like-sign vortex in the dipole.

3.2 Out of equilibrium and disordered systems

Many out of equilibrium systems in Nature can be described by effective random processes. From the diffusing trajectories of dust particles or proteins on the cell membrane (see Section 3.3), 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 present a few results obtained at LPT in the field of stochastic processes, out of equilibrium and disordered systems, and illustrate some of their applications.

Exclusion processes and KPZ universality

S. Prolhac

There has been much effort in the past 30 years to discover general laws that govern non-equilibrium systems, that are currently far less understood than systems at equilibrium. Two interesting examples of non-equilibrium systems are driven lattice gases and interface growth models.

The one-dimensional **Totally Asymmetric Simple Exclusion Process (TASEP)** is a strongly driven lattice gas featuring hard-core particles moving in the same direction. TASEP can be mapped to an interface growth model. The fluctuations of the interface observed at large scales are then described by a very singular stochastic partial differential equation called the Kardar-Parisi-Zhang (KPZ) equation. An important property of TASEP is that it is exactly solvable using Bethe ansatz. This makes TASEP a very useful tool to derive exact results in the KPZ universality class.

The KPZ universality class is characterized by a relaxation time t scaling with the system size L as $t \sim L^{3/2}$. Much is already known about fluctuations in the transient regime $t \ll L^{3/2}$, where distributions from random matrix theory appear, as well as in the stationary regime $t \gg L^{3/2}$ where large deviation functions obeying Gallavotti-Cohen fluctuation relation have been obtained. Far less is known about the crossover between the two regimes. Any calculation of fluctuations in the crossover regime would presumably require a precise knowledge of the eigenstates of TASEP on a finite lattice.

The Markov matrix of TASEP is the generator of the time evolution of the model. It is a real non-symmetric matrix. For large system

size L with finite density of particles, the eigenvalues fill a bounded domain $\mathcal{D}$ of the complex plane, see figure 3.3. The density of eigenvalues in $\mathcal{D}$ has been studied by Bethe ansatz for TASEP with periodic boundary conditions [100]. It was found to vanish close to the stationary eigenvalue $E = 0$ with an exponent $2/5$ directly related to the KPZ relaxation scale $t \sim L^{3/2}$. An explicit equation has also been obtained for the curve marking the boundary of $\mathcal{D}$. Interesting changes in the topology of this curve are observed numerically on small systems when interpolating between TASEP and its equilibrium counterpart.

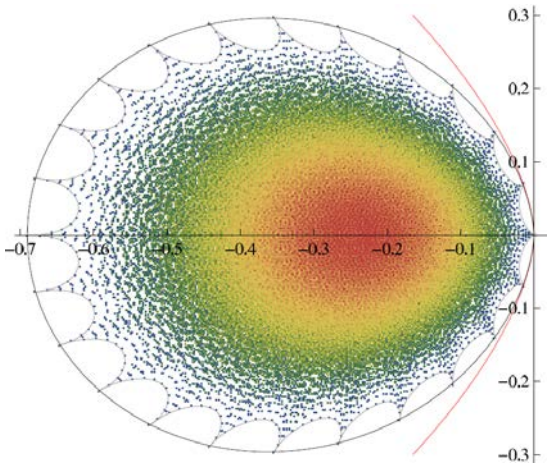

Figure 3.3 : *Spectrum of periodic TASEP with 12 particles on $L = 24$ sites. Each small square is colored according to the number of eigenvalues E such that E/L is in the square, with bigger numbers in the center.*

The first excited states of the matrix control the relaxation to the stationary state. They have an eigenvalue with real part scaling for large L as $L^{-3/2}$. Only the eigenvalue of the first excited state (gap) was previously know. A detailed study shows that each excited state is indexed by two integer partitions [114]. Explicit parametric expressions were obtained for all corresponding eigenvalues. This is a first step in calculating fluctuations in the crossover regime $t \sim L^{3/2}$.

Physics of society

C. Sire

Competitive systems

Following works on the dynamics of poker tournaments (with the faithful prediction of the wealth distribution of players), the fate of games with a tree-like structure of plays (like chess), or the generic number of different leaders in a competition (growing like the logarithm of the number of initial players), baseball and football (more recently) championships have been studied. In the context of baseball tournaments, a one-parameter model (characterizing the degree of competition/homogeneity of team strengths) has been introduced in [12]. The model allowed to identify two periods in actual US baseball championships (pre and post 1960), the competition becoming much more competitive in the most recent period. Along several quantities, the average fraction of wins (and its yearly fluctuations) as a function of the final rank, and the distribution of the number of streaks (number of victories in a raw) were quantitatively reproduced during both periods.

Collective motions in fish schools and human groups

In the framework of a new collaboration with G. Theraulaz' group at CRCA, a model describing the collective motion of fish in a school has been extensively studied in [121] (including a video abstract). This model was validated and calibrated on actual experiment (1 to 30 fish) conducted by the CRCA team. The dimensionless version of the model has essentially only two relevant parameters, characterizing the strength of the attraction and alignment forces between neighboring fish (the latter increasing almost linearly with the fish velocity).

The model reproduces the swarming (disordered) phase, the coherent aligned ("ferromagnetic") schooling phase, the rotating "milling" ("vortex") phase, all commonly observed in real fish schools (see Fig. 3.4). More surprisingly, in a narrow range of the phase diagram, a very elongated tubular phase (where fish travel in both directions and turn back at the edges of the tube) was found, which is also (but rarely) observed in real fish schools. The strong increase of the

alignement (similar to magnetic) susceptibility was investigated near the schooling-milling transition line, and it was noticed that common parameters for real fish schools (in particular those studied at CRCA) actually lie close to this line. This allows the fish to change their organization through a minimal change of velocity and hence easily adapt to their environment (including the presence of predators).

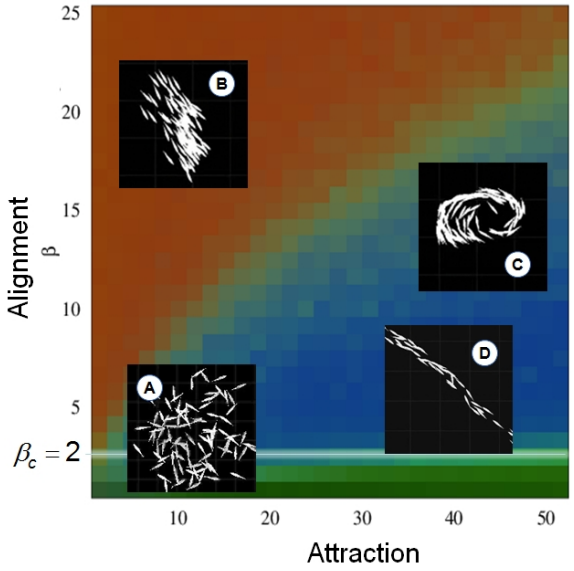

Figure 3.4 : *Phase diagram of the fish school model in the attraction-alignment (β) coupling constants plane, with the swarming phase (A; disordered; for $\beta < 2$), the coherent aligned (B; "ferromagnetic") schooling phase, the rotating "milling" phase (C; "vortex"), and the rare, but actually observed, tubular phase (D; a blowup of the full structure is shown).*

Another collaboration involving the CRCA team and the SOUK team at the LAAS addresses collective motion in human groups and the interplay with decision processes. One study addresses the dynamics of human "clusters" in cocktail parties (experiments performed by the LAAS team), which is quantitatively described by a diffusion-aggregation-evaporation model. In another series of experiments (among others) designed and performed during one week in February 2014 by the three teams at the LPT, CRCA, and LAAS, each person in a group of people (10 to 50) is allocated a color (red/blue; 50 % of each) unknown to all the participants. The people carry a beeping device, which beeps when there "environment" (in practice, the majority of their 1, 3, or 5 nearest neighbors, an information unknown to them) is not of the same color. In all cases, the dynamics finally ends (no one beeps anymore), leading to a partial separation which can be mapped to a physical phase separation at zero temperature.

Other applications of out of equilibrium random processes

D. Dean, C. Sire, V. Démery (PhD student), C. Touya (PhD student)

Other problems in out of equilibrium statistical physics were addressed in the PhyStat group, that we briefly review.

A notoriously difficult problem is the evaluation of the effective diffusion constant of a (group of) random walker in a disordered environment. This environment can be a static random potential, the coupling to a dynamical field, or the effect of the interaction with other walkers. In different contexts (dipole diffusion in a random electric field, diffusion of active and passive tracers in fluctuating fields...), this problem has been addressed using perturbative and non perturbative methods (non Markovian methods, field theory, path integrals...) [19, 77, 78].

Another problem is the study of forces emerging from a fluctuating environment. For instance, the drag force necessary to move a spin in a magnetic system (with its own thermal fluctuations) has been studied, with the calculation of the force-velocity relation for different such systems [45, 49, 79]. A related problem is the emergence of Casimir-like effects (originating in the imposition of physical boundary conditions) resulting from purely classical thermal fluctuations. Such effects have been studied in the context of a model of a polarizable material, or in the dynamics of an inclusion in an excited field, with possible applications to proteins, polymers, membranes (the experimental observation of the induced drag force experienced by the inclusion has also been discussed) [17, 43, 79, 97].

3.3 Statistical mechanics for biophysics and soft condensed matter

First applications of statistical mechanics to biophysics and/or biology problems where tackled more than 10 years ago in the PhyStat group, and have known a regular activity thus far. Published works range from fundamental research with a biophysical background and motivation, to more applied works and notably to publications in collaboration with experimental groups (in Toulouse and more recently in Germany), where questions raised by experimental facts are explored and solved.

Equilibrium statistical mechanics of DNA

M. Manghi, N. Destainville, J. Palmeri

Stretching, bending, torsion and finite size effects – DNA adsorbed on surfaces

We have developed a mesoscopic DNA model which couples the base-pairing degrees of freedom (using an Ising-like model) to the chain degrees of freedom (bending, torsion and stretching) [2]. Indeed the bending, torsion and stretching moduli, as well as the base-pair length, are drastically different in the double-helix (dsDNA) and the single-stranded DNA (ssDNA). This model allows us to characterize the denaturation transition (where both strands de-hybridize) as a function of the elastic moduli, as well as the statistical and mechanical properties as a function of the temperature. This is a natural generalization of previous works where only the bending was considered. By including the weight of forming a closed loop (a simple model for a denaturation bubble), we explain how the melting temperature increases when the DNA length increases, as observed in experiments.

Atomic Force Microscopy (AFM) is widely used to observe dsDNA adsorbed on surfaces. In recent experiments [3], "anomalies" have been detected in the distribution of bending angles along DNA (which measures its flexibility): an overabundance of large angles were found which are not predicted by the traditional statistical model of DNA chains, the Worm-Like Chain (WLC) model.

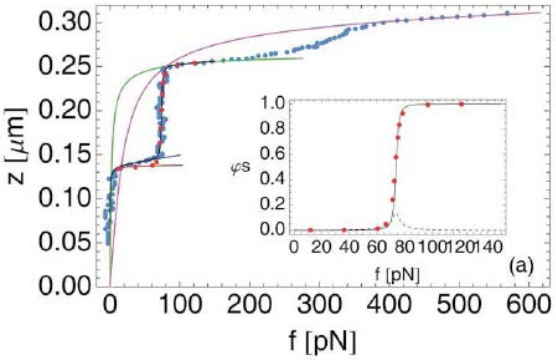

Figure 3.5 : *Force-extension curves of a poly(dG-dC) DNA of $\simeq 400$ base-pairs. Experimental data (blue symbols) are taken from Rief et al., Nat. Struct. Biol.* **6**, *346 (1999), where the stretching force is applied by AFM. The first transition at $\simeq 60-80$ pN corresponds to a B-to-S one, whereas the second one at $\simeq 300$ pN, is a transition from the S-form to a ssDNA. The different curves correspond to: the WLC model for dsDNA (in red) and the S-DNA (green), a non-linear extensible model for ss-DNA (pink) and the model for the B-to-S transition (black). The red dots correspond to a semi-analytic model by transfer matrix which does not take into account the finite extensibility of the S-form. Inset : Fraction of base-pairs in the S state, φ_S, and Ising correlation function (dots) vs applied force [82].*

We have explained these anomalies by the presence of small denaturation bubbles (or kinks) facilitated by the presence of the substrate which modifies interactions between DNA base-pairs [1]. We 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.

Stretching transitions of DNA under force

The nature of the transition of the dsDNA, when stretched in single molecule experiments,

3. Wiggins *et al.*, Nature Nanotech. **1**, 137 (2005).

is already a long standing issue. This issue was tackled using the previously mentioned mesoscopic coupled DNA model, which unexpected and original results [82]. For stretching forces larger than $60 - 80\,\mathrm{pN}$, it is generally assumed that the increase by almost a factor 2 of the DNA length (see Fig. 3.5) is associated to a transition from the natural B-form to a "stretched" S-form, where the double-helix is unwound and takes the form of a fluctuating ladder (instead of an helix). Alternatively, it has been proposed that the transition is a denaturation one, where the two strands are separated. The results are summarized as follows: (i) the experimental stretching curves of ssDNA are adjusted up to the nN, but the model requires surprisingly a monomer size ($\sim 0.2\,\mathrm{nm}$) smaller than the nucleotide one ($\sim 0.7\,\mathrm{nm}$), corresponding to chemical sub-units. (ii) Mesoscopic models are therefore not able to fit the transition B to ss, since the monomer unit should change during the transition. (iii) An analytical formula is derived to fit the B-to-S transition, thus generalizing the Marko and Siggia approach. We obtained an excellent agreement with exact transfer matrix results and with experiments on poly(dG-dC) (Fig. 3.5) and λ-DNA, thus showing, that it is indeed a B-to-S transition. (iv) However, the transition for poly(dA-dT) is different, probably a B-to-ss one. The nature of the transition is therefore sequence-dependent, *via* the H-bond strength of base-pairing.

Out-of-equilibrium DNA

M. Manghi, N. Destainville, A. K. Dasanna (PhD student), F. Sicard (postdoc)

TPM as a probe of DNA conformation changes (MM)

With our colleagues from the Institut de Pharmacologie et Biologie Structurale (IPBS), we aim at studying the DNA conformational changes using the Tethered Particle Motion (TPM) set-up (described in Fig. 3.6) (ANR TPM-on-a-chip project). Using kinetic Monte Carlo simulations and comparing them to experiments, we proposed a calibration of TPM at the dynamical level [25]. Indeed, the experimental set-up perturbs DNA dynamics due to several factors: (i) it is the dynamics of the complex DNA-particle (not the DNA alone) that is observed; (ii) the interactions between the particle and the surface modify the accessible DNA conformations; (iii) the hydrodynamic friction due to the particle and the proximity of the surface slows down the dynamics.

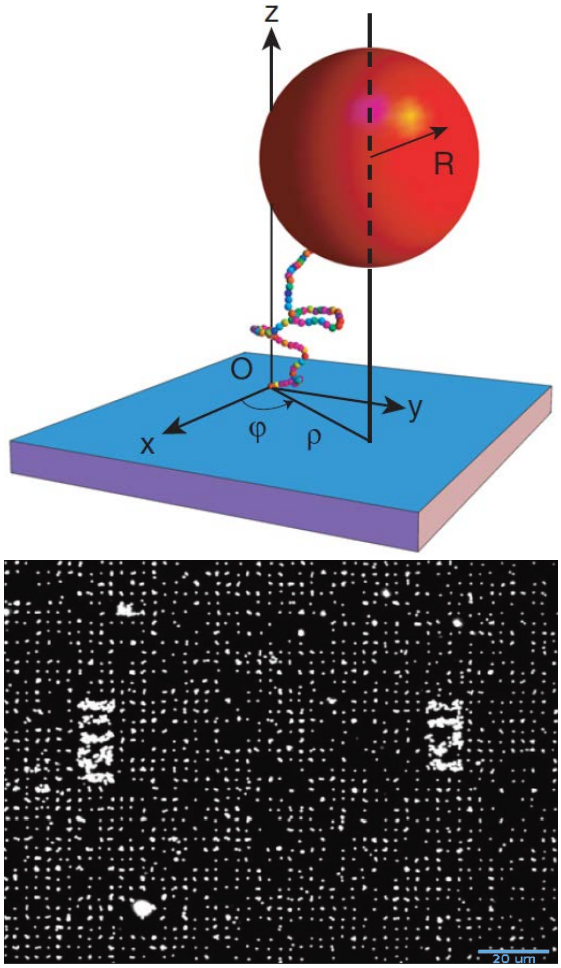

Figure 3.6 : **Top** *: Model for TPM simulations. The DNA is grafted to a surface at one end and to a colloidal particle (of 10 to 1000 nm) at the other end. The fluctuation amplitude of the particle parallel to the surface allows us to deduce the DNA end-to-end distance: the amplitude increases when this distance increases [25]. Each bead represents $\simeq 10$ base-pairs.* **Bottom** *: Micrograph of TPM particles (white dots) parallelized on a DNA chip "Nano-multiplex" (the scale bar corresponds to 20 μm).*

Including hydrodynamic interactions, we have shown that the dynamical calibration depends on the global chain relaxation time, which

increases when the DNA length and particle size increase. For particle sizes smaller than 20 nm, the friction is negligible, thus leading to a temporal resolution of about 20 ms [25]. This work is a first step towards the quantitative study of DNA conformation changes due to heating, changes in salt concentration or inserts of curved A-tracks (current Ph.D. of Annaël Brunet).

Two mesoscopic models for denaturation bubble closure

In our group, we have also studied the hybridization (or "renaturation") dynamics of the DNA double helix [83, 102]. Coupling internal and external degrees of freedom plays a fundamental role to explain the experimentally observed long hybridization times [4] ($\sim 100\ \mu$s). Following our previous works, we have numerically studied two mesoscopic models, the monomeric units of which are the nucleotides. The first one, without helicity (the molecule thus looks like a flexible ladder), led to insufficient closure times smaller than a few μs. Taking into account the helix character of the molecule enabled us to reach the 100 μs time scale, as desired, for realistic model parameters. Indeed, as we have confirmed it later by the use of MetaDynamics [122], a biassed numerical method that enables a refined characterization of the free-energy landscape in spite of large energy barriers, closure is associated to a collective twisting dynamics that could not be fully apprehended by the first, simpler model.

Biomembranes and interfaces

N. Destainville, M. Manghi, J. Palmeri, N. Meilhac (postdoc), S. Weitz (postdoc), L. Horvath (PhD student), G. Gueguen (PhD student), S. Buyukdagli (postdoc)

Stacked bilayers and their unbinding transition

In order to better understand the physical properties of biomembranes, it can be useful to work on model membranes, which are simpler to study than real cell membranes and in which it can be more easily conceivable to decipher elementary biophysical mechanisms and to compare experiments and theories. One of those model systems, finite**bilayers stacks** adhering on a substrate, have been studied by taking into account an Helfrich free energy to describe each bilayer and a non-linear interaction between adjacent bilayers (through a Morse potential). Thanks to a **variational approach**, the unbinding transition (when the temperature grows) has been fully characterized, leading to very rich phase diagrams [27]. In addition, when reaching the unbinding transition of the uppermost bilayer, it goes further away from the remainder of the stack, its fluctuations grow while its hydrodynamic interactions with the stack vanish. It thus looks more and more like a free bilayer, and thus becomes a more realistic model of free bilayer than a usual supported one.

Cluster phases of membrane proteins

With the ultimate motivation of giving a full picture of **biomembrane organization embracing both their proteinic and lipidic complexity**, membrane **nano-domains** have been studied by the PhyStat group for about 15 years now. Indeed, a cell membrane contains several thousand of different protein and lipid species that ensure a large variety of biological functions. To accomplish their task, they must interact with their biochemical partners, which often lie in the membrane themselves, and it is observed that parters must be co-localized in advance in small membrane **micro-** or **nano-domains**, of size ranging from 10 to 100 nm. To explain this compartmentalization, different approaches in the literature appeal either to proteins or to lipids.

When proteins are invoked, a new paradigm has been proposed in the group in 2008, where nano-domains result from the competition of effective short-range attractive forces and longer-range repulsive ones mediated by the elastic membrane, on the order of the thermal energy k_BT. The resulting **cluster phases**, first discovered in colloidal suspensions, have the required manometric size when realistic parameters are injected in the model, extracted either from experiments or numerical works.

In the past 5 years, this model has progressed in the PhyStat group in 3 directions: (i) In [53] and [60], the role of protein diversity has been studied analytically and confirmed by Monte Carlo simulations: when a great number

4. G. Altan-Bonnet, A. Libchaber, O. Krichevsky, Phys. Rev. Lett. **90**, 138101 (2003).

($N_F \sim 10^3$ to 10^4) of different protein families coexist in a same biomembrane, as in real cells, they segregate in different clusters provided the short-range affinity between proteins of a same family is slightly more favorable than between proteins of different families. *A difference of short-range binding energy as small as 2 to 3 k_BT is thus sufficient to ensure* **specialization of biological nano-domains** because a few protein species only (belonging to the same *family*) cohabit in each nano-domain (see Fig. 3.7).

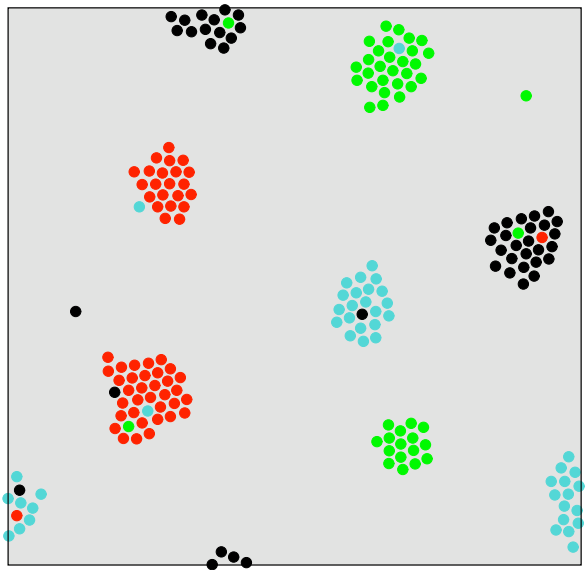

Figure 3.7 : *Nano-domain specialization mechanism. Different protein families, shown in different colors, are sorted in different nano-domains because proteins of alike families have a better short-range affinity than proteins of different families.*

This work appeals to the mean-field Flory theory which becomes exact in the large N_F limit of interest here. (ii) In [103], the nature of the long-range repulsion between proteins embedded in a biomembrane has been established on stronger theoretical grounds, by fully taking account non-trivial many-body effects in the entropic (Casimir) and elastic interactions. The main mechanism dwells on the up-down symmetry breaking due either to the proteins themselves or to the asymmetry of composition of the two leaflets of a cell membrane. Contrary to what was believed so far, it has been demonstrated that the *effective* repulsion always overcome the Casimir attraction, even for inclusions imposing a weak up-down symmetry breaking, provided that a non-vanishing surface tension exists. (iii) These theoretical findings have received a strong **experimental support in the tetraspanin-web context**, through a collaboration between the PhyStat group and two experimental groups in Germany, using notably sub-wavelength fluorescence microscopy (STED with < 50 nm spatial resolution) [115]. Notably, it has been observed that when the protein concentration grows, the size of clusters does not vary much while their number grows proportionally with the concentration, as predicted by the theory. The observations are also in agreement with the predictions of the item (i) above.

Coupling between curvature and local composition

Another kind of mechanism invoked to account for biomembrane micro- or nano-patterning involves *lipids*, in more direct connection with the celebrated "lipid raft" mechanism. Following the route paved by S. Safran, R. Lipowsky, W. Helfrich, or U. Seifert, a recent work published by researchers of the PhyStat group follows a field-theoretic approach, where the membrane height-fluctuation field $h(\mathbf{r})$ and its derivatives are coupled to *two* concentration fields, $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$, one for each leaflet. The membrane stiffness is written as a function of $\phi_1(\mathbf{r}) + \phi_2(\mathbf{r})$ while the curvature depends on $\phi_1(\mathbf{r}) - \phi_2(\mathbf{r})$ only. As compared to the previous item, the up-down symmetry can thus be broken by imposing directly different average concentrations in each leaflet. The model embraced nano-patterning through both (i) "raft"-like nano-domains, which are stiffer than the surrounding membrane but flat, and (ii) curved bud-like nano-domains when $\phi_1(\mathbf{r}) \neq \phi_2(\mathbf{r})$. A very rich phase diagram emerges, far richer in the spherical (vesicle) geometry than in the planar one, the only one to have been explored so far in this two-concentration fields context.

Ion partitioning and transport in nanoporous membranes

Using classical molecular dynamics simulations, we have studied water and **electrolytes near interfaces and in charged nanopores**,

focusing on effects due to specific ion characteristics (such as size, charge, polarizability) by studying via such microscopic simulations ionic distributions, transport, correlations, and fluctuations. This work has led to a clearer understanding of the essential role played by the competing multipolar contributions to the vapor-liquid and the solute-liquid interface electrical potentials in determining an important ion-specific electrostatic contribution to the solvation free energy. Furthermore, this work on nanopores has practical applications in the further development of our commercial modeling software, NanoFlux, used in the technologically important area of membrane nanofiltration (for the production of potable water and the treatment of industrial wastewater in the ceramic, chemical, and nuclear industries), a field in which one of us has been an industry consultant.

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 [13, 14, 48, 75, 76, 96]. 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. The PhyStat group benefitted of a fruitful collaboration with the team of M.-P. Rols at the IPBS Toulouse, one of the world leading experimental groups in the field. A PhD student (T. Portet) was co-supervised by D. S. Dean and M.-P. Rols and received a young scientist prize of the Bettencourt-Schueller foundation, in 2010.

It was shown that giant unilamellar vesicles subjected to electropermeabilizing pulses tend to shrink. 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. (3.8).

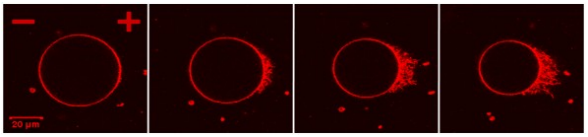

Figure 3.8 : *Confocal images of a lipid giant unilamellar vesicle subjected to electric pulses (360 V/cm; 0.5 Hz; 5 ms duration), exhibiting size decrease and the formation of tubular structures facing the anode. 6 pulses are applied between each snapshot.*

These 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). The permeabilization of cells in the presence of plasmid DNA (4.7 kb) has also been studied. 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). The transport of DNA in the region of a cell which is assumed to have a pore formed by electroporation has been modelized. 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.

Statistical physics of electrolytes closed to dielectric surfaces

Interfaces which separate an electrolyte (a solution of ions in water) and a medium such as air or a carbonated membrane present dielectric jumps which deform the electric field lines. Ions located at a few nanometers from the interface are thus repelled, due to the famous image-charge forces. Using a field-theoretic variational approach [26], we have studied the ionic distribution close to planar interfaces, slits and cylindrical nanopores [24, 59]. Three competing mechanisms are at play: the dielectric repulsion, the ion-ion correlations (or ionic solvatation), and the attraction of counter-ions by the

surface charge. For given parameters, a new good coion exclusion regime appears, where the dielectric repulsion overcomes the electrostatic attraction. It leads, in the cylindrical geometry, to a first order transition between a state where ions are excluded from the pore (the "Vapor" state) and a "Liquid" state where ions enter the pore (the phase diagram is shown in Fig. 3.9). We argue that this discontinuous transition, which subsists for small values of the surface charge, could provide a common physical mechanism, accounting for the experimentally observed conductivity fluctuations in synthetic and biological nanochannels (without the need to invoke any specific biochemical ones). The conductivity fluctuations would then be a manifestation of the fluctuation induced switching between the high (liquid) and low (vapor) density phases of the nano-confined electrolyte (see Fig. 3.9). This phase transition is the ionic analog of the confinement modified liquid-vapor water "capillary evaporation" transition occurring in hydrophobic nanopores [24].

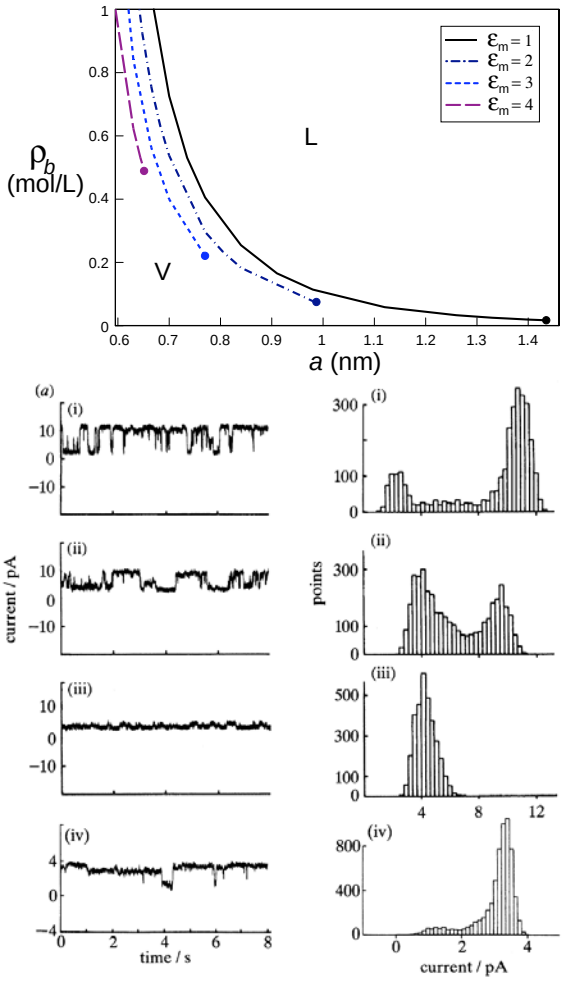

Figure 3.9 : **Top**: *Phase diagram for different values of pore dielectric constant* ϵ_{m}*, showing the coexistence lines which separate the ionic liquid (L) and vapor (V) phases in a cylindrical nanopore.* **Bottom**: *(a) Ionic current fluctuations observed through a PET membrane for a KCl solution at 0.1 mol/L (*$p\mathrm{H} = 7.4$*), and (b) histogram of the conductivity for different concentrations of divalent ions* $CaCl_2$ *(from top to bottom:* 3×10^{-4}*;* 3×10^{-3} *mol/L and without* $CaCl_2$ *but at* $p\mathrm{H} = 8$*). Taken from Lev et al. Proc. Roy. Soc. B* **252***, 187 (1993).*

4

Systèmes de Fermions Finis – Agrégats (Agrégats)

The core of the activity of the cluster group focuses on the microscopic description of irradiation processes in clusters and molecules. The understanding of irradiation processes is a key issue in many fields of physics and chemistry and has also key implications in biology. Let us cite as especially relevant examples irradiation of materials in relation to nuclear power plants or to space missions, or irradiation of molecules of biological interest in relation to cancer treatment. Microscopic mechanisms of irradiation dynamics are still poorly understood, even if numerous studies at various levels of refinement already exist, starting from isolated molecules and clusters up to pieces of bulk material, and including various combinations of active species coated by a more inert environment such as embedded clusters or solvated biomolecules. The group has developed a solid expertise in the field over the last two decades. The last five years have been devoted to further developments of the modeling with a special focus on formal and computational aspects, while still pursuing elaborate calculations of realistic cases in direct relation to ongoing experiments. The major axes of development can thus be sorted according to three categories: formal, methodological, and computational researches.

Formal developments

A major effort has been devoted to the formal improvement of current theoretical framework. The highly involved situations encountered in irradiation processes call for "simple", robust and fully time-dependent theories. Among the various available approaches Time-Dependent Density Functional Theory (TDDFT), solved in real time, offers an optimal compromise between cost and capabilities. The basic idea of (TD)DFT is to replace the many-body problem by an effective one-particle description in which the many-body effects of the system enter through an exchange-correlation potential that is a functional of the density of the system. This functional is not known and needs to be approximated. Therefore the application of TDDFT to modeling experimental situations relies on these approximations. We started working on TDDFT more than 20 years ago and developed one of the first real time calculations of irradiation dynamics, back in the mid 1990's. Since then, and especially in the last few years, the problem has been considered by several groups following basically the same strategy as ours, and the field is thus becoming highly competitive.

Although TDDFT, in its standard Local Density Approximation (TDLDA), provides a sound starting basis for such dynamical situations, it is still plagued by intrinsic limitations. We have attacked one of them, the so-called Self Interaction Correction (SIC) problem, in the second half of the 2000's. We could thus propose the first formally sound time-dependent theory of this prob-

lem. In the last five years, we mostly pursued these activities in terms of computational effort. Another major issue concerns the account of dissipative effects in the TDLDA dynamics. In electronic systems, such dissipative scenarios cover several aspects that we attacked in parallel, along different lines of formal developments.

First, we reformulated (to the best of our knowledge as the first sound formal proof) the so-called Trajectory Surface Hopping (TSH) approaches which provide a stochastic ensemble description of low energy dynamics [35]. TSH methods allow one to describe dynamics beyond mean field (TDLDA) by accommodating propagation on a set of potential energy surfaces. Such approaches are widely used in chemistry since more than two decades, but, surprisingly enough, mostly on a practical basis. While TSH is well suited to simple situations where the number of active surfaces is limited to a few, the case of highly dissipative scenarios (involving numerous potential energy surfaces, in molecular physics terminology) requires a radically different (although again of stochastic nature) approach. We have thus reformulated an old approach of ours, originally introduced in the context of nuclear collisions, in a simpler, but practically manageable, frame. The theory allows us to go beyond mean field dynamics by introducing a stochastic ensemble of mean-field transitions between mean-field states being decided on the basis of time-dependent perturbation theory at short time. It can be shown that such a theory can be reduced to a quantum kinetic equation complemented by a stochastic collision term which makes it extremely complete. The key assumption here is the loss of coherence of mean-field states over such a perturbative time, a situation typically encountered at high energies. This theory, originally dubbed Stochastic TDHF, provides a well founded extension of TDLDA and displays the expected dissipative features. It thus certainly provides a promising basis for extending TDLDA in the dissipative regime. It will be intensively developed in the forthcoming years [53].

It should also be noted here that we explored two alternative paths to STDHF. First, we developed a computational version of Time-Dependent Current-DFT (TDCDFT). In TDCDFT, the basic quantity is the electronic current density of the system, on top of the density as in TDDFT. Within this framework, instead of looking for approximations that are non-local in the density, to improve over TDLDA, one can look for approximations to the exchange-correlation potential that are local functionals of the current density. This has been shown to offer an adequate account of dissipation in the linear domain. The purpose of this work was to extend TDCDFT at higher excitation energies, and of course in real time, as compared to previous, linear response approaches. TDCDFT in real time is certainly worth being further investigated but also limited to moderate excitations as it raises complex formal as well as computational questions. Beside dissipation, TDCDFT also allows one to give a proper description of the polarization in solids and to treat the response to transverse fields, which is important to describe magnetic excitations. This represents as well a research line in our group, in collaboration with our colleagues of the Laboratoire de Chimie et Physique Quantiques at the University P. Sabatier through a Ph.D position funded by the LABEX NEXT (see Ph.D thesis [5]).

We also investigated another path to dissipation following standard relaxation time ansatz of kinetic theory, on top of TDLDA. Again, such approaches are limited to moderate excitations but turn out to offer practical solutions to the problem, with a limited amount of parameters. It will thus be developed further as well.

The last line of development beyond TDLDA was devoted to Green's functions approaches within the framework of Many-Body Perturbation Theory (MBPT). In this framework, the many-body effects of the system are contained in the self-energy, which thus plays a similar role as the exchange-correlation potential in a density-functional context. Also the self-energy needs to be approximated. MBPT approximations can be found in a systematic way, although MBPT in itself is too costly for realistic systems. Therefore, passing through MBPT has the advantage that approximations with a clear physical meaning can be designed more easily than in the context of density functionals and introduced

in a second-step into the more efficient TDDFT [10, 25] or to (TD) density-matrix functional theory (TDDMFT), see Ph.D thesis [6], the connection between TDDFT (or TDDMFT) and MBPT being direct via the time-dependent density (or density-matrix of the system). Therefore much effort is put in exploring better approximations to correlation in MBPT [9, 26, 39, 40].

Methodological developments

In parallel to formal developments, we pursued our detailed analysis of electron dynamics in irradiated clusters and molecules. These many studies were recently gathered in a long paper prepared for Physics Reports [60]. One can grossly identify three major directions of investigations in the last few years, all concerning electronic signals. Electron emission can be analyzed at various levels of details, ranging from the simpler total ionization down to energy- and/or angular-resolved cross-sections. All these signals can furthermore be analyzed in a time-resolved manner, possibly leading to pump-and-probe scenarios in which a pump laser excites a system and a probe laser tests its response.

The first line of investigation focused on a better description of Photo-Electron Spectra (PES), namely energy-resolved electron emission. While we have developed such studies since more than 10 years, we extended the applicability of our method to larger laser intensities and explored PES in elaborate SIC approaches mentioned above. In relation to experiments, we also performed calculations in the case of fullerenes for which numerous data become available. To the best of our knowledge, such calculations, covering various dynamical scenarios, were the first of their kind.

The second focus concerned angular distributions. In the gas phase, molecule or cluster orientations are unknown so that a proper comparison between theory and experiments requires an averaging over molecule/cluster orientation with respect to laser polarisation. In the one-photon regime (one single photon needed to reach ionization), it is well known that the angular differential cross-section (or Photo-Angular Distribution, PAD) reduces to a simple form involving one single parameter, the so-called anisotropy parameter β. We devoted systematic studies to β and showed how sensitive it is to details of the description of the system [18, 19, 30]. We furthermore extended our calculations to the multi-photon regime (several photons needed to reach ionization) where only direct averaging is feasible [50]. Again, we performed the first realistic computations of PAD in fullerenes, in direct relation to experiments, and covering all ionisation (mono- and multi-photon) regimes (Ph.D thesis [3]). Although such calculations may appear rather simple, it should be noted that they remain at the limit of today's computer possibilities, even with optimized codes as we use (see below and Sec. 4.3).

Finally, and again in relation with experiments, we started to work on attosecond-resolved dynamics (see Sec. 4.2). Experiments mostly access total ionization, the new line of development being to address more and more complex molecules rather than atoms. We performed some systematic studies in a simple dimer molecule and could show that we perfectly reproduce the trends observed in experiments [45]. The details of the underlying mechanism are still a matter of debate but our recent investigations showed that the tools we have developed over the years could very well bring invaluable information on the detail of these mechanisms. Work along that line will of course be pursued in the next years.

Technical developments

The last major axis of our activities concerns the development of computational tools to address the various formal and methodological developments in the most efficient manner. We invested along 3 major directions concerning these computational efforts. The first one again concerns the Self Interaction Correction (SIC) discussed in the formal developments. A full Time-Dependent inclusion of SIC (TDSIC) has required a significant computational effort. This full TDSIC is based on the propagation of a double set of wave functions (see Ph.D thesis [1]) and needs elaborate propagation techniques with very short time steps. We finally succeeded in obtaining a stable, practical, although demanding, scheme which allowed us to propose the first full TDSIC computations in real time TDDFT [42]. This specific aspect will by the way become part

of the second major effort we devoted to the preparation of the open source package "TELEMAN" (for "Time-dependent ELectronic dynamics in Molecules And Nanosystems") based on the real-time TDDFT codes developed in our group since two decades. In the framework of a French-German-Chinese collaboration, we dedicated a lot of efforts to a major upgrade of our codes with the aim at opening them to the scientific community. This covers several complementing aspects. The first completed one was a further optimization of our codes: i) optimization of FFT packages; ii) partial use of GPU cores; iii) enhanced parallelization of some sections of the codes. Adding up the various improvements allowed us to gain a significant speedup, from 2 to 15, depending on the considered systems. The second aspect concerns the user interface which was very rough, as our codes were in constant development since 20 years. This simplification phase was accompanied by the preparation of a dedicated webpage. We hope to be able to open a beta version of this web page mid 2014, only little delayed as compared to the originally scheduled project. It should be noted that our website will offer several original features among the growing number of real-time TDDFT codes, mostly in terms of access to dedicated ionization observables (PES and PAD in particular) but also in terms of TDSIC and TDCDFT, although these two last items will remain in a restricted area, only open to colleagues willing to fully participate in the technical developments. A last computational project, presently in development, will consist in coupling TELEMAN with a major Molecular Dynamics package developed in Frankfurt ("MesoBioNano Explorer") with the aim at developing a general purpose Quantum-Classical code allowing the treatment of irradiation processes including environment effects.

These various axes of research are gathered in Table 1.2 which provides in a compact manner a general vision of our activities. It includes the various supports associated to these projects, in particular in terms of national, European and international fundings (see Insert 1.1). It also indicates how the various members of the group (permanent and non permanent) were included in these various tasks. We finally give a rough estimate of the duration of each of these projects, which shows the complementarity and the continuity of the various research axes. As can be seen from Table 1.2, several of these axes will continue in the years to come, in view of their relevance.

Funding: Since 2009, the AGRÉGATS group has been funded by

❍ 5 *ANR contracts* : MIRRAMO (Irradiation of Biological Molecules, 2007-2009, PI : Prof. Michel Farizon, IPNL), COLDIRR (Irradiation of Cold Molecular Nanosystems, 2009-2013, PI : Prof. Michel Farizon, IPNL), MUSES (Multiscale Electron Dynamics, 2010-2014, PI : Dr. Franck Lépine, ILM Lyon), PWTELEMAN (Beijing(Pékin) -Wuxi-Toulouse-Erlangen-Le Mans collaboration on Time dependent Electronic dynamics in Molecules And Nanosystems, 2011-2014, PI : Prof. Calvayrac, LPEC Le Mans), and LASCAR (Étude expérimentale et théorique de l'interaction d'une impulsion ultracourte avec un nanocone de carbone, 2014-2017, PI : Dr. Béatrice Châtel, LCAR, Toulouse);

❍ 1 *Marie Curie contract* : CORINF (Correlated Multielectron Dynamics in Intense Light Fields, 2011-2015, PI : Prof. Misha Ivanov, Imperial College of London, et Dr. Olga Smirnova, Max Born Institute Berlin);

❍ 2 fellowships from the *Institut Universitaire de France (IUF)*;

❍ 1 position of Adjunct Professor at State University New York, University at Buffalo (UB), NY, USA, since 2013;

❍ Postdoctoral fellowships funded by ANR (see above);

❍ PhD fellowships awarded by the doctoral school *Sciences de la Matière* of the University of Toulouse, by the LABEX *NEXT* (Nano – EXtreme measurements – Theory), and by the *Midi-Pyrénées Region* and *CNRS*.

Main visitors: Scientists who have visited the AGRÉGATS group for a period of at least one month since 2009 include Prof. Valentin NESTERENKO (Dubna, Russia), Dr. Peter KLÜPFEL (Reykjavik, Iceland) They were funded by visiting professor fellowships from the University of Toulouse, CNRS guest scientist fellowships, or by means of the IUF grants.

Insert 4.1 : *Funding of the AGRÉGATS group and its main foreign visitors.*

Topics		Publi.	Dates						Financ. support	Perm.	Non-perm.	Related organized conferences
			2009	2010	2011	2012	2013	2014	2015			
Formal developments	Stoch. meth. TSH STDHF	[35, 53]							MUSES CORINF IUF, UB	PMD PR ES	JME NS LL	ThDays 2011
	Dissipation, TDCDFT	[53]							MUSES CORINF IUF, UB NEXT	PMD PR ES	JME MV NR	ThDays 2011 ThDays 2012 ThDays 2012
	Green's functions	[25, 39, 9] [26, 40]								PR	SDS	GF 2013
Methodology : Ionization in detail	Photo-electron spectra	[13, 31, 32] [41, 42, 43] [44, 45, 60]							LASCAR IUF UB	PMD PR ES	SV PW CZG	ThDays 2014 ThDays 2014
	OA-PAD	[14, 19] [20, 30]							MUSES UB	PMD ES	PW CZG	Buffalo 2013
	Attopulses FEL	[45]							MUSES CORINF	PMD ES	TR CZG	ThDays 2011
Computational and numerical developments	TD 2setSIC	[3, 4, 17] [24, 42] [46, 58]								PMD PR ES	JM MV	ThDays2014
	Open source								TELEMAN IUF	PMD ES	JME PW LL	Le Mans 2014
	QM/MM	[1, 5, 12] [14, 18, 29] [33, 34]							COLDIRR IUF	PMD ES	TR MV	ThDays 2009 ThDays 2013

PMD : Phuong Mai Dinh
PR : Pina Romaniello
ES : Eric Suraud

JME : Jose-Maria Escartin
TR : Thomas Raitza

JM : Jérémie Messud
SV : Sylvain Vidal
PW : Philipp Wopperer
NS :Nader Slama
NR :Nathaniel Raimbault

SDS : Stefano Di Sabatino
CZG : Cong Zhang Gao
LL : Lionel Lacombe
MV : Marc Vincendon

Nota Bene : Prof. Dr. (Dr. h.c.) Paul-Gerhard Reinhard, from the University of Erlangen, is also associated to most of these research topics.

Insert 4.2 : *Synthesis of achievements, collaborations and financial supports of the* Agrégats *group.*

The above presentation aimed at introducing the activity of the group in a general manner. We would like now to discuss in more details a few illustrative examples of particularly interesting results. We have thus chosen three highlights, one among each type of activity: formal, methodological, and technical developments. We shall thus illustrate our achievements on the three following examples: beyond standard approximations in MBPT, attosecond spectroscopy in N_2, and the TELEMAN project.

4.1 Beyond standard approximations in MBPT

S .Di Sabatino, P. Romaniello

Approximations to correlation in MBPT are explored following two strategies: i) by improving existent approximations to the self-energy; ii) exploring innovative routes which take implicitly into account correlation by calculating a set of nonlinear, first order coupled functional differential equations, without introducing the self-energy. Both strategies are based on physically motivated approximations to the fundamental equations of MBPT. This has allowed us to elucidate various aspects behind standard approximations in MBPT and to go beyond [9, 26, 39, 40]. In particular the second strategy has allowed us to describe multiple satellites in the photoelectron spectrum of silicon, with an unprecedented excellent agreement with the experiments [26]. Figure 4.1 shows the photoemission spectrum of silicon, integrated over the Brillouin zone. Experiment (blue crosses) shows prominent quasi-particle structures (which are related to one-particle energies), followed by a series of satellites (which are related to neutral excitations of the system). Standard approximations (dashed red line) are in fair agreement with experiment in the quasi-particle region, but produce only one "averaged" satellite. The new approximation (green dot-dashed line), instead, can capture the essential physics of multiple satellites. The same strategy is now being used within TDDMFT.

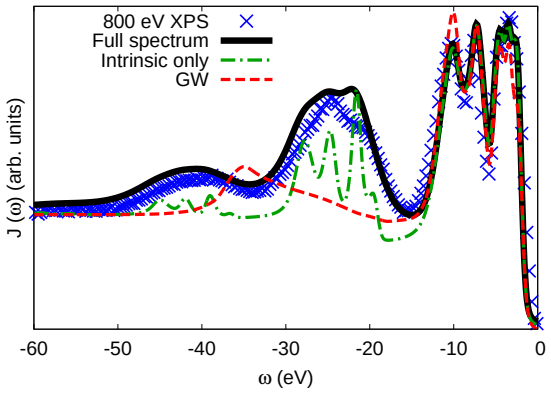

Figure 4.1 : *Experimental XPS spectrum of Si at 800 eV photon energy (blue crosses), compared to the theoretical photoelectron spectrum calculated from standard approximations (red dashed), and from our new approximation (green dot-dashed). On top of the latter the black solid line also includes extrinsic and interference effects. All calculated spectral functions are supplemented with cross sections and a secondary electrons background. From [26]*

4.2 Attosecond spectroscopy in simple dimer molecules

P. M. Dinh, C. Z. Gao, T. Raitza, É. Suraud

The time-resolved analysis of electron dynamics has focused numerous investigations over the years. The recent availability of lasers producing trains of attosecond pulses clearly opens the door to such investigations. Early convincing tests were performed in simple atoms such as He and Ar on the basis of an IR fs laser pulse topped by an UV atto-train. Such measurements exhibited marked oscillations (with period half the IR period) as a function of the delay between UV train and IR signals. The associated theoretical investigations relied on simple simulations using the Time-Dependent Schrödinger Equation (TDSE) with a single active electron. A robust many-electron theory is not yet available to explain the observations.

Experiments were generalized to simple molecules with qualitatively similar results as in the atomic case and a somewhat similar IR+UV setup. We have thus started computations in

real-time TDDFT to understand experimental results and we obtained a remarkable agreement between theory and experiments as illustrated in Figure 4.2. We consider here the N_2 molecule as a test case [45] and use an IR pulse complemented by an UV attopulse train (with 20 attopulses of duration 0.29 fs each and separated by 1.3 fs), first with polarization aligned along the molecular axis. With the choice of laser parameters the pure IR does not ionize but when combined to the UV train ionization occurs and is modulated with delay between IR and UV, with a period half the IR period, as in the above mentioned atomic case. Ionization maxima then appear for minima and maxima of the IR pulse (see panel (a) of Figure 4.2). Conversely, minima are reached when the attopulse train is synchronized with the zero crossings of the laser electric field. As in gas phase, the relative orientation of molecules with respect to laser polarization is unknown, it is interesting to check the impact of alignment, as shown in panel (b) of Figure 4.2. The amplitude of ionization oscillations is decreased when the laser is polarized perpendicular to the molecular axis but they nevertheless subsist, so that the original pattern is preserved.

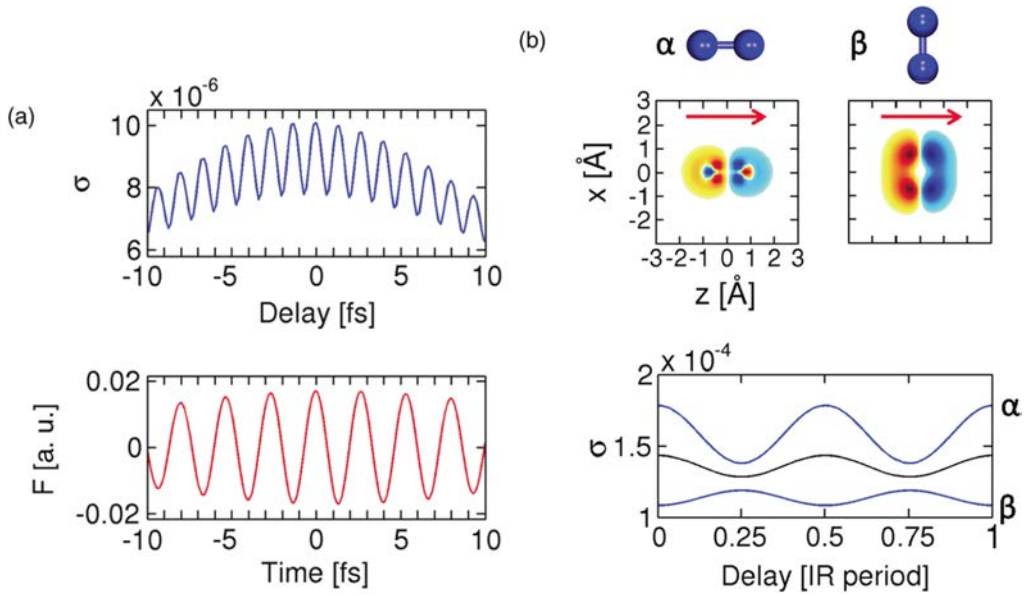

Figure 4.2 : *(a) Plot of ionization as a function of delay between UV atto train and IR pulses. The time axis corresponds to the instant where the atto train is synchronized. Maximum ionization is observed when the atto train is synchronized with the extrema of the IR field, which thus produces an oscillatory pattern with period twice the IR period. (b) Effect of molecular orientation with respect to the laser polarization axis. Color maps correspond to density plots in the presence of an electric field as indicated. The lower panel shows the results of calculations for longitudinal, transverse and alignment-averaged configurations. From [45].*

Details of the ionization mechanisms are still to be understood in full detail as they can be interpreted in various frameworks. Most importantly, systematic computations of various systems should help to unravel such mechanisms. In this respect, the dedicated analysis tools developed in the group, especially the PES and PAD technology [18, 19, 30, 50, 51, 60], are of crucial importance for the study of these phenomena. We thus pursue an active research on this topic.

4.3 The TELEMAN open-source package

P. M. Dinh, J. M. Escartín, L. Lacombe, T. Raitza, É. Suraud, P. Wopperer, M. Vincendon

The TELEMAN project aims at providing to

the public a package of efficient (sub-) routines for simulations of the electronic and ionic dynamics of complex molecules at the level of time-dependent density functional theory coupled to molecular dynamics for the ions (TDDFT-MD). It is based on the PW-TELEMAN collaboration between Beijing (China), Wuxi (China), Toulouse, Erlangen (Germany), and Le Mans (France), and funded by an joint ANR-China contract. Although this package has been very successful for exploratory studies over the last 20 years, it has required an effort of standardization and documentation to make it more efficient and user friendly. Such an optimization also constitutes a crucial step to apply the forthcoming developments of the theory, as the inclusion of dissipative effect beyond mean field.

We here briefly describe the various achievements attained during the past three years. The first step consisted in optimizing the FFT routines. Historically the NETLIB library was used. In 2012, a move to the FFTW3 library, optionally coupled to the Intel's MKL library, has been successfully implemented, and has allowed a typical speedup by 50 %. A second effort, done in parallel to the previous step, was devoted to a further parallelization of the code. A MPI parallelization already existed since more than 15 years, with a distribution of the wave functions over the processors. The implementation of OMP in the same spirit has been also achieved in 2012. However, the migration from FFTW3 to FFTW3-OMP does not bring a significant speedup of the calculations. Another implementation, using MPI instead, has been done on the grid points, on top of that done on the wave functions. Indeed, the size of the computation box is one of the major bottlenecks of our code. One can occasionally uses about 250 000 grid points, but the standard is more close to a million, and sometimes even more than a million and a half. Meanwhile, the CPU time almost linearly scales with the number of points. This is why in 2013, a MPI parallelization on the grid points has been implemented. The speedup compared with a serial calculation, using FFTW3, ranges from 2 (for 24 wave functions, box size of 96^3, and 16 processors) to 15 (for 240 wave functions, box size of 96^3 and 48 processors). There is of course a compromise between the number of processors, the box size and the number of wave functions to be found. Indeed, increasing the number of processors does not systematically enhance the speedup because one then increases the number of communications between the processors. One also, at the same time, consumes significantly more CPU serial hours with only a minor gain in the real calculation time. We have now to explore in a more systematic way the speedup for various clusters and molecules to establish a kind of rule of thumb for the evaluation of this compromise.

During the past two years, the use of GPU cores has also been tested, in NETLIB and FFTW3. With one GPU core per CPU core, the typical gain is about a factor 3 in NETLIB, while it is rather about 1.5 in FFTW3. When using a MPI parallelization on the wave functions on top of the use of GPU/CPU cores, a speedup by a factor 3 is also attained. Therefore, the use of GPU, which had implied a non-trivial coding, is probably not more competitive than the use of MPI/CPU. Moreover, calculations on GPU/CPU need specific machines which are not easily accessible, while multi-node machines are more widely used (even with a 4-core PC).

In parallel to these hardware developments, a dedicated web page has been prepared, in view of the forthcoming opening of the package. The objectives of this web page are threefold: downloading the TELEMAN package, from a GIT repository located in Le Mans with the latest version, as well as older ones; downloading a detailed documentation on the installation, compilation options, input and typical output files; accessing tutorials on benchmark test cases, with scripts that can automatically check whether the output files are correct or not. The web page already exists but is accessible for the moment to the PW-TELEMAN collaboration only. The official opening of the TELEMAN package will be materialized by the organization of an international conference, funded by our ANR-China contract, in Le Mans (France) next September, gathering experts and developers of TDDFT codes.

5

Articles published in peer-reviewed journals

The diversity of subjects treated at LPT translates into an equally large variety of scientific journals and conferences where LPT scientists publish and present their work.

The LPT scientists have published around 420 articles in peer-reviewed journals during the past five years. Number of publication per LPT thematic group (including a few preprints):

- **Fermions Fortement Corrélés (FFC): 113**
- **Cohérence Quantique (Quantware): 128**
- **Physique Statistique des Systèmes Complexes (PhyStat): 123**
- **Systèmes de Fermions Finis – Agrégats (Agrégats): 60**

❍ The **average number of authors** on a LPT article is close to 3: 1.4 permanent researcher at LPT, 0.4 LPT postdoc or PhD student, 1.4 non LPT researcher (including LPT visitors). The names of LPT permanent researchers are underlined and those of LPT postdocs/PhD students are dash-underlined in the publication list below and elsewhere in this document.

❍ Since 2009, more than **300 different authors** are involved in the LPT publications (excluding LPT permanent staff, postdocs, and PhD students). They work in **nearly 200 different institutions**[1] including **9 laboratories on the Toulouse campus**.

❍ Percentage of LPT publications since 2009 having **at least one author from a foreign institution**[2] **(32 countries involved)**: Germany ∼20 %, USA ∼10 %, Russia ∼6 %, Italy, Slovenia, UK (∼5 % each), Argentina, Belgium, Switzerland (∼4 % each)... The home institution of the main French collaborators outside Toulouse of the LPT scientists are the Université Paris-Sud, CEA Saclay, Université Pierre et Marie Curie, Université & ENS Lyon, Université de Montpellier, and ENS Paris.

❍ The following publication list includes, among others, 34 articles published in *Physical Review Letters* (and around 140 *Physical Review A-E*), and 1 in *Nature Communications*[2]. The LPT publications listed below have already attracted ∼3000 citations (900 in 2013), in ∼1800 citing articles without self-citations.

❍ 11 LPT articles solely published in APS journals were highlighted as *APS Editors' suggestion* and 6 were featured in *Physics*.

❍ Most LPT publications since 2006 are referenced on ArXiv and on the CNRS HAL repository.

1. Analyzing search results for LPT publications on ISI Web of Sciences.

2. In addition to APS journals (accounting for almost half of LPT publications), the main journals where LPT scientists publish their work are (cited according to the number of published articles): *European Physical Journal B, D, E, +*, *Journal of Physics A-C*, *New Journal of Physics*, *Europhysics Letters*, *Journal of Chemical Physics*, *Journal of Statistical Mechanics*...

5.1 Fermions Fortement Corrélés (FFC)

[1] J. Jacobsen, and F. Alet, *The semiflexible fully-packed loop model and interacting rhombus tilings*, Physical Review Letters **102**, 145702 (2009).

[2] 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).

[3] 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).

[4] 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 **80**, 094407 (2009).

[5] P. Azaria, S. Capponi, and P. Lecheminant, *Three-Component Fermi Gas in a one-dimensional Optical Lattice*, Physical Review A **80**, 041604(R) (2009).

[6] D. Schwandt, F. Alet, and S. Capponi, *Quantum Monte Carlo simulations of fidelity at magnetic quantum phase transitions*, Physical Review Letters **103**, 170501 (2009).

[7] K. S. D. Beach, F. Alet, M. Mambrini, and S. Capponi, *SU(N) Heisenberg model on the square lattice: a continuous-N quantum Monte Carlo study*, Physical Review B **80**, 184401 (2009).

[8] Manuela Capello and Didier 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).

[9] Marcin Raczkowski, Manuela Capello and Didier Poilblanc, *Unidirectional Charge Instability of the d-wave RVB Superconductor*, Acta Phys. Polon. **115**, 77 (2009).

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

[11] A. Ralko, M. Mambrini, and D. Poilblanc, *A Generalized Quantum Dimer Model Applied to the Frustrated Heisenberg Model on the Square Lattice: Emergence of a Mixed Columnar-Plaquette Phase*, Physical Review B **80**, 184427 (2009).

[12] Revaz Ramazashvili, *Kramers degeneracy in a magnetic field and Zeeman spin-orbit couplingin antiferromagnetic conductors*, Physical Review B **79**, 184432 (2009).

[13] Revaz Ramazashvili, *Electric excitation of spin resonance in antiferromagnetic conductors*, Physical Review B **80**, 054405 (2009).

[14] Revaz Ramazashvili, *Kramers degeneracy in a magnetic field and zeeman spin-orbit coupling in antiferromagnetic conductors*, Physica B **404**, 360 (2009).

[15] I. Affleck, N. Laflorencie and Erik S. Sorensen, *Entanglement entropy in quantum impurity systems and systems with boundaries*, J. Phys. A: Math. Theor. **42**, 504009 (2009).

[16] J. Bobroff, N. Laflorencie, L. K. Alexander, A. V. Mahajan, B. Koteswararao and P. Mendels, *Impurity-induced magnetic order in low dimensional spin gapped materials*, Physical Review Letters **103**, 047201 (2009).

[17] J. Sirker and N. Laflorencie, *NMR Response in quasi one-dimensional Spin-1/2 Antiferromagnets*, Europhysics Letters **86**, 57004 (2009).

[18] N. Laflorencie and F. Mila, *Theory of the field-induced BEC in the frustrated spin-1/2 dimer compound $BaCuSi_2O_6$* Physical Review Letters **102**, 060602 (2009).

[19] M.Moliner, D.C. Cabra, A. Honecker, P. Pujol and F. Stauffer, *Magnetization Process of the Classical Shastry-Sutherland Lattice* Physical Review B **79**, 144401 (2009).

[20] H. Nonne, P. Lecheminant, S. Capponi, G. Roux, and E. Boulat, *Haldane charge conjecture in one-dimensional multicomponent fermionic cold atoms*, Physical Review B **81**, 020408(R) (2010).

[21] L.K. Alexander, J. Bobroff, A.V. Mahajan, B. Koteswararao, N. Laflorencie and F. Alet, *Impurity effets in coupled-ladder $BiCu_2PO_6$: NMR and QMC*, Physical Review B **81**, 054438 (2010).

[22] T. Fabritius, S. Wessel, N. Laflorencie, *Finite temperature ordering of diluted graphene antiferromagnet*, Physical Review B **82**, 035402 (2010).

[23] A. F. Albuquerque, F. Alet, C. Sire, and S. Capponi, *Quantum Critical Scaling of Fidelity Susceptibility*, Physical Review B **81**, 064418 (2010).

[24] D. Charrier, and F. Alet, *Phase diagram of an extended classical dimer model*, Physical Review B **82**, 014429 (2010).

[25] D. Charrier, S. Capponi, M. Oshikawa, and P. Pujol, *Quantum phase transitions in three-leg spin tubes*, Physical Review B **82**, 075108 (2010).

[26] F. Alet, I. P. McCulloch, S. Capponi, and M. Mambrini, *Valence bond entanglement entropy of frustrated spin chains*, Physical Review B **82**, 094452 (2010).

[27] A. Banerjee, K. Damle and F. Alet, *Impurity spin texture at a deconfined quantum critical point*, Physical Review B **82**, 155139 (2010).

[28] H. Nonne, E. Boulat, S. Capponi, and P. Lecheminant, *Competing orders in the generalized Hund chain model at half-filling*, Physical Review B **82**, 155134 (2010).

[29] D. N. Aristov, C. Brünger, F. F. Assaad, M. N. Kiselev, A. Weichselbaum, S. Capponi, and F. Alet, *Asymmetric spin-1/2 two-leg ladders*, Physical Review B **82**, 174410 (2010).

[30] J.-M. Stéphan, G. Misguich and F. Alet, *Geometrical entanglement of critical XXZ and Ising chains and Affleck-Ludwig boundary entropies*, Physical Review B **82**, 180406(R) (2010).

[31] A. F. Albuquerque, and F. Alet, *Critical correlations for short-range valence-bond wavefunctions on the square lattice*, Physical Review B **82**, 180408(R) (2010).

[32] D. Poilblanc, M. Mambrini, and D. Schwandt, *Effective Quantum Dimer Model for the Kagome Heisenberg Antiferromagnet: Nearby Quantum Critical Point and Hidden Degeneracy*, Physical Review B **81**, 180402 (RC) (2010).

[33] A. Ralko, F. Trousselet, and D. Poilblanc, *Quantum Melting of Valence Bond Crystal Insulators and Novel Supersolid Phase at Commensurate Density*, Physical Review Letters **104**, 127203 (2010).

[34] D. Schwandt, M. Mambrini, and D. Poilblanc, *Generalized Hardcore Dimer Models approach to low-energy Heisenberg frustrated antiferromagnets: general properties and application to the kagome antiferromagnet*, Physical Review B **81**, 214413 (2010).

[35] J. Almeida, G. Roux, and D. Poilblanc, *Pair Density Waves in Coupled Doped Two-Leg Ladders*, Physical Review B **82**, 041102(R) (2010).

[36] Didier Poilblanc, *Entanglement spectra of quantum Heisenberg ladders*, *Entanglement spectra of quantum Heisenberg ladders*, Physical Review Letters **105**, 077202 (2010).

[37] D. Poilblanc and A. Ralko, *Impurity-doped Kagome Antiferromagnet: A Quantum Dimer Model Approach*, Physical Review B **82**, 174424 (2010).

[38] Revaz Ramazashvili, *Quantum Oscillations in Antiferromagnetic Conductors with Small Carrier Pockets*, Physical Review Letters **105**, 216404 (2010).

[39] A. Banerjee, K. Damle and F. Alet, *Impurity spin texture at a Néel-Valence Bond Solid critical point in $d = 2$ SU(3) quantum antiferromagnets*, Physical Review B **83**, 235111 (2011).

[40] F. Alet, S. Capponi, H. Nonne, P. Lecheminant, and I. P. McCulloch, *Quantum criticality in the SO(5) bilinear-biquadratic Heisenberg chain*, Physical Review B **83**, 060407(R) (2011).

[41] A. F. Albuquerque, D. Schwandt, B. Hetényi, S. Capponi, M. Mambrini, and A. M. Läuchli, *Phase Diagram of a Frustrated Quantum Antiferromagnet on the Honeycomb Lattice: Magnetic Order versus Valence-Bond Crystal formation*, Physical Review B **84**, 024406 (2011).

[42] H. Nonne, P. Lecheminant, S. Capponi, G. Roux, and E. Boulat, *Competing orders in one-dimensional half-filled multicomponent fermionic cold atoms: The Haldane-charge conjecture*, Physical Review B **84**, 125123 (2011).

[43] C. A. Lamas, S. Capponi, and P. Pujol, *Combined analytical and numerical approach to study magnetization plateaux in doped quasi-one-dimensional antiferromagnets*, Physical Review B **84**, 115125 (2011).

[44] S. Capponi, F. Alet, and M. Mambrini, *Entanglement of quantum spin systems: a valence-bond approach*, Modern Physics Letters B **25**, 917 (2011).

[45] H. Nonne, E. Boulat, S. Capponi, and P. Lecheminant, *Phase diagram of one-dimensional alkaline-earth cold fermionic atoms*, Modern Physics Letters B **25**, 955 (2011).

[46] Andreas W. W. Ludwig, Didier Poilblanc, Simon Trebst and Matthias Troyer, *Two-dimensional quantum liquids from interacting non-Abelian anyons*, New Journal of Physics **13**, 045014 (2011).

[47] Didier Poilblanc, *Out-of-equilibrium Correlated Systems: Bipartite Entanglement as a Probe of Thermalization*, Physical Review B **84**, 045120 (2011).

[48] Didier Poilblanc, Andreas W. W. Ludwig, Simon Trebst and Matthias Troyer, *Quantum Spin Ladders of non-Abelian anyons*, Physical Review B **83**, 134439 (2011).

[49] Yasir Iqbal, Federico Becca, Didier Poilblanc, *Valence-bond crystal in the extended kagome spin-1/2 quantum Heisenberg antiferromagnet: A variational Monte Carlo approach*, Physical Review B **83**, 100404(R) (2011).

[50] J. Ignacio Cirac, Didier Poilblanc, Norbert Schuch, Frank Verstraete, *Entanglement spectrum and boundary theories with projected entangled-pair states*, Physical Review B **83**, 245134 (2011).

[51] Yasir Iqbal, Federico Becca, Didier Poilblanc, *Projected wave function study of Z2 spin liquids on the kagome lattice for the spin-1/2 quantum Heisenberg antiferromagnet*, Physical Review B **84**, 020407(R) (2011), *Editor's suggestion*.

[52] Didier Poilblanc, Grégoire Misguich, *Competing Valence Bond Crystals in the Kagome Quantum Dimer Model*, Physical Review B **84**, 214401 (2011).

[53] A. Lavarélo, G. Roux and N. Laflorencie, *Melting of a frustration-induced dimer crystal and incommensurability in the J_1-J_2 two-leg ladder*, Physical Review B **84**, 144407 (2011).

[54] F. Crépin, N. Laflorencie, G. Roux and P. Simon, *Hard-core bosons on a 2-leg ladder: Mott insulator, Luttinger liquid, and Bose glass*, Physical Review B **84**, 054517 (2011).

[55] N. Laflorencie and F. Mila, *Condensate-free bosonic fluid induced by frustrated proximity effect*, Physical Review Letters **107**, 037203 (2011).

[56] H. F. Song, N. Laflorencie, S. Rachel and K. Le Hur, *Entanglement Entropy of the Two-Dimensional Heisenberg Antiferromagnet* Physical Review B **83**, 224410 (2011).

[57] A. F. Albuquerque, N. Laflorencie, J.-D. Picon and F. Mila, *Phase separation vs supersolid behavior in frustrated antiferromagnets*, Physical Review B **83**, 174421 (2011).

[58] J. Hoyos, N. Laflorencie, A. Vieira and T. Vojta, *Protecting clean critical points by local disorder correlations*, Europhysics Letters **93**, 30004 (2011).

[59] A.F. Albuquerque, F. Alet, and R. Moessner, *Coexistence of long-range and algebraic correlations for short-range valence-bond wave functions in three dimensions*, Physical Review Letters **109**, 147204 (2012).

[60] P. Corboz, S. Capponi, A. M. Läuchli, B. Bauer, and R. Orús, *Comment on "Topological quantum phase transitions of attractive spinless fermions in a honeycomb lattice" by Poletti D. et al.*, Europhysics Letters **98**, 27005 (2012).

[61] X. Plat, S. Capponi, and P. Pujol, *Combined analytical and numerical approach to magnetization plateaux in one-dimensional spin tube antiferromagnets*, Physical Review B **85**, 174423 (2012).

[62] K. Totsuka, P. Lecheminant, and S. Capponi, *Semiclassical Approach to Competing Orders in Two-leg Spin Ladder with Ring-Exchange*, Physical Review B **86**, 014435 (2012).

[63] H.-Y. Yang, A. F. Albuquerque, S. Capponi, A. M. Läuchli, K. P. Schmidt, *Effective Spin Couplings in the Mott Insulator of the Honeycomb Lattice Hubbard Model*, New Journal of Physics **14**, 115027 (2012).

[64] Didier Poilblanc, Matthias Troyer, Eddy Ardonne, Parsa Bonderson, *Fractionalization of itinerant anyons in one dimensional chains*, Physical Review Letters **108**, 207201 (2012).

[65] C. A. Lamas, A. Ralko, D. C. Cabra, D. Poilblanc, P. Pujol, *Statistical transmutation in doped quantum dimer models*, Physical Review Letters **109**, 016403 (2012).

[66] Didier Poilblanc, Norbert Schuch, David Pérez-García, J. Ignacio Cirac, *Topological and Entanglement Properties of Resonating Valence Bond wavefunctions*, Physical Review B **86**, 014404 (2012).

[67] Yasir Iqbal, Federico Becca, Didier Poilblanc, *Valence-bond crystals in the kagome spin-1/2 Heisenberg antiferromagnet: Symmetry classification and projected wave function study*, New Journal of Physics **14**, 115031 (2012).

[68] Norbert Schuch, Didier Poilblanc, J. Ignacio Cirac, David Perez-Garcia, *Resonating valence bond states in the PEPS formalism*, Physical Review B **86**, 115108 (2012), Editor's suggestion.

[69] Revaz Ramazashvili, *Zeeman coupling in low-carrier antiferromagnetic conductors with strong spinÐorbit interaction*, Physica B **407**, 1930 (2012).

[70] N. Laflorencie, *Sliding phase in randomly stacked 2D superfluids/superconductors*, Europhysics Letters **99**, 66001 (2012).

[71] T. Coletta, N. Laflorencie and F. Mila, *Semiclassical approach to ground-state properties of hard-core bosons in two dimensions*, Physical Review B **85**, 104421 (2012).

[72] S. Rachel, N. Laflorencie, H. F. Song, K. LeHur, *Detecting Quantum Critical Points using Bipartite Fluctuations*, Physical Review Letters **108**, 116401 (2012).

[73] H. F. Song, S. Rachel, C. Flindt, I. Klich, N. Laflorencie and K. Le Hur, *Bipartite Fluctuations as a Probe of Many-Body Entanglement*, Physical Review B **85**, 035409 (2012).

[74] N. Bartolo, D.J. Papoular, L. Barbiero, C. Menotti, A. Recati, *Dipolar-Induced Resonance for Ultracold Bosons in a Quasi-1D Optical Lattice*, Physical Review A **88**, 023603 (2013).

[75] M. Di Dio, L. Barbiero, A. Recati, M. Dalmonte, *Spontaneous Peierls dimerization and emergent bond order in one-dimensional dipolar gases* , preprint arXiv:1304.5200.

[76] S. Pujari, K. Damle and F. Alet, *Néel-State to Valence-Bond-Solid Transition on the Honeycomb Lattice: Evidence for Deconfined Criticality*, Physical Review Letters **111**, 087203 (2013).

[77] S. Pujari,and M. Lawler, *Effect of Dirac spinons on angle-resolved photoemission signatures of herbertsmithite*, Physical Review B **87**, 104415 (2013).

[78] S. Capponi, V. R. Chandra, A. Auerbach, and M. Weinstein, *p6 - Chiral Resonating Valence Bonds in the Kagome Antiferomagnet*, Physical Review B **87**, 161118(R) (2013).

[79] H. Nonne, M. Moliner, S. Capponi, P. Lecheminant, and K. Totsuka, *Symmetry-protected topological phases of alkaline-earth cold fermionic atoms in one dimension*, Europhysics Letters **102**, 37008 (2013).

[80] S. Capponi, P. Lecheminant, and M. Moliner, *Quantum phase transitions in multileg spin ladders with ring exchange*, Physical Review B **88**, 075132 (2013).

[81] S. Capponi, O. Derzhko, A. Honecker, A. M. Läuchli, J. Richter, *Numerical study of magnetization plateaus in the spin-1/2 kagome Heisenberg antiferromagnet* , Physical Review B **88**, 144416 (2013).

[82] C. A. Lamas, A. Ralko, M. Oshikawa, D. Poilblanc, and P. Pujol, *Statistics of holes and nature of the superfluid phases in quantum dimer models*, Physical Review B **87**, 104512 (2013).

[83] Yasir Iqbal, Federico Becca, Sandro Sorella and Didier Poilblanc, *Gapless spin-liquid phase in the kagome spin-1/2 Heisenberg antiferromagnet*, Physical Review B **87**, 060405(R) (2013).

[84] Norbert Schuch, Didier Poilblanc, J. Ignacio Cirac, and David Perez-Garcia, *Topological order in the PEPS formalism: Transfer operator and boundary Hamiltonians*, Physical Review Letters **111**, 090501 (2013).

[85] H.J. Changlani, S. Ghosh, S. Pujari, and C. L. Henley, *Emergent Spin Excitations in a Bethe Lattice at Percolation*, Physical Review Letters **111**, 157201 (2013).

[86] Didier Poilblanc, Adrian Feiguin, Matthias Troyer, Eddy Ardonne, and Parsa Bonderson, *One-dimensional itinerant interacting non-Abelian anyons*, Physical Review B **87**, 085106 (2013).

[87] Ling Wang, Didier Poilblanc, Gu Wen, and F. Verstraete, *Constructing gapless spin liquid state for the spin-1/2 $J_1 - J_2$ Heisenberg model on a square lattice*, Physical Review Letters **111**, 037202 (2013).

[88] Didier Poilblanc and Norbert Schuch, *Simplex $\mathbb{Z}_2$ spin liquids on the Kagome lattice with Entangled Pair States: spinon and vison coherence lengths, topological entropy and gapless edge modes*, Physical Review B **87**, 140407 (2013).

[89] Didier Poilblanc, Norbert Schuch, and J. Ignacio Cirac, *Field-induced superfluids and Bose liquids in projected entangled pair states*, Physical Review B **88**, 144414 (2013).

[90] S. Krämer, N. Laflorencie, R. Stern, M. Horvatić, C. Berthier, H. Nakamura, T. Kimura, and F. Mila, *Spatially Resolved Magnetization in Bose-Einstein Condensed state of $BaCuSi_2O_6$: Evidence for Imperfect Frustration*, Physical Review B **87**, 180405(R) (2013).

[91] J.-P. Álvarez Zúñiga, and N. Laflorencie, *Bose glass transition and spin-wave localization for 2D bosons in a random potential* , Physical Review Letters **111**, 160403 (2013).

[92] A. Lavarélo, G. Roux, and N. Laflorencie, *Magnetic responses of randomly depleted spin ladders*, Physical Review B **88**, 134420 (2013).

[93] H. D. Rosales, D. C. Cabra, C. A. Lamas, P. Pujol, M. E. Zhitomirsky, *Broken discrete symmetries in a frustrated honeycomb antiferromagnet*, Physical Review B **87**, 104402 (2013).

[94] A. Petković and V. Vinokur, *Fluctuation-induced noise in out-of-equilibrium disordered superconducting films* , Annals of Physics **339**, 412 (2013).

[95] R. Nath, K.M. Ranjith, J. Sichelschmidt, M. Baenitz, Yu. Skourski, F. Alet, I. Rousochatzakis and A.A. Tsirlin, *Hindered magnetic order from multiple dimensionalities in Cu_2PO_6*, Physical Review B **89**, 014407 (2014).

[96] D.J. Luitz, F. Alet, and N. Laflorencie, *Universal behavior beyond multifractality in quantum many-body systems*, Physical Review Letters **112**, 057203 (2014).

[97] D. Schwandt, F. Alet, and M. Oshikawa, *Valence bond distribution and correlation in bipartite Heisenberg antiferromagnets*, Physical Review B **89**, 104416 (2014).

[98] D.J. Luitz, F. Alet, and N. Laflorencie, *Shannon-Rényi entropies and participation spectra across 3d $O(3)$ criticality*, Physical Review B **89**, 165106 (2014).

[99] H. Casa Grande, N. Laflorencie, F. Alet, and A.P. Viera, *Analytical and numerical studies of disordered spin-1 Heisenberg chains with aperiodic couplings*, Physical Review B **89**, 134408 (2014).

[100] S. Capponi, S. S. Jahromi, F. Alet, and K. P. Schmidt, *Baxter-Wu model in a transverse magnetic field*, Physical Review E **89**, 069136 (2014).

[101] S. Yang, L. Lehman, D. Poilblanc, K. Van Acoleyen, F. Verstraete, J.I. Cirac, and N. Schuch, *Edge theories in Projected Entangled Pair State models*, Physical Review Letters **112**, 036402 (2014).

[102] Yasir Iqbal, Didier Poilblanc, and Federico Becca, *Vanishing spin gap in a competing spin-liquid phase in the kagome Heisenberg antiferromagnet*, Physical Review B **89**, 020407(R) (2014).

[103] M. V. Kartsovnik, V. N. Zverev, D. Andres, W. Biberacher, T. Helm, P. D. Grigoriev, R. Ramazashvili, N. D. Kushch, and H. Mülcer, *Magnetic quantum oscillations in the charge-density-wave state of the organic metals α-(BEDT-TTF)$_2$MHg(SCN)$_4$ with $M = K$ and Tl*, Low Temperature Physics/Fizika Nizkikh Temperatur **40**, 484 (2014).

[104] D. Huerga, J. Dukelsky, N. Laflorencie, and G. Ortiz, *Chiral phases of two-dimensional hard-core bosons with frustrated ring-exchange*, Physical Review B **89**, 094401 (2014).

[105] J.-P. Álvarez Zúñiga, G. Lemarié, and N. Laflorencie, *Spin wave theory for 2D disordered hard-core bosons*, to appear in AIP Conference Proceedings TIDS15 conference, arXiv:1310.0601 (2013).

[106] D.J. Luitz, N. Laflorencie, and F. Alet, *Participation spectroscopy and entanglement Hamiltonian of quantum spin models*, J. Stat. Mech. (2014) P08007.

[107] D. Poilblanc, P. Corboz, N. Schuch and I. Cirac, *RVB superconductors with fermionic projected entangled pair states*, Physical Review B **89**, 241106 (2014).

[108] S. Pujari and C.L. Henley, *Boson features in STM spectra of cuprate superconductors: Weak-coupling phenomenology*, Physical Review B **90**, 085129 (2014).

[109] Z. Ristivojevic, A. Petković, P. Le Doussal and T. Giamarchi, *Superfluid-Bose glass transition in one dimension*, preprint arXiv:1404.06788.

[110] D.J. Luitz, X Plat, N. Laflorencie, and F. Alet, *Improving entanglement and thermodynamic Rényi entropy measurements in quantum Monte Carlo*, Physical Review B **90**, 125105 (2014).

[111] A. Petrescu, H. F. Song, S. Rachel, Z. Ristivojevic, C. Flindt, N. Laflorencie, I. Klich, N. Regnault, and K. Le Hur, *Fluctuations and Entanglement spectrum in quantum Hall states*, preprint arXiv:1405.7816.

[112] T. Picot, and D. Poilblanc, *Nematic and supernematic phases in Kagome quantum antiferromagnets under a magnetic field*, preprint arXiv:1406.7205.

[113] Mohsin Iqbal, D. Poilblanc and Norbert Schuch, *Semionic resonating valence bond states*, preprint arXiv:1407.7773.

5.2 Cohérence Quantique (Quantware)

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

[2] 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 Societies **395**, 1934 (2009).

[3] 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).

[4] I. Garcia-Mata, and D.L. Shepelyansky, *Nonlinear delocalization on disordered Stark ladder*, European Physical Journal B **71**, 121 (2009).

[5] M. Mulansky, K. Ahnert, A. Pikovsky, and D.L. Shepelyansky, *Dynamical thermalization of disordered nonlinear lattices*, Physical Review E **80**, 056212 (2009).

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

[7] 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).

[8] A.D. Chepelianskii and D.L. Shepelyansky, *Microwave stabilization of edge transport and zero-resistance states*, Physical Review B **80**, 241308(R) (2009).

[9] K.M. Frahm, and D.L. Shepelyansky, *Diffusion and localization for the Chirikov typical map*, Physical Review E **80**, 016210 (2009).

[10] I.B. Khriplovich, and D.L. Shepelyansky, *Capture of dark matter by the Solar System*, International Journal of Modern Physics D **18**, N0.12, 1903 (2009).

[11] D.L. Shepelyansky, *Chirikov criterion*, Scholarpedia **4(9)**, 8567 (2009).

[12] I. Nechita, and Cl'ement Pellegrini, *Quantum Trajectories in Random Environment: the Statistical Model for a Heat Bath*, Confluentes Mathematici **1**, No. 2, 249-289 (2009).

[13] F. Benaych-Georges, and I. Nechita, *A permutation model for free random variables and its classical analogue*, Pacific Journal of Mathematics **242**, No. 1, 33-51 (2009).

[14] G. Aubrun, and I. Nechita, *Stochastic domination for iterated convolutions and catalytic majorization*, Annales de l'Institut Henri Poincaré: Probability and Statistics **45**, No. 3, 611-625 (2009).

[15] L. Arnaud and D. Braun, *Efficiency of Producing Random Unitary Matrices with Quantum Circuits*, Physical Review A **80**, 062329 (2009); arXiv:0807.0775v1

[16] L. Arnaud and D. Braun, *Distribution of Interference in the Presence of Decoherence*, Physical Review A **80**, 062329 (2009); arXiv:0910.1826

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

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

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

[20] O. Giraud, M. Znidaric and B. Georgeot *Quantum circuit for three-qubit random states* Physical Review A **80**, 042309 (2009).

[21] O. Giraud, J. Martin and B. Georgeot *Entanglement and localization of wavefunctions* Complex Phenomena in Nanoscale Systems, NATO Science for Peace and Security Series B : Physics and Biophysics (Springer Netherlands), 51 (2009).

[22] D.L. Shepelyansky and O.V. Zhirov, *Google matrix, dynamical attractors and Ulam networks*, Physical Review E **81**, 036213 (2010).

[23] L. Ermann, and D.L. Shepelyansky, *Google matrix and Ulam networks of intermittency maps*, Physical Review E **81**, 036221 (2010).

[24] L. Ermann, and D.L. Shepelyansky, *Ulam method and fractal Weyl law for Perron-Frobenius operators*, Eur. Phys. J. B **75**, 299 (2010).

[25] M.V. Entin, L.I. Magarill, and D.L. Shepelyansky, *Theory of resonant photon drag in monolayer graphene*, Physical Review B **81**, 165441 (2010).

[26] B. Georgeot, O. Giraud, and D.L. Shepelyansky, *Spectral properties of the Google matrix of the World Wide Web and other directed networks*, Physical Review E **81**, 056109 (2010).

[27] O.V. Zhirov, and D.L. Shepelyansky, *Towards Google matrix of brain*, Physics Letters A **374**, 3206 (2010).

[28] K.M. Frahm, and D.L. Shepelyansky, *Ulam method for the Chirikov standard map*, European Physical Journal B **76**, 57 (2010).

[29] A.O. Zhirov, O.V. Zhirov, and D.L. Shepelyansky, *Two-dimensional ranking of Wikipedia articles*, European Physical Journal B **77**, 523 (2010).

[30] D.L. Shepelyansky, *Poincaré recurrences in Hamiltonian systems with a few degrees of freedom*, Physical Review B **82**, 055202(R) (2010).

[31] B. Collins, and I. Nechita, *Eigenvalue and Entropy Statistics for Products of Conjugate Random Quantum Channels*, Entropy **12**, No. 6, 1612-1631 (2010).

[32] B. Collins, I. Nechita, and K. Życzkowski, *Random graph states, maximal flow and Fuss-Catalan distributions*, Journal of Physics A **43**, 275303 (2010).

[33] B. Collins, and I. Nechita, *Random quantum channels I: graphical calculus and the Bell state phenomenon*, Communications in Mathematical Physics **297**, No. 2, 345-370 (2010).

[34] D. Braun, *Versatile cold-atom simulator of non-Abelian gauge potentials*, Physical Review A **82**, 013617 (2010); arXiv:1002.1322

[35] D. Braun, *Parameter estimation with mixed quantum states*, European Physical Journal D **59**, 521 (2010); arXiv:1002.1323v1

[36] O. Giraud, P. A. Braun, D. Braun, *Quantifying Quantumness and the Quest for Queens of Quantum*, New Journal of Physics **12**, 063005 (2010), arXiv:1002.2158v1

[37] J. Martin, O. Giraud, P. A. Braun, D. Braun, and T. Bastin, *Multiqubit symmetric states with high geometric entanglement*, Physical Review A **81**, 062347 (2010), arXiv:1003.0593v1

[38] B. Roubert, P. A. Braun, and D. Braun, *Large effects of boundaries on spin amplification in spin chains*, Physical Review A **82**, 022302 (2010), arXiv:1003.5863

[39] B. Georgeot and F. Mila *Chirality of triangular antiferromagnetic clusters as a qubit* Physical Review Letters **104**, 200502 (2010).

[40] G. L. Gattobigio, A. Couvert, B. Georgeot and D. GuÃ©ry-Odelin *Interaction of a propagating guided matter wave with a localized potential* New Journal of Physics **12** 085013 (2010).

[41] N. Destainville, B. Georgeot and O. Giraud *Quantum algorithm for exact Monte Carlo sampling*, Physical Review Letters **104**, 250502 (2010).

[42] J. Martin, I. Garcia-Mata, O. Giraud, and B. Georgeot*Multifractal wave functions of simple quantum maps*,Physical Review E **82**, 046206 (2010).

[43] F. Lignières, B. Georgeot and J. Ballot *P-modes in rapidly rotating stars : Looking for regular patterns in synthetic asymptotic spectra*, Astronomische Nachrichten **331**, 1053 (2010) .

[44] O. Giraud and K. Thas *Hearing shapes of drums : Mathematical and physical aspects of isospectrality* Review of Modern Physics **82**, 2213 (2010).

[45] O.V. Zhirov, A.S. Pikovsky, and D.L. Shepelyansky, *Quantum vacuum of strongly nonlinear lattices*, Physical Review E **83**, 016202 (2011).

[46] L. Ermann, A.D. Chepelianskii, and D.L. Shepelyansky, *Fractal Weyl law for Linux kernel architecture*, European Physical Journal B **79**, 115 (2011).

[47] M.W. Abel, and D.L. Shepelyansky, *Google matrix of business process management*, European Physical Journal B **84**, 493 (2011).

[48] L. Ermann, and D.L. Shepelyansky, *Relativistic graphene ratchet on semidisk Galton board*, European Physical Journal B **79**, 357 (2011).

[49] J. Lages, and D.L. Shepelyansky, *Superinsulator as a phase of bi-particle localized states*, European Physical Journal B **81**, 237 (2011).

[50] O.V. Zhirov, and D.L. Shepelyansky, *Wigner crystal in snaked nanochannels*, European Physical Journal B **82**, 63 (2011).

[51] M. Mulansky, K.Ahnert, A.Pikovsky, and D.L. Shepelyansky, *Strong and weak chaos in weakly nonintegrable many-body Hamiltonian systems*, Journal of Statistical Physics **145**, 1256 (2011).

[52] L. Ermann, and D.L. Shepelyansky, *Google matrix of the world trade network*, Acta Physica Polonica A **120**, N0. 6A, A158 (2011).

[53] K.M. Frahm, B. Georgeot, and D.L. Shepelyansky, *Universal emergence of PageRank*, Journal of Physics A **44**, 465101 (2011) **(selected as Insight by the Editor)**.

[54] S. Attal, and I. Nechita, *Discrete approximation of the free Fock space*, Séminaire de Probabilités XLIII **2006/2011**, 379-394 (2011).

[55] K. Życzkowski, K. Penson, I. Nechita, and B. Collins, *Generating random density matrices*, Journal of Mathematical Physics **52**, 062201 (2011).

[56] B. Collins, and I. Nechita, *Random quantum channels II: Entanglement of random subspaces, RÃ©nyi entropy estimates and additivity problems*, Advances in Mathematics **226**, 1181-1201 (2011).

[57] B. Collins, and I. Nechita, *Gaussianization and eigenvalue statistics for Random quantum channels (III)*, Annals of Applied Probability **21**, No. 3, 1136-1179 (2011).

[58] G. Aubrun, and I. Nechita, *The multiplicative property characterizes ℓ_p and L_p norms*, Confluentes Mathematici **3**, No. 4, 637-647 (2011).

[59] D. Braun and J. Martin, *Heisenberg-limited sensitivity with decoherence-enhanced measurements*, Nature Communications, **2**, 223 (2011), arXiv:1005.4443

[60] D. Braun, J. Hoffman, and E. Tiesinga, *Superradiance of cold atoms coupled to a superconducting circuit*, Physical Review A **83**, 062305 (2011), arXiv:1101.5300v1

[61] D. Braun, *Ultimate quantum bounds on mass measurements with a nano-mechanical oscillator*, Europhysics Letters **94**, 68007 (2011), arXiv:1009.5020

[62] P. Nalbach, D. Braun, and M. Thorwart, *How "quantum" is the exciton dynamics in the Fenna-Matthews-Olson complex?*, Physical Review E **84**, 041926 (2011); arXiv:1104.2031

[63] G. L. Gattobigio, A. Couvert, B. Georgeot, and D. Guéry-Odelin*Exploring classically chaotic potentials with a matter wave quantum probe*, Physical Review Letters **107**, 254104 (2011). **(This article made the cover of the issue of the journal)**.

[64] M. Pasek, B. Georgeot, F. Lignieres, D. R. Reese *Regular modes in rotating stars*, Physical Review Letters **107**, 121101 (2011) .

[65] L. Ermann, A.D. Chepelianskii, and D.L. Shepelyansky, *Toward two-dimensional search engines*, Journal of Physics A **45**, 275101 (2012).

[66] L. Ermann, and D.L. Shepelyansky, *The Arnold cat map, the Ulam method and time reversal*, Physica D **241**, 514 (2012).

[67] K.M. Frahm, and D.L. Shepelyansky, *Poincaré recurrences of DNA sequences*, Physical Review E **85**, 016214 (2012).

[68] O.V. Zhirov, and D.L. Shepelyansky, *Wigner crystal in snaked nanochannels: outlook*, Physica B **407**, 1909 (2012).

[69] D.L. Shepelyansky, *Kolmogorov turbulence, Anderson localization and KAM integrability*, European Physical Journal B **85**, 199 (2012).

[70] V. Kandiah, and D.L. Shepelyansky, *PageRank model of opinion formation on social networks*, Physica A **391**, 5779 (2012).

[71] K.M. Frahm, A.D. Chepelianskii, and D.L. Shepelyansky, *PageRank of integers*, Journal of Physics A **45**, 405101 (2012).

[72] K.M. Frahm, and D.L. Shepelyansky, *Google matrix of Twitter*, European Physical Journal B **85**, 355 (2012).

[73] D.L. Shepelyansky, *Microwave ionization of hydrogen atoms*, Scholarpedia **7(1)**, 9795 (2012).

[74] I. Nechita, and C. Pellegrini, *Random repeated quantum interactions and random invariant states*, Probability Theory and Related Fields **151**, 299-320 (2012).

[75] T. Banica, I. Nechita, and K. Życzkowski, *Almost Hadamard matrices: general theory and examples*, Open Systems & Information Dynamics **19**, No. 4, 1250024 (2012).

[76] G. Aubrun, and I. Nechita, *Realigning random states*, Journal of Mathematical Physics **53**, 102210 (2012).

[77] B. Collins, I. Nechita, and D. Ye, *The absolute positive partial transpose property for random induced states*, Random Matrices: Theory and Applications **01**, 1250002 (2012).

[78] B. Collins, M. Fukuda, and I. Nechita, *Towards a state minimizing the output entropy of a tensor product of random quantum channels*, Journal of Mathematical Physics **53**, 032203 (2012).

[79] S. Belinschi, B. Collins, and I. Nechita, *Laws of large numbers for eigenvectors and eigenvalues associated to random subspaces in a tensor product*, Inventiones mathematicae **190**, No. 3, 647-697 (2012).

[80] O. Pinel, J. Fade, D. Braun, P. Jian, N. Treps, and C. Fabre, *Ultimate sensitivity of precision measurements with Gaussian quantum light : a multi-modal approach*, Physical Review A (Rapid Communications) **85**, 010101 (2012); arXiv:1105.2644

[81] Olivier Giraud, P. A. Braun, D. Braun, *Parametrization of spin-1 classical states*, Physical Review A **85**, 032101 (2012); arXiv:1110.0325

[82] N. Wiebe, D. Braun, and S. Lloyd, *Quantum Algorithm for Data Fitting*, Physical Review Letters **109**, 050505 (2012); arXiv:1204.5242; **(synopsis by the Editors in "Physics — spotlighting exceptional research")**

[83] Heng-Na Xiong, Wei-Min Zhang, Matisse Wei-Yuan Tu, and D. Braun, *Dynamically stabilized decoherence-free states in non-Markovian open fermionic systems*, Physical Review A **86**, 032107 (2012); arXiv:1207.1538

[84] B. Georgeot and O. Giraud *The game of go as a complex network*, Europhysics Letters **97**, 68002 (2012) **(selected as Editor's choice)**.

[85] G. L. Gattobigio, A. Couvert, G. Reinaudi, B. Georgeot and D. Guéry-Odelin *Optically guided beam splitter for propagating matter waves*,Physical Review Letters **109**, 030403 (2012) **(selected as Editor's suggestion; synopsis by the Editors in "Physics — spotlighting exceptional research")**.

[86] M. Pasek, F. Lignières, B. Georgeot and D. R. Reese *Regular Oscillation Subspectrum of Rapidly Rotating Stars*, Astronomy & Astrophysics **546**, A11 (2012) **(the paper made the cover of the october 2012 issue of the journal)** .

[87] I. Garcia-Mata, J. Martin, O. Giraud and B. Georgeot *Multifractality of quantum wave packets*, Physical Review E **86**, 056215 (2012).

[88] L. Ermann, and D.L. Shepelyansky, *Ecological analysis of world trade*, Physics Letters A **377**, 250 (2013).

[89] J. Lages, and D.L. Shepelyansky, *Dark matter chaos in the Solar System*, Monthly Notices of the Royal Astronomical Society Letters **430**, L25 (2013).

[90] L. Ermann, A.D. Chepelianskii, and D.L. Shepelyansky, *Symmetry breaking for ratchet transport in presence of interactions and magnetic field*, Physical Review E **87**, 022912 (2013).

[91] L. Ermann, K.M. Frahm, and D.L. Shepelyansky, *Spectral properties of Google matrix of Wikipedia and other networks*, European Physical Journal B **86**, 193 (2013).

[92] V. Kandiah, and D.L. Shepelyansky, *Google matrix analysis of DNA sequences*, PLoS ONE **8(5)**, e61519 (2013).

[93] K.M. Frahm, and D.L. Shepelyansky, *Poincaré recurrences and Ulam method for the Chirikov standard map*, European Physical Journal B **86**, 322 (2013).

[94] O.V. Zhirov, A.D. Chepelianskii, and D.L. Shepelyansky, *Towards a synchronization theory of microwave-induced zero-resistance states*, Physical Review B **88**, 035410 (2013).

[95] Y.-H. Eom, K.M. Frahm, A.Benczur, and D.L. Shepelyansky, *Time evolution of Wikipedia network ranking*, European Physical Journal B **86**, 492 (2013).

[96] L.Chakhmakhchyan, and D.L. Shepelyansky, *PageRank model of opinion formation on Ulam networks*, Physics Letters A **377**, 3119 (2013).

[97] Y.-H. Eom, and D.L. Shepelyansky, *Highlighting entanglement of cultures via ranking of multilingual Wikipedia articles*, PLoS ONE **8(10)**, e74554 (2013).

[98] L. Ermann, and D.L. Shepelyansky, *Quantum Gibbs distribution from dynamical thermalization in classical nonlinear lattices*, New Journal of Physics **15**, 123004 (2013).

[99] O.V. Zhirov, and D.L. Shepelyansky, *Thermoelectricity of Wigner crystal in a periodic potential*, Europhysics Letters **103**, 68008 (2013).

[100] D.L. Shepelyansky, *Chaos at Fifty Four in 2013*, arXiv:1306.6570[nlin.CD] (2013); short version at Phys. Today **67(3)**, 9 (2014).

[101] D.L. Shepelyansky, *Oriol Bohigas*, Scholarpedia **8(12)**, 31656 (2013).

[102] T. Banica, and I. Nechita, *Asymptotic eigenvalue distributions of block-transposed Wishart matrices*, Journal of Theoretical Probability **26**, 855-869 (2013).

[103] B. Collins, I. Nechita, and K. Życzkowski, *Area law for random graph states*, Journal of Physics A **46**, 305302 (2013).

[104] T. Banica, andI. Nechita, *Almost Hadamard matrices: the case of arbitrary exponents*, Discrete Applied Mathematics **161**, No. 16-17, 2367-2379 (2013).

[105] I. Nechita, C. Pellegrini, *Random pure quantum states via unitary Brownian motion*, Electronic Communications in Probability **18**, No. 27, 1-13 (2013).

[106] B. Collins, M. Fukuda, and I. Nechita, *Low entropy output states for products of random unitary channels*, Random Matrices: Theory and Applications **02**, 1250018 (2013).

[107] G. Lemarié, A. Kamlapure, D. Bucheli, L. Benfatto, J. Lorenzana, G. Seibold, S. C. Ganguli, P. Raychaudhuri, and C. Castellani, *Universal scaling of the order-parameter distribution in strongly disordered superconductors*, Physical Review B **87**, 184509 (2013).

[108] M. Lopez, J.-F. Clément, G. Lemarié, D. Delande, P. Szriftgiser and J. C. Garreau, *Phase diagram of the anisotropic Anderson transition with the atomic kicked rotor: theory and experiment*, New Journal of Physics **15**, 065013 (2013).

[109] J. P. Álvarez Zúñiga, G. Lemarié, N. Laflorencie, *Spin wave theory for 2D disordered hard-core bosons*, to appear in AIP Conference Proceedings TIDS15 conference, arXiv:1310.0601 (2013).

[110] F. Benatti, D. Braun, *Sub-shot noise sensitivities without entanglement*, Physical Review A **87**, 012340 (2013)

[111] O. Pinel, P. Jian, C. Fabre, N. Treps, D. Braun, *Quantum parameter estimation using general single-mode Gaussian states*, Physical Review A **88**, 040102(R) (2013)

[112] U. Marzolino, D. Braun, *Precision Measurements of Temperature and Chemical Potential of Quantum Gases*, Physical Review A **88**, 063609 (2013)

[113] P. Cheiney, F. Damon, G. Condon, B. Georgeot and D. Guéry-Odelin, *Realization of tunnel barriers for matter waves using spatial gaps*, Europhysics Letters **103**, 50006 (2013) .

[114] A. Pikovsky, *Robust synchronization of spin-torque oscillators with an LCR load*, Physical Review E **88**, 032812 (2013) .

[115] K.M. Frahm, Y.-H.Eom, and D.L. Shepelyansky, *Google matrix of the citation network of Physical Review*, arXiv:1310.5624 [physics.soc-ph], submitted to Physical Review E (2014).

[116] V. Kandiah, and D.L. Shepelyansky, *Google matrix analysis of C.elegans neural network*, Physics Letters A **378**, 1932 (2014)

[117] K.M. Frahm, and D.L. Shepelyansky, *Poisson statistics of PageRank probabilities of Twitter and Wikipedia networks*, European Physical Journal B, **87**, 93 (2014).

[118] G. Rollin, J.Lages, and D.L. Shepelyansky, *"Chaotic enhancement of dark matter density in binary systems and galaxies*, submitted to MNRAS Letters arXiv:1403.0254 [astro-ph.EP] (2014).

[119] L. Ermann, and D.L. Shepelyansky, *Destruction of Anderson localization by nonlinearity in kicked rotator at different effective dimensions*, Journal of Physics A (submitted) arXiv:arXiv:1403.2692 [cond-mat.dis-nn] (2014).

[120] Y.-H.Eom, and H.-H. Jo, *Generalized friendship paradox in complex networks: The case of scientific collaboration*, Scientific Reports **4**, 4603 (2014).

[121] H.-H. Jo and Y.-H.Eom, *Generalized friendship paradox in networks with tunable degree-attribute correlation*, arxiv:1405.1279.

[122] D. Braun, O. Giraud, I. Nechita, C. Pellegriini, and M. Znidaric, *A universal set of qubit quantum channels*, Journal of Physics A **47**, 135302 (2014).

[123] T. Banica, I. Nechita, and J.-M. Schlenker, *Submatrices of Hadamard matrices: complementation results*, Electronic Journal of Linear Algebra **27**, 197-212 (2014).

[124] T. Banica, andI. Nechita, *Block-modified Wishart matrices and free Poisson laws*, to appear in Houston Journal of Mathematics .

[125] M. Fukuda, and I. Nechita, *Asymptotically well-behaved input states do not violate additivity for conjugate pairs of random quantum channels*, to appear in Communications in Mathematical Physics .

[126] R. Dubertrand, I. García-Mata, B. Georgeot, O. Giraud, G. Lemarié and J. Martin *Two scenarios for quantum multifractality breakdown* Physical Review Letters **112**, 234101 (2014)

[127] V. Kandiah, B. Georgeot and O. Giraud *Move ordering and communities in complex networks describing the game of go* submitted to Physical Review E .

[128] R. Dubertrand and A. Goussev *Origin of the exponential decay of the Loschmidt echo in integrable systems*, Physical Review E **89**, 022915 (2014).

5.3 Physique Statistique des Systèmes Complexes (PhyStat)

[1] N. Destainville, M. Manghi, and J. Palmeri, *Microscopic mechanism for experimentally observed anomalous elasticity of DNA in 2D*, Biophysical Journal **96**, 4464-4469 (2009).

[2] M. Manghi, J. Palmeri, and N. Destainville, *Coupling between denaturation and chain conformations in DNA: stretching, bending, torsion and finite size effects*, Journal of Physics: Condensed Matter **21**, 034104 (2009).

[3] S. Prolhac, M. R. Evans and K. Mallick, *Matrix product solution of the multispecies partially asymmetric exclusion process*, Journal of Physics A **42**, 165004 (2009).

[4] S. Prolhac and K. Mallick, *Cumulants of the current in a weakly asymmetric exclusion process*, Journal of Physics A **42**, 175001 (2009).

[5] S. Prolhac, *A combinatorial solution for the current fluctuations in the exclusion process*, arXiv:0904.2356 (2009).

[6] 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).

[7] 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).

[8] 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).

[9] P.-H. Chavanis, *Dynamical and thermodynamical stability of two-dimensional flows: variational principles and relaxation equations*, European Physical Journal B **70**, 73 (2009).

[10] P.-H. Chavanis, *Statistics of the gravitational force in various dimensions of space: from Gaussian to Levy laws*, European Physical Journal B **70**, 413 (2009).

[11] F. Staniscia, P.-H. Chavanis, G. De Ninno, and D. Fanelli, *Out-of-equilibrium phase re-entrance(s) in long-range interacting systems*, Physical Review E **80**, 021138 (2009).

[12] C. Sire and S. Redner, *Understanding baseball team standings and streaks*, European Physical Journal B **67**, 473 (2009).

[13] T. Portet, F. Camps Febrer, J.-M. Escoffre, C. Favard, M.-P. Rols, and D. S. Dean, *Visualization of membrane loss during the shrinkage of giant vesicles under electropulsation*, Biophysical Journal **96**, 4109 (2009).

[14] J.-M. Escoffre, T. Portet, L. Wasungu, J. Teissié, 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).

[15] D. S. Dean, *Thermal Casimir effect with soft boundary conditions*, Physical Review E **79**, 011108 (2009).

[16] 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).

[17] D. S. Dean, R. R. Horgan, A. Naji, and R. Podgornik, *The thermal Casimir effect between random layered dielectrics*, Physical Review A **79**, 040101 (2009).

[18] D. S. Dean and A. Gopinathan, *The non-equilibrium behavior of pseudo-Casimir forces*, Journal of Statistical Mechanics, L08001 (2009).

[19] C. Touya, D. S. Dean, and C. Sire, *Dipole diffusion in a random electric field*, Journal of Physics A **42**, 375001 (2009).

[20] 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).

[21] 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).

[22] J. Palmeri, N. Ben Amar, H. Saidani, and A. Deratani, *Process modeling of brackish and seawater nanofiltration*, Desalination and Water Treatment **9**, 263 (2009).

[23] S. Prolhac, *Tree structures for the current fluctuations in the exclusion process*, Journal of Physics A **43**, 105002 (2010).

[24] S. Buyukdagli, M. Manghi, and J. Palmeri, *Ionic capillary evaporation in weakly charged nanopores*, Physical Review Letters **105**, 158103 (2010).

[25] M. Manghi, C. Tardin, J. Baglio, P. Rousseau, L. Salomé, and N. Destainville, *Probing DNA conformational changes with high temporal resolution by tethered particle motion*, Physical Biology **7**, 046003 (2010).

[26] S. Buyukdagli, M. Manghi, and J. Palmeri, *Variational approach for electrolyte solutions: from dielectric interfaces to charged nanopores*, Physical Review E **81**, 041601 (2010).

[27] M. Manghi, and N. Destainville, *Statistical mechanics and dynamics of two supported stacked lipid bilayers*, Langmuir **26**, 4057-4068 (2010).

[28] P.-H. Chavanis, *A stochastic Keller-Segel model of chemotaxis*, Communication in Nonlinear Science and Numerical Simulations **15**, 60 (2010).

[29] P.-H. Chavanis, *Hydrodynamics of Brownian particles*, Physica A **389**, 375 (2010).

[30] P.-H. Chavanis, *Kinetic theory of stellar systems, two-dimensional vortices and HMF model*, Theoretical Computational Fluid Dynamics **24**, 217 (2010).

[31] M. Lemou and P.-H. Chavanis, *Escape of stars from gravitational clusters in the Chandrasekhar model*, Physica A **389**, 1021 (2010).

[32] P.-H. Chavanis and L. Delfini, *Phase transitions in self-gravitating systems and bacterial populations with a screened attractive potential*, Physical Review E **81**, 051103 (2010).

[33] A. Naso, R. Monchaux, P.-H. Chavanis, and B. Dubrulle, *Statistical mechanics of Beltrami flows in axisymmetric geometry: Theory reexamined*, Physical Review E **81**, 066318 (2010).

[34] A. Campa and P.-H. Chavanis, *Dynamical stability criterion for inhomogeneous quasi-stationary states in long-range systems*, Journal of Statistical Mechanics P06001 (2010).

[35] P.-H. Chavanis, *Kinetic equations for systems with long-range interactions: a unified description*, Journal of Statistical Mechanics P05019 (2010).

[36] F. Staniscia, A. Turchi, D. Fanelli, P.-H. Chavanis, and G. De Ninno, *Negative specific heat in the canonical statistical ensemble*, Physical Review Letters **105**, 010601 (2010).

[37] A. Naso, S. Thalabard, G. Collette, P.-H. Chavanis, and B. Dubrulle, *Statistical mechanics of Beltrami flows in axisymmetric geometry: equilibria and bifurcations*, Journal of Statistical Mechanics P06019 (2010).

[38] P. Carcaud, P.-H. Chavanis, M. Lemou, and F. Mehats, *Evaporation law in kinetic gravitational systems described by simplified Landau models*, Discrete and Continuous Dynamical Systems **14**, 907 (2010).

[39] P.-H. Chavanis and A. Campa, *Inhomogeneous Tsallis distributions in the HMF model*, European Physical Journal B **76**, 581 (2010).

[40] P.-H. Chavanis, A. Naso, and B. Dubrulle, *Relaxation equations for two-dimensional turbulent flows with a prior vorticity distribution*, European Physical Journal B **77**, 167 (2010).

[41] A. Naso, P.-H. Chavanis, and B. Dubrulle, *Statistical mechanics of two-dimensional Euler flows and minimum enstrophy states*, European Physical Journal B **77**, 187 (2010).

[42] P.-H. Chavanis and R. Mannella, *Self-gravitating Brownian particles in two dimensions: the case of N=2 particles*, European Physical Journal B **78**, 139 (2010).

[43] A. Naji, D. S. Dean, J. Sarabadani, R. R. Horgan, and R. Podgornik, *Thermal Casimir-van der Waals interaction between randomly charged dielectrics*, Physical Review Letters **104**, 060601 (2010).

[44] A. F. Albuquerque, F. Alet, C. Sire, and S. Capponi, *Quantum critical scaling of fidelity susceptibility*, Physical Review E **81**, 064418 (2010).

[45] V. Démery and D. S. Dean, *Drag forces in classical fields*, Physical Review Letters **104**, 080601 (2010).

[46] D. S. Dean and A. J. Gopinathan, *Out-of-equilibrium behavior of Casimir-type fluctuation-induced forces for free classical fields*, Physical Review E **81**, 041126 (2010).

[47] D. S. Dean, R. R. Horgan, A. Naji, and R. Podgornik, *The effects of dielectric disorder on van der Waals interactions in slab geometries*, Physical Review E **81**, 051117 (2010).

[48] M. Golzio, J.-M. Escoffre, T. Portet, C. Mauroy, J. Teissié, D. S. Dean, and M.-P. Rols, *Observations of the mechanism of electromediated DNA uptake – from vesicles to tissues*, Current Gene Therapy **10**, 256 (2010).

[49] V. Démery and D. S. Dean, *Drag forces on inclusions in classical fields with dissipative dynamics*, European Journal of Physics E **32**, 377 (2010).

[50] J. Sarabadani, A. Naji, D. S. Dean, R. R. Horgan, and R. Podgornik, *Non-monotonic fluctuation-induced interactions between dielectric slabs carrying charge disorder*, Journal of Chemical Physics **133**, 174702 (2010).

[51] 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 **26**, 2574 (2010).

[52] P.-A. Cazade, J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Molecular Simulation of Ion-Specific Effects in Confined Electrolyte Solutions Using Polarizable Force fields*, Journal of Physical Chemistry C **114**, 12245 (2010).

[53] N. Destainville, *An alternative scenario for the formation of specialized protein nanodomains (cluster phases) in biomembranes*, Europhys. Lett. **91**, 58001 (2010).

[54] S. Prolhac and H. Spohn, *Two-point generating function of the free energy for a directed polymer in a random medium*, Journal of Statistical Mechanics P01031 (2011).

[55] S. Prolhac and H. Spohn, *The one-dimensional KPZ equation and the Airy process*, Journal of Statistical Mechanics P03020 (2011).

[56] C. Arita, A. Ayyer, K. Mallick and S. Prolhac, *Recursive structures in the multispecies TASEP*, Journal of Physics A **44**, 335004 (2011).

[57] S. Prolhac and H. Spohn, *The height distribution of the KPZ equation with sharp wedge initial condition: numerical evaluations*, Physical Review E **84**, 011119 (2011).

[58] S. Prolhac and H. Spohn, *The propagator of the attractive delta-Bose gas in one dimension*, Journal of Mathematical Physics **52**, 122106 (2011).

[59] S. Buyukdagli, M. Manghi, and J. Palmeri, *Ionic exclusion phase transition in neutral and weakly charged cylindrical nanopores*, Journal of Chemical Physics **134**, 074706 (2011).

[60] N. Meilhac, and N. Destainville, *Clusters of proteins in bio-membranes: insights into the roles of interaction potential shapes and of protein diversity*, Journal of Physical Chemistry B **115**, 7190 (2011).

[61] P.-H. Chavanis, *Brownian particles with long and short range interactions*, Physica A **390**, 1546 (2011).

[62] P.-H. Chavanis and C. Sire, *Exact analytical solution of the collapse of self-gravitating Brownian particles and bacterial populations at zero temperature*, Physical Review E **83**, 031131 (2011).

[63] P.-H. Chavanis, *Thermodynamics of the HMF model with a magnetic field*, European Physical Journal B **80**, 275 (2011).

[64] A. Naso, P.-H. Chavanis, and B. Dubrulle, *Statistical mechanics of Fofonoff flows in an oceanic basin*, European Physical Journal B **80**, 493 (2011).

[65] F. Staniscia, P.-H. Chavanis, and G. De Ninno, *Out-of-equilibrium phase transitions in the HMF model: a closer look*, Physical Review E **83**, 051111 (2011).

[66] P.-H. Chavanis, F. Baldovin, and E. Orlandini, *Noise-induced dynamical phase transitions in long-range systems*, Physical Review E **83**, 040101(R) (2011).

[67] P.-H. Chavanis, *The quantum HMF model: I. Fermions*, Journal of Statistical Mechanics P08002 (2011).

[68] P.-H. Chavanis, *The quantum HMF model: II. Bosons*, Journal of Statistical Mechanics P08003 (2011).

[69] P.-H. Chavanis, *Instability of a uniformly collapsing cloud of classical and quantum self-gravitating Brownian particles*, Physical Review E **84**, 031101 (2011).

[70] P.-H. Chavanis, *Mass-radius relation of Newtonian self-gravitating Bose-Einstein condensates with short-range interactions. I. Analytical results*, Physical Review D **84**, 043531 (2011).

[71] P.-H. Chavanis and L. Delfini, *Mass-radius relation of Newtonian self-gravitating Bose-Einstein condensates with short-range interactions. II. Numerical results*, Physical Review D **84**, 043532 (2011).

[72] P.-H. Chavanis, *BEC dark matter, Zeldovich approximation and generalized Burgers equation*, Physical Review D **84**, 063518 (2011).

[73] C. Sire, P.-H. Chavanis and J. Sopik, *Effective merging dynamics of two and three fluid vortices: Application to two-dimensional decaying turbulence*, Physical Review E **84**, 056317 (2011).

[74] D. S. Dean, A. Naji, and R. Podgornik, *Sample-to-sample fluctuations of electrostatic forces generated by quenched charge disorder*, Physical Review E **83**, 011102 (2011).

[75] T. Portet, C. Favard, J. Teissié, D. S. Dean, and M.-P. Rols, *Insights into the mechanisms of electromediated gene delivery and application to the loading of giant vesicles with negatively charged macromolecules*, Soft Matter **7**, 3872 (2011).

[76] J.-M. Escoffre, T. Portet, C. Favard, J. Teissié, D. S. Dean, and M.-P. Rols, *Electromediated formation of DNA complexes with cell membranes and its consequences for gene delivery*, Biochimica et Biophysica Acta **1808**, 1534 (2011).

[77] D. S. Dean and V. Démery, *Diffusion of active tracers in fluctuating fields*, Journal of Physics C **23**, 234114 (2011).

[78] V. Démery and D. S. Dean, *Perturbative path integral study of active and passive tracer diffusion in fluctuating fields*, Physical Review E **84**, 011148 (2011).

[79] V. Démery and D. S. Dean, *Thermal Casimir drag in fluctuating classical fields*, Physical Review E **84**, 010103(R) (2011).

[80] D. Boyer and D. S. Dean, *On the distribution of estimators of diffusion constants for Brownian motion*, Journal of Physics A **44**, 335003 (2011)

[81] C. Arita, A. Ayyer, K. Mallick and S. Prolhac, *Generalized matrix Ansatz in the multispecies exclusion process in the partially asymmetric case*, Journal of Physics A **45**, 195001 (2012).

[82] M. Manghi, N. Destainville, and J. Palmeri, *Mesoscopic models for DNA stretching under force: New results and comparison with experiments*, European Physical Journal E **35**, 110 (2012).

[83] A. K. Dasanna, N. Destainville, J. Palmeri, and M. Manghi, *Strand diffusion-limited closure of denaturation bubbles in DNA*, Europhysics Letters **98**, 38002 (2012).

[84] P.-H. Chavanis, *Growth of perturbations in an expanding universe with Bose-Einstein condensate dark matter*, Astronomy and Astrophysics **537**, A127 (2012).

[85] P.-H. Chavanis, *Kinetic theory of spatially homogeneous systems with long-range interactions: I. General results*, European Physical Journal Plus **127**, 19 (2012).

[86] P.-H. Chavanis, *Kinetic theory of two-dimensional point vortices with collective effects*, Journal of Statistical Mechanics, P02019 (2012).

[87] P.-H. Chavanis, *Kinetic theory of long-range interacting systems with angle-action variables and collective effects*, Physica A **391**, 3680 (2012).

[88] P.-H. Chavanis, *Kinetic theory of Onsager's vortices in two-dimensional hydrodynamics*, Physica A **391**, 3657 (2012).

[89] P.-H. Chavanis, *Virial theorem for rotating self-gravitating Brownian particles and two-dimensional point vortices*, International Journal of Modern Physics B **26**, 1241002 (2012).

[90] C. Herbert, B. Dubrulle, P.-H. Chavanis and D. Paillard, *Phase transitions and marginal ensemble equivalence for freely evolving flows on a rotating sphere*, Physical Review E **85**, 056304 (2012).

[91] C. Herbert, B. Dubrulle, P.-H. Chavanis and D. Paillard, *Statistical mechanics of quasi-geostrophic flows on a rotating sphere*, Journal of Statistical Mechanics, P05023 (2012).

[92] P.-H. Chavanis, *Dynamical stability of infinite homogeneous self-gravitating systems and plasmas: application of the Nyquist method*, European Physical Journal B **85**, 229 (2012).

[93] P.-H. Chavanis, *Virial theorem for Onsager vortices in two-dimensional hydrodynamics*, European Physical Journal Plus **127**, 159 (2012).

[94] P.-H. Chavanis and T. Harko, *Bose-Einstein condensate general relativistic stars*, Physical Review D **86**, 064011 (2012).

[95] C. Sire and P.-H. Chavanis, *Collapse and evaporation of a canonical self-gravitating gas*, in *Proceedings of the 12th Marcel Grossmann Meeting*, Eds. T. Damour, R. T. Jantzen, and R. Ruffini (World Scientific, Singapore, 2012).

[96] T. Portet, C. Mauroy, V. Démery, T. Houles, J.-M. Escoffre, D. S. Dean, and M.-P. Rols, *Destabilizing giant liposomes with electric fields: an overview of current applications*, Journal of Membrane Biology **245**, 555 (2012).

[97] D. S. Dean, V. Démery, V. A. Parsegian, and R. Podgornik, *Out-of-equilibrium relaxation of the thermal Casimir effect in a model polarizable material*, Physical Review E **85**, 031108 (2012).

[98] J. Dweik, B. Coasne, J. Palmeri, P. Jouanna, and P. Gouze, *Inner and subsurface distribution of water and ions in weakly and highly hydrophilic uncharged nanoporous materials: a molecular dynamics study of a confined NaI electrolyte solution*, Journal of Physical Chemistry C **116**, 726 (2012).

[99] R. Moliner-Salvador, A. Deratani, J. Palmeri, and E. Sanchez, *Use of nanofiltration membrane technology for ceramic industry wastewater treatment*, Boletin de la Sociedad Espanola de Ceramica y Vidrio **51**, 103 (2012).

[100] S. Prolhac, *Spectrum of the totally asymmetric simple exclusion process on a periodic lattice - bulk eigenvalues*, Journal of Physics A **46**, 415001 (2013).

[101] L. Horvath, T. A. Beu, M. Manghi, and J. Palmeri, *The vapor-liquid interface potential of (multi)polar fluids and its influence on ion solvation*, Journal of Chemical Physics **138**, 154702 (2013).

[102] A. K. Dasanna, N. Destainville, J. Palmeri, and M. Manghi, *Slow closure of denaturation bubbles in DNA: twist matters*, Physical Review E **87**, 052703 (2013).

[103] S. Weitz, and N. Destainville, *Attractive asymmetric inclusions in elastic membranes under tension: cluster phases and membrane invaginations*, Soft Matter **9**, 7804 (2013).

[104] A. Campa and P.-H. Chavanis, *Caloric curves fitted by polytropic distributions in the HMF model*, European Physical Journal B **86**, 170 (2013).

[105] P.-H. Chavanis, *Linear response theory for hydrodynamic and kinetic equations with long-range interactions*, European Physical Journal Plus **128**, 38 (2013).

[106] P.-H. Chavanis, *Efficiency of coherent vortices to trap dust particles in the solar nebula*, European Physical Journal Web of Conferences **46**, 06004 (2013).

[107] P.-H. Chavanis, *A cosmological model based on a quadratic equation of state unifying vacuum energy, radiation, and dark energy*, Journal of Gravity, 682451 (2013).

[108] P.-H. Chavanis, *A simple model of universe describing the early inflation and the late accelerated expansion in a symmetric manner*, AIP Conference Proceedings **1548**, 75 (2013).

[109] P.-H. Chavanis, *Kinetic theory of spatially inhomogeneous stellar systems without collective effects*, Astronomy and Astrophysics **556**, A93 (2013).

[110] P.-H. Chavanis, *Initial value problem for the linearized mean field Kramers equation with long-range interactions*, European Physical Journal Plus **128**, 106 (2013).

[111] P.-H. Chavanis, *Kinetic theory of spatially homogeneous systems with long-range interactions: II. Historic and basic equations*, European Physical Journal Plus **128**, 126 (2013).

[112] P.-H. Chavanis, *Kinetic theory of spatially homogeneous systems with long-range interactions: III. Application to power law potentials, plasmas, stellar systems, and to the HMF model*, European Physical Journal Plus **128**, 128 (2013).

[113] C. Ferreira Esmi, L. Schrive, Y. Barre, J. Palmeri, and Andre Deratani, *Using nanofiltration in a zero-rejection process: the removal of Ni2+ and Co2+ from salty wastewater*, Desalination and Water Treatment **51**, 476 (2013).

[114] S. Prolhac, *Spectrum of the totally asymmetric simple exclusion process on a periodic lattice - first excited states*, Journal of Physics A **47**, 375001 (2014).

[115] Y. Homsi, J. G. Schloetel, K. D. Scheffer, T. H. Schmidt, N. Destainville, L. Florin, and T. Lang, *The extracellular δ-domain is essential for the formation of CD81 tetraspanin webs*, Biophysical Journal **107**, 100 (2014).

[116] P.-H. Chavanis, *Gravitational phase transitions with an exclusion constraint in position space*, European Physical Journal B **87**, 9 (2014).

[117] P.-H. Chavanis, *Models of universe with a polytropic equation of state: I. The early universe*, European Physical Journal Plus **129**, 38 (2014).

[118] P.-H. Chavanis, *Statistical mechanics of two-dimensional point vortices: relaxation equations and strong mixing limit*, European Physical Journal B **87**, 81 (2014).

[119] P.-H. Chavanis and L. Delfini, *Random transitions described by the stochastic Smoluchowski-Poisson system and by the stochastic Keller-Segel model*, Physical Review E **89**, 032139 (2014).

[120] Y. Pomeau, M. LeBerre, P.-H. Chavanis and B. Denet, *Supernovae: an example of complexity in the physics of compressible fluids*, European Physical Journal E, **37**, 26 (2014).

[121] D. Calovi, U. Lopez, S. Ngo, C. Sire, H. Chaté, and G. Theraulaz, *Swarming, schooling, milling: phase diagram of a data-driven fish school model*, New Journal of Physics **16**, 015026 (2014).

[122] F. Sicard, N. Destainville and E. Manghi, *DNA denaturation bubbles: free-energy landscape and nucleation/closure rates*, arXiv:1405.3867 (2014).

[123] G. Gueguen, N. Destainville and E. Manghi, *Mixed lipid bilayers with locally varying spontaneous curvature and bending*, European Physical Journal E **37**, 76 (2014).

5.4 Systèmes de Fermions Finis – Agrégats (Agrégats)

[1] P. M. Dinh, F. Fehrer, P.-G. Reinhard, N. Rösch, and E. Suraud, *Dipole excitations of Ar substrate in contact with Na clusters*, Surface Science **603**, 400 (2009).

[2] Z. P. Wang, P. M. Dinh, P.-G. Reinhard, E. Suraud, G. Bruny, C. Montano, S. Feil, S. Eden, H. Abdoul-Carime, B. Farizon, M. Farizon, S. Ouaskit, and T.D. Maerk, *Production of intense beams of mass-selected water cluster ions and theoretical study of atom-water interactions*, International Journal of Mass Spectrometry **285**, 143 (2009).

[3] J. Messud, Z. P. Wang, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Polarizabilities as a test of localized approximations to the self-interaction correction*, Chemical Physics Letters **479**, 300 (2009).

[4] J. Messud, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Simplification of the time-dependent generalized self-interaction correction method using two sets of orbitals : Application of the optimized effective potential formalism*, Physical Review A **80**, 044503 (2009).

[5] M. Bär, P. M. Dinh, L. V. Moskaleva, P.-G. Reinhard, N. Rösch, and E. Suraud, *Deposition of Na Clusters on MgO(001)*, Physical Review B **80**, 195404 (2009).

[6] V. O. Nesterenko, A. N. Novikov, A. Yu Cherny, F. F. de Souza Cruz, and E. Suraud, *An adiabatic transport of Bose-Einstein condensates in double-well traps*, Physical Review B **42**, 235303 (2009).

[7] J. Messud, M. Bender and E. Suraud, *Density functional theory and Kohn-Sham scheme for self-bound systems*, Physical Review C **80**, 054314 (2009).

[8] T. Raitza, H. Reinholz, G. Röpke, I. Morozov and E. Suraud, *Laser Excited Expanding Small Clusters: Single Time Distribution Functions*, Contributions to Plasma Physics **49**, 496(2009).

[9] P. Romaniello, S. Guyot and L. Reining, *The self-energy beyond GW: Local and nonlocal vertex corrections*, Journal of Chemical Physics **131**, 154111 (2009).

[10] P. Romaniello, D. Sangalli, J. A. Berger, F. Sottile, L. Molinari, L. Reining, and G. Onida, *The self-energy beyond GW: Local and nonlocal vertex corrections*, Journal of Chemical Physics **130**, 044108 (2009)

[11] P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Dynamics of clusters and molecules in contact with an environment*, Physics Reports **485**, 43 (2010).

[12] T. Fennel, K.-H. Meiwes-Broer, J. Tiggesbäumker, P.-G. Reinhard, P. M. Dinh, and E. Suraud, *Laser-driven nonlinear cluster dynamics : from single- and multiphoton excitations to the strong-field domain*, Review of Modern Physics **82**, 1793 (2010).

[13] M. Baer, P. M. Dinh, L. V. Moskaleva, P.-G. Reinhard, N. Roesch, and E. Suraud, *Angular distributions of electrons emitted from free and deposited Na_8 clusters*, Physica Status Solidi B **247**, 1122 (2010).

[14] U. F. Ndongmouo-Taffoti, P. M. Dinh, P.-G. Reinhard, E. Suraud, and Z. P. Wang, *Exploration of dynamical regimes of irradiated small water clusters*, European Journal of Physics D **58**, 131 (2010).

[15] S. Vidal, Z. P. Wang, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Frequency dependence of level depletion in Na clusters and in C_2H_4*, Journal of Physics B **43**, 165102 (2010).

[16] P. M. Dinh, J. Messud, P.-G. Reinhard, and E. Suraud, *The self-interaction correction in the time domain*, Journal of Physics : Conference Series **248**, 012024 (2010).

[17] M. Baer, B. Faber, P.-G. Reinhard, P. M. Dinh, E. Suraud, and P. Wopperer, *Dynamics of Na clusters in/on insulating substrates*, Journal of Physics : Conference Series **248**, 012023 (2010).

[18] P. Wopperer, B. Faber, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Angular distributions of photo-electrons from free Na clusters*, Physical Review A **82**, 063416 (2010).

[19] P. Wopperer, B. Faber, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Orientation averaged angular distributions of photo-electrons from free Na clusters*, Physics Letters A **375**, 39 (2010).

[20] V. O. Nesterenko, A. N. Novikov, E. Suraud, and J Kvasil, *Tunneling and transport dynamics of trapped Bose-Einstein condensates*, Journal of Physics : Conference Series **248**, 012033 (2010).

[21] V. O. Nesterenko, A. N. Novikov, and E. Suraud, *Adiabatic transport of Bose-Einstein condensates in a double-well trap: Case of weak nonlinearity*, Laser Physics **20**, 1149 (2010).

[22] P. Romaniello, M. C. D'Andria, and F. Lelj, *Nonlinear optical properties of $Ni(Me_6pzS_2)MX$ (M=Ni, Pd, Pt; X=Me_2timdt, mnt)*, Journal of Physical Chemistry A **114**, 5838 (2010).

[23] Z. P. Wang, P. M. Dinh, P.-G. Reinhard, E. Suraud, and F. S. Zhang, *Non-adiabatic effects in the irradiation of ethylene*, International Journal of Quantum Chemistry **111**, 480 (2011).

[24] J. Messud, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *The Generalized SIC-OEP formalism and the Generalized SIC-Slater approximation (stationary and time-dependent cases)*, Annalen der Physik **523**, 270 (2011).

[25] D. Sangalli, P. Romaniello, G. Onida, and A. Marini, *Double excitations in correlated systems: a many-body approach)*, Journal of Chemical Physics **134**, 034115 (2011).

[26] M. Guzzo, G. Lani, F. Sottile, P. Romaniello, M. Gatti, J.J. Kas, J. J. Rehr, M. G. Silly, F. Sirotti, and L. Reining, *Valence Electron Photoemission Spectrum of Semiconductors: Ab Initio Description of Multiple Satellites)*, Physical Review Letters **107**, 166401 (2011).

[27] E. DelRe, P. Di Porto, S. Di Sabatino, and B. Crosignani, *Reduced statistical fluctuations of the position of an object partitioning in two its environment*, AIP Conference Proceedings **1411** (2011).

[28] E. DelRe, B. Crosignani, P. Di Porto, and S. Di Sabatino, *Built-in reduction of statistical fluctuations of partitioning objects*, Physical Review Letters **84**, 021112 (2011).

[29] P. M. Dinh, J. Douady, F. Fehrer, B. Gervais, E. Giglio, A. Ipatov, P.-G. Reinhard, and E. Suraud, *A hierarchical approach for the dynamics of Na clusters in contact with an Ar substrate*, chapter in Theoretical and Computational Developments in Modern Density Functional Theory, Editors : Amlan K. Roy, Nova Science Publishers, pp. 391-424 (2012).

[30] P. Wopperer, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Frequency dependence of photoelectron angular distributions in small Na clusters*, Physical Review A **85**, 015402 (2012).

[31] P. M. Dinh, S. Vidal, P.-G. Reinhard, and E. Suraud, *Fingerprints of level depletion in photoelectron spectra of small sodium cluster in the UV domain*, New Journal of Physics **14**, 063015 (2012).

[32] M. Baer, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Photoelectron spectra : a tool of analysis of irradiation dynamics*, Journal of Physics : Conference Series **373**, 012011 (2012).

[33] D. Berger, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *A study of colour centers in MgO using a hierarchical model*, European Journal of Physics D **66**, 164 (2012).

[34] B. Faber, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Na clusters on metal supported Ar layers*, European Journal of Physics D **66**, 194 (2012).

[35] J. M. Escartín, P. Romaniello, L. Stella, P.-G. Reinhard, and E. Suraud, *On transition rates in surface hopping*, Journal of Chemical Physics **137**, 234113 (2012)

[36] V. O. Nesterenko, A. N. Novikov, and E. Suraud, *Strong coupling dynamics of Bose Einstein condensate in a double-well trap*, Journal of Physics B **45**, 225503s (2012).

[37] P. M. Dinh, D. Berger, B. Faber, P.-G. Reinhard, and E. Suraud, *Variations on a QM/MM approach to cluster dynamics*, Journal of Physics : Conference Series **393**, 012002 (2012).

[38] P. Wopperer, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Laser excitation from clusters: observables from electron emission*, Journal of Physics : Conference Series **393**, 012001 (2012).

[39] G. Lani, P. Romaniello, and L. Reining, *Approximations for many-body Green's functions: insights from the fundamental equations*, New Journal of Physics **14**, 013056 (2012).

[40] P. Romaniello, F. Bechstedt, and L. Reining, *Beyond the GW approximation: Combining correlation channels*, Physical Review B **85**, 155131 (2012).

[41] P. M. Dinh, P. Romaniello, P.-G. Reinhard, and E. Suraud, *Calculation of photoelectron spectra : A mean-field-based scheme*, Physical Review A **87**, 032514 (2013).

[42] M. Vincendon, P. M. Dinh, P. Romaniello, P.-G. Reinhard, and E. Suraud, *Photoelectron spectra from time-dependent fully self-interaction corrected density functional theory*, European Journal of Physics D **67**, 97 (2013).

[43] P. Wopperer, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Dynamics of irradiation : from clusters to nano-objects and from material science to biology*, Journal of Physics : Conference Series **410**, 012158 (2013).

[44] P. Wopperer, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *On the role of resonances in photoionization of metal clusters*, Journal of Physics : Conference Series **438**, 012010 (2013).

[45] Ch. Neidel, J. Klei, C.-H. Yang, A. Rouzée, M. J. J. Vrakking, K. Klünder, M. Miranda, C. L. Arnold, T. Fordell, A. L'Huillier, M. Gisselbrecht, P. Johnsson, P. M. Dinh, E. Suraud, P.-G. Reinhard, V. Despré, M. A. L. Marques, and F. Lépine, *Probing Time-Dependent Molecular Dipoles on the Attosecond Time Scale*, Physical Review Letters **111**, 033001 (2013).

[46] P. Kluepfel, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Koopmans condition in self-interaction corrected density functional theory*, Physical Review A **88**, 052501 (2013).

[47] C. Z. Gao, J. Wang, F. S. Zhang, *Collision of H^++ CH_4 at 30 eV : A simulation study*, Nuclear Instruments and Methods B **307**, 225 (2013).

[48] C. Z. Gao, J. Wang, F. S. Zhang, *Dynamics of proton collisions with acetylene, ethylene and ethane at 30 eV*, Chemical Physics **410**, 9 (2013).

[49] S. Denifl, G. Garcia, B. A. Huber, B. P. Marinovic, N. Mason, J. Postler, H. Rabus, G. Rixon, A. V. Solov'yov, E. Suraud, and A. V. Yakubovitch, *Radiation damage of biomolecules (RADAM) database development: current status*, Journal of Physics : Conference Series **438**, 012016 (2013).

[50] P. Wopperer, P.-G. Reinhard, and E. Suraud, *On photo-electron angular distributions from clusters*, Annalen der Physik (Berlin) **525**, 309 (2013).

[51] P.-G. Reinhard, P. Wopperer, P. M. Dinh, and E. Suraud, *On Electronic Photoemission from Irradiated C_{60}* (online only).

[52] P. Di Porto, S. Di Sabatino, B. Crosignani, and E. DelRe, *Power-Law Relaxation and Cumulative Information*, Journal of Statistical Physics **153**, 479 (2013).

[53] N. Slama, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Dissipation in quantum time dependent mean field*, Journal of Physics : Conference Series, in press (2014).

[54] C. Z. Gao, J. Wang, F. S. Zhang, *Theoretical study on collision dynamics of H^++ CH_4 at low energies*, Journal of Chemical Physics **140**, 054308 (2014).

[55] F. Mao, C. Zhang, C. Z. Gao, J. Dai, and F. S. Zhang, *The effects of electron transfer on the energy loss of slow He^{2+}, C^{2+}, and C^{4+} ions penetrating a graphene fragment*, Journal of Physics : Condensed Matter **26**, 085402 (2014).

[56] J. Wang, C. Z. Gao, F. Calvayrac, and F. S. Zhang, *Collision dynamics of proton with formaldehyde: Fragmentation and ionization*, Journal of Chemical Physics **140**, 124306 (2014).

[57] G. Reitsma, O. Gonzalez-Magana, O. Versolato, M. Door, R. Hoekstra, E. Suraud, B. Fischer, N. Camus, M. Kremer, R. Moshammer, and T. Schlathölter, *Femtosecond laser induced ionization and dissociation of gas-phase protonated leucine enkephalin*, International Journal of Mass Spectrometry, in press (2014).

[58] P. M. Dinh, C. Z. Gao, P. Kluepfel, P.-G. Reinhard, E. Suraud, M. Vincendon, J. Wang, and F. S. Zhang, *A density functional theory study of $Na(H_2O)_n$: an example of the impact of self-interaction corrections*, European Journal of Physics D **68**, 239 (2014).

[59] F. Berthias, V. Buridon, H. Abdoul-Carime, B. Farizon, M. Farizon, P. M. Dinh, P.-G. Reinhard, E. Suraud, and T.D. Märk, *Collision induced dissociation of protonated water clusters*, Physical Review A, **89**, 062705 (2014).

[60] P. Wopperer, P. M. Dinh, P.-G. Reinhard, and E. Suraud, *Electrons as probes of dynamics in molecules and clusters : a contribution from Time Dependent Density Functional Theory*, Physics Reports, in press (2014).

6

International and national conferences

The LPT scientists have intervened in more than 350 international and national conferences during the past five years. Number of presentations per LPT thematic group:

- **Fermions Fortement Corrélés (FFC): 100**
- **Cohérence Quantique (Quantware): 89**
- **Physique Statistique des Systèmes Complexes (PhyStat): 68**
- **Systèmes de Fermions Finis – Agrégats (Agrégats): 94**

The diversity of subjects treated at LPT translates into an equally large variety of conferences where LPT scientists present their work.

6.1 Fermions Fortement Corrélés (FFC)

[1] F. Alet, *Entanglement and fidelity of quantum spin systems : a valence bond approach*, talk at the *Joint European Japanese Conference : Frustration in Condensed Matter* (Lyon, France, May 2009).

[2] F. Alet, *Entanglement and fidelity of quantum spin systems : a valence bond approach*, talk at the *Workshop "Topological Order: From Quantum Hall Systems to Magnetic Materials"* (MPI Dresden, Germany, July 2009).

[3] S. Capponi, *Effective Theory of Magnetization Plateaux in the Shastry-Sutherland Lattice*, talk at the *Joint European Japanese Conference : Frustration in Condensed Matter* (Lyon, France, May 2009).

[4] S. Capponi, *Three-Component Fermi Gas in a one-dimensional Optical Lattice*, talk at the *ICAM International Workshop on "Emergent Quantum Phenomena from the Nano- to the Macro-World"* (Cargèse, France, July 2009).

[5] 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"* (Cargèse, France, July 2009).

[6] 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 *mesoscopic physics GDR meeting* (Aussois, France, October 2009).

[7] S. Capponi, *Entanglement & Fidelity of quantum spin systems: a Valence-Bond approach*, invited talk at the *CTS Condensed Matter Program 2009* (Mahabaleshwar, India, December 2009).

[8] N. Laflorencie, *Field-induced triplet BEC in frustrated bilayers, application to the Han Purple pigment $BaCuSi_2O_6$*, talk at the *Joint European Japanese Conference : Frustration in Condensed Matter* (Lyon, France, May 2009).

[9] M. Mambrini, *From Frustrated Heisenberg Quantum Antiferromagnets to Quantitative Generalized Quantum Dimer Models*, invited talk at the Condensed-matter school and workshop "ICTS Condensed Matter Programme 2009" (ICMP09), Mahabaleshwar, India, 5-23 December 2009.

[10] D. Poilblanc, 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.

[11] D. Poilblanc, invited talk at the International Workshop on "The Next Generation of Quantum Simulations", Richard B. Gump South Pacific Research Station (Univ. of Berkeley), Moorea, French Polynesia, 2-7 May 2009.

[12] D. Poilblanc, International Workshop "Emergence of inhomogeneous phases in strongly correlated electron systems", University of Florida Paris Research Center, Paris, France June 30 - July 3, 2009.

[13] D. Poilblanc, invited talk at the Max-Plank-Institute Dresden workshop on "Topological Order, From Quantum Hall Systems to Magnetic Materials", , APCTP-MPIPKS Seminar and Workshop - July 19-24, 2009.

[14] D. Poilblanc, 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'Etudes Scientifiques de Cargèse, Corsica, France, 6-19 July 2009.

[15] D. Poilblanc, invited talk at the KITP Workshop "The Physics of Higher Temperature Superconductivity"„ UC Santa Barbara, August 8 - Sept. 11 2009.

[16] D. Poilblanc, invited talk at the Réunion d'Aspet, GDR MICO„ octobre 12-15, 2009.

[17] D. Poilblanc, invited talk at the Condensed-matter school and workshop "ICTS Condensed Matter Programme 2009" (ICMP09), Mahabaleshwar, India, 5-23 December 2009.

[18] F. Alet, *Measuring entanglement with valence bonds*, invited talk at the conference *New trends in quantum magnetism* (Orsay, France, June 2010).

[19] F. Alet, *Quantum critical scaling of fidelity susceptibility revisited*, invited talk at the *workshop Quantum Information Concepts for Condensed Matter Problems* (MPI Dresden, Germany, June 2010).

[20] F. Alet, *Entanglement & Fidelity of quantum spin systems: a Valence-Bond approach*, invited *Theoretical Physics colloquium* (Kaiserslautern, Germany, July 2010)

[21] F. Alet, *Short-range Valence Bond physics : old wave-functions, new results*, invited talk at the *ICTS Condensed Matter Programme 2010 workshop* (Mysore, India, December 2010).

[22] S. Capponi, *Exotic phases of matter*, poster presented at the *4th Japanese-French Symposium Frontiers of Science* (Poitiers, France, January 2010).

[23] 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 *"Time-dependent dynamics and non-equilibrium quantum systems" conference* (Budapest, Hungary, May 2010).

[24] S. Capponi, *Exotic phases with one-dimensional multicomponent fermionic cold atoms*, invited talk at the *Theory of Quantum Gases and Quantum Coherence workshop* (Nice, France, June 2010).

[25] S. Capponi, *Entanglement & Fidelity of quantum spin systems: a Valence-Bond approach*, invited talk at the *International Conference on Frustrated Spin Systems, Cold Atoms and Nanomaterials* (Hanoi, Vietnam, July 2010); *Modern Physics Letters B* **25**, 917 (2011).

[26] S. Capponi, *Effective models with contractor-renormalization technique*, invited talk at the *International workshop on "Density Matrix Renormalization Group and other Advances in Numerical renormalization Group Methods"* (Beijing, China, October 2010).

[27] S. Capponi, *Computing fidelity with Quantum Monte-Carlo*, talk at the *KITP workshop "Disentangling Quantum Many-body Systems"* (Santa Barbara, USA, October 2010).

[28] N. Laflorencie, *Gapped Quantum Magnets at High Magnetic Field*, invited talk at the *Rencontres LPS-LPTMS* (Orsay, March 2010).

[29] N. Laflorencie and F. Mila, *Superfluididty without condensate*, invited talk at the *Perspectives in Highly Frustrated Magnetism* (Dresden, April 2010).

[30] N. Laflorencie, *Field-induced exotic triplet BEC in the frustrated bilayers* $BaCuSi_2O_6$, poster presentation and organisation of the conference *New trends in quantum magnetism* (Orsay, France, June 2010).

[31] N. Laflorencie, *Entanglement in 1D quantum spins systems: impurities and disorder effects*, invited talk at the *workshop Quantum Information Concepts for Condensed Matter Problems* (MPI Dresden, Germany, June 2010).

[32] N. Laflorencie, *Superfluididty without Bose Condensation for frustrated bosons*, talk at the *workshop Condensed Matter in Paris* (IHP Paris, France, November 2010).

[33] M. Mambrini, *A Generalized Quantum Dimer Model for the singlet sector of the kagome antiferromagnet*, invited talk at the International Workshop " Novel Physics on the kagome network", Univ. Paris-Sud, Orsay, 18-20 January 2010,.

[34] M. Mambrini, *From frustrated Heisenberg antiferromagnets to generalized quantum dimer models : an exact projection scheme*, invited talk at the International Workshop "New trends in Quantum Magnetism", Orsay, June 1-3 2010.

[35] D. Poilblanc, invited talk at the International Workshop " Novel Physics on the kagome network", Univ. Paris-Sud, Orsay, 18-20 January 2010,.

[36] D. Poilblanc, invited talk at the International Workshop "New trends in Quantum Magnetism", Orsay, June 1-3 2010.

[37] D. Poilblanc, invited talk at the International Workshop "Quantum Information Concepts for Condensed Matter Problems", Max-Planck-Institute PKS Dresden, 14-19 January 2010.

[38] D. Poilblanc, invited talk at the International Workshop "Emergence of New States of Matter in Magnetic Systems and Beyond", ICTP Trieste, 5-9 July 2010.

[39] D. Poilblanc, invited talk at the International Conference Superstripes, Majorana Theoretical Physics Center, Erice, 19-24 July 2010.

[40] D. Poilblanc, invited talk at the International Workshop "Resonating Valence Bond Physics: Spin Liquids and Beyond", Budapest, 13-15 October 2010.

[41] D. Poilblanc, invited talk (and Scientific Adviser) at the International Workshop "Disentangling Quantum Many-body Systems: Computational and Conceptual Approaches", KITP & UC Santa Barbara, 21 nov. – 18 déc. 2010.

[42] P. Pujol, *Topological transition in quantum spin tubes*, invited talk at the *"Advanced Study Group 2010 on Unconventional Magnetism on High Fields" workshop* (Dresde, Germany, June 2010).

[43] F. Alet, *A second look at short-range valence bond physics*, invited talk at the *Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter workshop* (ICTP Trieste, Italy, July 2011).

[44] F. Alet, *Coulomb phase of hardcore dimers: phase transitions and reminiscence in spin systems*, invited talk at the conference *Topological materials conference* (ILL Grenoble, France, October 2011).

[45] S. Capponi, *Exotic phases of matter*, poster presented at the *France-Taiwan Frontiers of Science Symposium* (Nice, France, June 2011).

[46] N. Laflorencie, *Condensate-free superfluidity induced by a frustrated proximity effect*, talk at the *Congrès génréal de la SFP* (Bordeaux, France, July 2011).

[47] N. Laflorencie, *Low-D and frustrated models of hard-core bosons: recent results*, invited talk at the *Mini-Workshop on Quantum Magnetism* (LPT Toulouse, France, July 2011).

[48] D. Poilblanc, Cours à l'Ecole des Houches, 11–21 avr. 2011, "Electrons fortement corrélés, au-delà de la théorie des liquides de Fermi".

[49] D. Poilblanc, invited talk at the International Workshop on "Topological Order and Quantum Computation", Richard B. Gump South Pacific Research Station (Univ. of Berkeley), Moorea, French Polynesia, 23–29 mai 2011.

[50] D. Poilblanc, invited talk at the International Workshop "Quantum Information", Centro de ciencias de Benasque Pedro Pascual, Benasque, Espagne, 13–28 juin 2011.

[51] D. Poilblanc, invited talk at the ICTP International Workshop on "Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter", Trieste, Italy, 25–29 juillet 2011.

[52] D. Poilblanc, invited talk at the International Workshop on "Novel Quantum States in Condensed Matter: Correlation, Frustration and Topology" (NQS2011), Yukawa Institute for Theoretical Physics, Kyoto University, Japan, 8–18 nov. 2011.

[53] P. Pujol, *Statistical transmutation in quantum dimer models*, invited talk at the *"Geometrically Frustrated Magnets: From Spin Ice to Kagome Planes" workshop* (Natal, Brazil, December 2011).

[54] R. Ramazashvili, invited talk at the *International Conference on Electron Crystals (ECRYS-2011)*, (Cargèse, France, August 2011).

[55] F. Alet, *Impurity spin texture at deconfined quantum critical points*, invited talk at the *workshop Impurities and textures in unconventional magnets* (MPI Dresden, Germany, April 2012).

[56] S. Capponi, *Emergent U(1) Symmetry in Square Lattice Quantum Dimer Models*, talk at the *APS March Meeting* (Boston, USA, March 2012).

[57] S. Capponi, H. Nonne, P. Lecheminant, and E. Boulat, *Mott insulating phases in 1D four-component fermionic cold atoms*, poster presented at the conference *Theory of quantum gases and quantum coherence BEC2012* (Lyon, France, June 2012).

[58] S. Capponi, *Effective Spin Couplings in the Mott Insulator of the Honeycomb Lattice Hubbard*, talk at the *KITP workshop "Frustrated Magnetism and Quantum Spin Liquids"* (Santa Barbara, USA, August 2012).

[59] S. Capponi, *Emergent U(1) Symmetry in Square Lattice Quantum Dimer Models*, invited talk at the *XXXVI International Conference of Theoretical Physics* (Ustron, Poland, September 2012).

[60] N. Laflorencie, *Disorder effects in spin gapped antiferromagnets*, invited talk at the workshop *Mott Physics Beyond Heisenberg* (EPFL, Switzerland, June 2012).

[61] M. Mambrini, *A round-trip from spin to quantum dimer models*, talk at the *APS March Meeting* (Boston, USA, March 2012).

[62] D. Poilblanc, invited talk at the International Workshop "New quantum states of matter in and out of equilibrium", May 21-25, 2012, Galileo Galilei Institute for Theoretical Physics, Florence.

[63] D. Poilblanc, invited talk at the International Workshop "Networking tensor networks: many-body systems and simulations", May 06-19, 2012, Centro de Ciencias de Benasque "Pedro Pascual".

[64] D. Poilblanc, invited talk at the International workshop "Frustrated Magnetism and Quantum Spin Liquids: From Theory and Models to Experiments", KITP, UC Santa Barbara, August 12-31, 2012.

[65] D. Poilblanc, invited talk at the International Workshop on "Topological Order and Quantum Computation", UC Berkeley Richard B. Gump South Pacific Research Station, Moorea, September 9-15, 2012.

[66] D. Poilblanc, invited talk at the International Workshop "Entanglement Spectra in Complex Quantum Wavefunctions", 12 - 16 November 2012, Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany.

[67] F. Alet, *Accessing localization properties of many-body systems with quantumÂăMonte Carlo*, invited talk at the *"Statistical Physics and Low Dimensional Systems" workshop* (Pont-à-Mousson, France, May 2013).

[68] F. Alet, *Néel - Valence Bond Crystal transition on honeycomb lattice*, invited talk at the *Topological Phases in Condensed Matter and Cold Atom Systems workshop* (Cargese, France, July 2013).

[69] F. Alet, *Accessing localization properties of many-body systems with quantumÂăMonte Carlo*, invited talk at the *conference "Statistical Physics of Quantum Matter"* (Taipei, Taiwan, July 2013).

[70] F. Alet, *Mini-revue sur l'intrication dans les systèmes magnétiques quantiques*, invited review at the *GDR MICO meeting* (Gif-sur-Yvette, France, November 2013).

[71] S. Capponi, *Symmetry-protected topological phases of alkaline-earth cold fermionic atoms in one dimension*, talk at the *APS March Meeting* (Baltimore, USA, March 2013).

[72] S. Capponi, *p6 - Chiral Resonating Valence Bonds in the Kagome Antiferromagnet*, talk at the *APS March Meeting* (Baltimore, USA, March 2013).

[73] H. Nonne, M. Moliner, S. Capponi, P. Lecheminant, and K. Totsuka, *Symmetry-protected topological phases of alkaline-earth cold fermionic atoms in one dimension*, poster presented at the *workshop on Frontier between atomic and solid state physics* (Paris, France, July 2013).

[74] S. Capponi, V. R. Chandra, A. Auerbach, and M. Weinstein, *p6 chiral Resonating Valence Bond in the kagome antiferromagnet*, poster presented at the *conference "Statistical Physics of Quantum Matter"* (Taipei, Taiwan, July 2013).

[75] H. Nonne, M. Moliner, S. Capponi, P. Lecheminant, and K. Totsuka, *Symmetry-protected topological phases of alkaline-earth cold fermionic atoms in one dimension*, poster presented at the *BEC2013 Conference* (Sant Feliu de Guixols, Spain, September 2013).

[76] N. Laflorencie, *Quantum antiferromagnets in strong magnetic fields: a playground for unconventional bosonic states of matter*, invited talk at the workshop *New magnetic field frontiers in atomic/molecular and solid-state physics* (Les Houches, May 2013).

[77] J.-P. Alvarez and N. Laflorencie, *Bose glass transition and spin wave localization for 2D bosons in a random potential*, talk at the conference *Disorder in Condensed Matter and Ultracold Atoms* (Varenna, Italy, June 2013).

[78] N. Laflorencie, *Superfluid-insulator transition and spin-wave localization for disordered 2D bosons*, talk at the conference *Transport in Interacting Disordered Systems* (Barcelona, September 2013).

[79] M. Mambrini, *Tour d'horizon de la théorie des systèmes magnétiques bidimensionnels frustrés*, invited review at the *GDR MICO meeting* (Roscoff, France, January 7-10 2013).

[80] D. Poilblanc, participation (as co-organiser) to: Symposium "Topological Quantum Information", Centro de Ciencias de Benasque Pedro Pascual (Espagne), 12-16 février 2013.

[81] D. Poilblanc, invited talk at the CECAM Workshop "Tensor network algorithms in computational physics and numerical analysis", ETH-Zürich, 15 – 17 mai 2013.

[82] D. Poilblanc, participation (as co-organizer) to: Workshop International "Topological Phases in Condensed Matter and Cold Atom Systems", Institut d'Etudes Supérieures de Cargèse, June 24-July 6, 2013.

[83] D. Poilblanc, invited talk at the International Workshop "Quantum Information", Centro de Ciencias de Benasque "Pedro Pascual", 7 – 14 juillet 2013.

[84] D. Poilblanc, invited talk at the International Workshop "Perspectives on Quantum Many-Body Entanglement", Johannes-Gutenberg Universität, Mainz, September 25-27 2013.

[85] D. Poilblanc, invited talk at the Japan-Swiss workshop on "Trends in Theory of Correlated Materials", Oct. 2-5, 2013 - EPFL, Lausanne.

[86] P. Pujol, *Statistics of Holes in quantum dimer models*, invited talk at the *"Statistical Physics and Low Dimensional Systems" workshop* (Pont-à-Mousson, France, May 2013).

[87] P. Pujol, *Lattice gauge theories for dimer models*, invited lecture at the *"Quantum spin liquids: from theory to numerical simulations" international school* (Trieste, Italy, September 2013).

[88] R. Ramazashvili, *Electron magnetism of antiferromagnetic conductors*, invited lecture course at the *Summer School on Topological Materials*, (ITAP, Turunç, Turkey, July 2013).

[89] F. Alet, *Universal behavior beyond multifractality in quantum many-body systems*, poster presented at the *workshop "Recent Progress and Perspectives in Scaling, Multifractality, Interactions, and Topological Effects Near Anderson Transitions"* (MPI Dresden, Germany, March 2014).

[90] S. Capponi, *Baxter-Wu model in transverse magnetic field*, invited talk at the *"Statistical Physics and Low Dimensional Systems" workshop* (Pont-à-Mousson, France, May 2014).

[91] D. Poilblanc, invited talk at the Spring Meeting Dresden 2014, Focus Session "Advanced Algorithms for Strongly Correlated Quantum Matter", March 30-April 3, 2014.

[92] D. Poilblanc, invited talk at the International Workshop "Tensor Networks and Simulations", Simons Center Berkeley, April 21 to 25, 2014.

[93] D. Poilblanc, invited talk at the International Workshop on "Topological Phases and Quantum Computation", Moorea Institute for Advanced Studies at the Richard B. Gump South Pacific Research Station (Univ. of Berkeley), Moorea, French Polynesia, May 26 – June 1, 2014.

[94] D. Poilblanc, invited talk at the International Workshop "Quantum Matter", Centro de Ciencias de Benasque, Benasque, Spain, June 15-18, 2014.

[95] D. Poilblanc, invited talk at the International Conference on "Topology and Entanglement in Correlated Quantum Systems", Max Planck Institute for the Physics of Complex Systems in Dresden, 21 - July 25, 2014.

[96] D. Poilblanc, participation (as co-organizer) to: International Workshop "Numerical and analytic methods for strongly correlated systems", Centro de Ciencias de Benasque, Benasque, Spain, August 24-September 13, 2014.

[97] D. Poilblanc, invited talk at International Workshop on " Correlations, criticality, and coherence in quantum systems" Évora, Portugal, 6-10 October 2014.

[98] D. Poilblanc, invited talk at International Workshop on "Novel Quantum States in Condensed Matter 2014" (NQS2014), November 4 - December 5, 2014, Yukawa Institute for Theoretical Physics, Kyoto University, Japan.

[99] A. Petković, *Superfluid-Insulator Transition of Interacting Disordered Bosons in One Dimension*, invited talk at the *"Statistical Physics and Low Dimensional Systems" workshop* (Pont-à-Mousson, France, May 2014).

[100] N. Laflorencie, *Theory of the frustrated Bose condensate of triplets in $BaCuSi_2O_6$ at high magnetic field*, poster at the *"International Conference on Strongly Correlated Electron Systems"* (Grenoble, France, July 2014).

6.2 Cohérence Quantique (Quantware)

[1] D.L.Shepelyansky, *Interplay of nonlinearity, interactions and Anderson localization*, invited talk at Workshop *Anderson localization in nonlinear and many-body systems* (Max Planck Institute for the Physics of Complex Systems, Dresden, March 16-20, 2009).

[2] D.L.Shepelyansky, *Delocalization by nonlinearity and interactions in systems with disorder*, invited talk at *DPG Spring Meeting of the Condensed Matter Section* (TU Dresden, Germany, March 22 - 27, 2009).

[3] D.L.Shepelyansky, *Delocalization tranzition for the Google Matrix*, invited talk at *SFB Symposium "Analysis of complex systems"* (Fritz Haber Inst. MPG, Berlin, Germany, July 3, 2009).

[4] D.L.Shepelyansky, *Google Matrix, dynamical attractors and Ulam networks*, invited talk at *ICPT Workshop "Pseudochaos and Stable-Chaos in Statistical Mechanics and Quantum Physics"* (Trieste, Italy, 21-25 September, 2009).

[5] D.L.Shepelyansky, *Spreading and thermalization in disordered nonlinear chains*, invited talk at *Workshop "Mesoscopic Physics of Waves for Imaging in Complex Media"* (Institut Henri Poincracé, Paris, 29-30 Oct, 2009).

[6] K.M.Frahm, *University networks, Ulam method and Chirikov standard map*, invited talk at *Workshop "PageRank Matrix Days"* (Univ. P.Sabatier, Toulouse, 10 - 11 December, 2009).

[7] O.Giraud, *PageRank algorithm and delocalization transition for network models*, invited talk at *Workshop "PageRank Matrix Days"* (Univ. P.Sabatier, Toulouse, 10 - 11 December, 2009).

[8] B.Georgeot, *Localization properties of the Google matrix for real networks*, invited talk at *Workshop "PageRank Matrix Days"* (Univ. P.Sabatier, Toulouse, 10 - 11 December, 2009).

[9] L.Ermann, *Google Matrix and Ulam networks*, invited talk at *Workshop "PageRank Matrix Days"* (Univ. P.Sabatier, Toulouse, 10 - 11 December, 2009).

[10] I. Nechita, *Random matrix models in quantum information theory*, invited talk at the *Canadian Mathematical Society Winter Meeting* (Windsor, Canada, December 2009).

[11] I. Nechita, *Random quantum channels: graphical calculus*, invited talk at the *Fields Workshop on Operator Structures in Quantum Information* (Toronto, Canada, July 2009).

[12] I. Nechita, *Majorization, entanglement catalysis, stochastic domination and ℓ_p-norms*, invited talk at the *Fields Workshop on Operator Structures in Quantum Information* (Toronto, Canada, July 2009).

[13] I. Nechita, *A graphical calculus for random quantum channels in quantum information theory*, invited talk at the *Atelier Décohérence et information quantique* (Grenoble, France, June 2009).

[14] I. Nechita, *Random repeated quantum interactions and random invariant states*, invited talk at the *Journées Systèmes Ouverts* (Grenoble, France, March 2009).

[15] I. Nechita, *A new diagrammatic approach to matrix integrals with applications to quantum information theory, Student talk at the winter school Geneva-Lyon on mathematical physics* (Les Diablerets, Switzerland, February 2009).

[16] D. Braun *French-Taiwanese Workshop on Theoretical Sciences, Oct. 2009, Hsinchu, Taiwan Decoherence: foe or friend?* (invited talk)

[17] D. Braun *DAMOP Meeting, Charlottesville, VA, May 2009 Decoherence enhanced measurements*

[18] B. Georgeot invited talk at the conference *Colloque Blanc de l'ANR*, february 2009, Paris.

[19] B. Georgeot invited talk at the conference *First Meeting of the GDR Quantum Dynamics 2009*, september 2009, Lyon.

[20] D.L.Shepelyansky, *Turbulent flows on complex networks*, invited talk at *Advanced Workshop "Anderson localization, Nonlinearity and Turbulence: a Cross-Fertilization"* (ICTP, Trieste, Italy, August 23 - September 3, 2010).

[21] I. Nechita, *Random quantum states*, invited talk at the *Open Quantum Systems conference* (Grenoble, France, November 2010).

[22] I. Nechita, *Graphical calculus for random quantum channels*, invited talk at the *Mittag-Leffler program on QIT* (Stockholm, Sweeden, November 2010).

[23] I. Nechita, *Entanglement of random subspaces*, invited talk at the *Workshop on Groups and Group Actions in Operator Theory* (Ottawa, Canada, July 2010).

[24] I. Nechita, *Random graph states and area laws*, invited talk at the *Random Matrix Techniques in Quantum Information Theory workshop* (Waterloo, Canada, July 2010).

[25] I. Nechita, *Free probability techniques in quantum information theory, QIP 2010 Rump Session* (Zürich, Switzerland, January 2010).

[26] D. Braun *"Quantum information in Paris" Workshop, Sept. 23, 2010, Decoherence-enhanced measurements* (invited talk)

[27] D. Braun *Nonlinear Sciences Perspectives 2010 Workshop: Quantum Chaos and Quantum Information, July 21-25, IIT Madras, Chennai, India, Quantifying Quantumness and the Quest for Queens of Quantum* (invited talk)

[28] D. Braun *Joint Colloquium Laboratoire de Physique Théorique and Institut de Mathématique de Toulouse, June 11, 2010, Quantifying Quantumness and the Quest for Queens of Quantum* (invited talk)

[29] D. Braun *GDR de Dynamique Quantique, Grenoble, France, June 17-19, 2010, Quantifying Quantumness and the Quest for Queens of Quantum*

[30] D. Braun *SFB workshop on Quantum Information, Innsbruck, Austria, May 2010, Quantifying Quantumness and the Quest for Queens of Quantum* (invited talk)

[31] D. Braun *DAMOP meeting, Houston (TX), USA, May 2010,* talk *Quantifying Quantumess and the Quest for Queens of Quantum*

[32] D. Braun *Candadian Institute of Advanced Research Conference, Seefeld, Austria, May 2010, Collectively enhanced quantum measurements* (invited talk)

[33] D. Braun *SOLID kick-off meeting, Bilbao, Spain, Feb. 2010,* talk *Quantifying Quantumess and the Quest for Queens of Quantum*

[34] B. Georgeot invited talk at the conference *Atom Laser Conference* , april 2010, Les Houches, France.

[35] B. Georgeot invited talk at the conference *Nonlinear Sciences Perspectives 2010 Workshop: Quantum Chaos and Quantum Information,*, July 21-25, IIT Madras, Chennai, India.

[36] D.L.Shepelyansky, *Google matrix of the world trade network*, invited talk at *Workshop "Quantum chaos and localisation phenomena"* (IFPAN, Warsaw, 20 - 22 May, 2011).

[37] D.L.Shepelyansky, *Wigner crystal in snaked nanochannels*, invited talk at *International conference Electronic Crystals, ECRYS-2011* (Cargese, Corse, 15 - 27 August, 2011).

[38] D.L.Shepelyansky, *Quantum chaos applications: from simple models to quantum computers and Google matrix*, lectures (12 hours) at *XXVII Graduate Physics Days* (Heidelberg University, October 4-7, 2011).

[39] D.L.Shepelyansky, *Google matrix of the world trade network*, invited talk at *4th Annual Research Conference "Complex systems: Towards a better understanding of financial stability and crises"* (3-4 November 2011, De Nedelandsche Bank, Amsterdam).

[40] D.L.Shepelyansky, *Google matrix of social networks*, invited talk at *VII Brunel-Bielefeld Workshop "Random Matrix Theory and Applications in Theoretical Sciences"* (15-17 Dec 2011, Bielefeld, Germany).

[41] I. Nechita, *Block-modified Wishart matrices and applications to entanglement theory*, invited talk at the *GDR IQFA Workshop* (Paris, France, November 2011).

[42] I. Nechita, *Block-modified Wishart matrices and applications to entanglement theory*, invited talk at the *Joint EMS-RMSE Mathematical Weekend* (Bilbao, Spain, October 2011).

[43] I. Nechita, *Block-modified Wishart matrices and applications to entanglement theory*, invited talk at the *14th Non-commutative harmonic analysis Workshop* (Bedlewo, Poland, September 2011).

[44] I. Nechita, *Positivity in Quantum Information Theory*, invited talk at the *Positivity Workshop, Fields Institute* (Toronto, Canada, August 2011).

[45] I. Nechita, *Additivité de la capacité des canaux quantiques, ou comment l'intrication peut aider la transmission de l'information*, *Annual meeting between the Mathematics and Physics departments at the Univeristy of Toulouse* (Toulouse, France, April 2011).

[46] D. Braun *Open Quantum Systems and Quantum Information Theory workshop, Toulouse Nov. 2011*, *Towards a universal set of quantum channels* (invited talk)

[47] D. Braun *QED2 meeting, Siegen, Germany, September 2011*, *Quantumness versus Entanglement* (invited talk)

[48] D. Braun *Young European Physicists meeting, Marie Curie International Training Network FASTQUAST, Toulouse, July 2011*, *Ultimate limits of sensitivity of physical measurements* (invited talk)

[49] D. Braun *Benasque Workshop on Quantum Simulations, Benasque, Spain, Feb. 28-March 4, 2011, Versatile cold-atom simulator of non-abelian gauge fields* (invited talk)

[50] D. Braun *Workshop on New Trends in Quantum Dynamics and Quantum Entanglement, Trieste, Italy, Feb. 21-25, 2011*, *Heisenberg limited sensitivity with decoherence-enhanced measurements* (invited talk)

[51] D. Braun *GdR "Quantum Information: from foundations to applications" meeting, Paris, November 2011,* talk *Heisenberg-limited sensitivity without entanglement*

[52] B. Georgeot invited talk at the conference *Siroco workshop*, june 2011, Paris, France.

[53] B. Georgeot invited talk at the conference *COMUL 2011*, september 2011, Toulouse School of Economics, Toulouse, France.

[54] B. Georgeot invited talk at the conference *JDEV 2011*, september 2011, ENSEEIHT, Toulouse, France.

[55] B. Georgeot contributed talk at the conference *The Impact of Asteroseismology across Stellar Astrophysics*, october 2011, KITP, Santa Barbara, Ca, USA.

[56] D.L.Shepelyansky, *Google matrix of Markov chains*, invited talk at *workshop in honor of Alexander Its "Integrable systems and random matrices"* (Institut Henri Poincare, Paris 21 - 23 May, 2012).

[57] D.L.Shepelyansky, *Kolmogorov turbulence, Anderson localization and KAM integrability*, invited talk at *Workshop "Mathematics and Physics of Anderson localization: 50 Years After", follow up meeting,* (Newton Institute, Cambridge, UK, 17 - 21 Sept, 2012).

[58] D.L.Shepelyansky, *NADINE - New tools and Algorithms for DIrected NEtwork analysis*, invited talk at *International Workshop on Search Computing* (Brussels 25-26 September, 2012).

[59] K.M.Frahm, *Google matrix of directed networks*, invited talk at *ECT Workshop "Spectral Properties of Complex Networks"* (Trento, Italy, July 2012).

[60] B.Georgeot, *The game of go as a complex network*, invited talk at *ECT Workshop "Spectral Properties of Complex Networks"* (Trento, Italy, July 2012).

[61] V.Kandiah, *PageRank model of opinion formation on social networks*, contributed talk at *ECT Workshop "Spectral Properties of Complex Networks"* (Trento, Italy, July 2012).

[62] I. Nechita, *Positive and completely positive maps via free additive powers of probability measures*, invited talk at the *Operator Spaces and Quantum Information Theory workshop* (Lyon, France, October 2012).

[63] I. Nechita, *Random subspaces of a tensor product and the additivity problem*, invited talk at the *DMV Annual Meeting* (Saarbrücken, Germany, September 2012).

[64] I. Nechita, *Random subspaces of a tensor product and the additivity problem*, invited talk at the *XIème Colloque Franco-Roumain de Mathḿatiques Appliquées* (Bucuresti, Romania, August 2012).

[65] I. Nechita, *Random subspaces of a tensor product and the additivity problem*, invited talk at the *Operator Spaces, Quantum Probability and Applications Workshop* (Wuhan, China, June 2012).

[66] I. Nechita, *Random Subspaces of a Tensor Product and the Additivity Problem*, invited talk at the *Probabilistic Methods in Quantum Mechanics Workshop* (Lyon, France, May 2012).

[67] I. Nechita, *Block-modified Wishart matrices and applications to entanglement theory*, invited talk at the *Random matrices and integrable systems winter school* (Les Houches, France, March 2012).

[68] I. Nechita, *Statistical properties of random quantum channels*, invited lecture at the *CIRM workshop on the Geometry of Quantum Entanglement* (Luminy, France, January 2012).

[69] D. Braun *Physics of Quantum Electronics Conference 2012, Snowbird, Utah, Jan. 2012, Heisenberg limited sensitivity without entanglement* (invited talk)

[70] D. Braun *Quantum Information and Measurement, Optical Society of America Conference, Berlin, March 2012, Heisenberg limited metrology without entanglement*

[71] D. Braun *Quantum Information and Measurement, Optical Society of America Conference, Berlin, March 2012, Optimal Mass-sensing with a Nano-mechanical Resonator*

[72] D. Braun *DPG-Frühjahrstagung, DAMOP section, Stuttgart, Germany, March 2012,* talk *Heisenberg-limited metrology without entanglement*

[73] D. Braun *DPG-Frühjahrstagung, DAMOP section, Stuttgart, Germany, March 2012,* talk *Ultimate quantum bounds on mass measurements with a nano-mechanical resonator*

[74] D.L.Shepelyansky, *Synchronization theory of microwave induced zero-resistance states*, invited talk at *International Workshop "MIRO and all that"* (Montpellier, France, 13 - 16 May, 2013).

[75] D.L.Shepelyansky, *Google matrix and fractal Weyl law*, invited talk at *workshop "Advances in quantum chaotic scattering: from (non-)linear waves to few-body systems"* (6 - 13 Sept 2013, MPI Complex systems, Dresden, Germany).

[76] K.M.Frahm, *Spectral analysis of Wikipedia and PhysRev networks*, invited talk at *workshop Directed networks days* (LAW Computer Science Department, Universita degli studi di Milano, Italy 13 - 14 June 2013).

[77] B.Georgeot, *The network of Go game*, invited talk at *workshop Directed networks days* (LAW Computer Science Department, Universita degli studi di Milano, Italy 13 - 14 June 2013).

[78] Y.-H.Eom, *Highlighting cultural distinctions from multilingual Wikipedia*, invited talk at *workshop Directed networks days* (LAW Computer Science Department, Universita degli studi di Milano, Italy 13 - 14 June 2013).

[79] Y.-H.Eom, *Highlighting cultural diversity via ranking of multilingual Wikipedia articles*, invited talk at *European conference on complex system 2013* (16-20 September 2013, Barcelona).

[80] V.Kandiah, D.Shepelyansky, *Google matrix analysis of DNA sequences*, invited talk at *workshop Directed networks days* (LAW Computer Science Department, Universita degli studi di Milano, Italy 13 - 14 June 2013).

[81] I. Nechita, *Random matrix theory with a view towards free probability, and connections to quantum information*, invited lectures at the *New Mathematical Directions for Quantum Information workshop, Newton Institute* (Cambridge, UK, September 2013).

[82] I. Nechita, *Entanglement of random subspaces*, invited talk at the *Advances on Open Quantum Systems summer school* (Autrans, France, July 2013).

[83] I. Nechita, *On the additivity of the minimum entropy of certain subspaces of tensor products*, invited talk at the *Workshop on Operator Spaces, Harmonic Analysis and Quantum Probability* (Madrid, Spain, June 2013).

[84] I. Nechita, *Intrication pour les états bipartis mélangés*, *Cogit meeting* (Rouen, France, June 2013).

[85] I. Nechita, *Positive and completely positive maps via free additive powers of probability measures*, invited talk at the *EMS-DMF joint mathematical weekend* (Aarhus, Denmark, April 2013).

[86] D. Braun *Matariki quantum science workshop*, Tübingen, Germany, June 2013, *Quantum-enhanced measurements — beyond entanglement assisted schemes* (invited talk)

[87] D.L.Shepelyansky, *Spectral properties of Google matrix*, invited talk at *Colloquium in memory of Oriol Bohigas "Wandering from Nuclei to Chaos"* (13 - 14 March 2014, LPTMS, Orsay).

[88] G. Lemarié, *Universal scaling of the order-parameter distribution in strongly disordered superconductors*, contributed oral presentation at the *Workshop on Coherent Phenomena in Disordered Optical Systems* (ICTP, Trieste, Italy, 26-30 May 2014).

[89] B. Georgeot, contributed oral presentation and poster at the *March meeting of the American Physical Society* March 2014, Denver, Co, USA.

6.3 Physique Statistique des Systèmes Complexes (PhyStat)

[1] C. Sire, *Collapse dynamics of self-gravitating gas*, invited talk at the *Workshop on Velocity and Density Collapse in Kinetic and Diffusion Models: Chemotaxis, Gravitation, Swarming* (IHP, Paris, October 2009).

[2] C. Sire, *Collapse and evaporation of a canonical self-gravitating gas*, invited talk at the *12th Marcel Grossmann Meeting* (UNESCO/IAP/ENS, Paris, 12-18 July 2009); C. Sire and P.-H. Chavanis, in *Proceedings of the 12th Marcel Grossmann Meeting*, Eds. T. Damour, R. T. Jantzen, and R. Ruffini (World Scientific, Singapore, 2012).

[3] P.-H. Chavanis, *Critical dimension of the self-gravitating radiation*, invited talk at the *XIIth Marcel Grossmann Meeting on "General Relativity"* (Paris, France, 13-18 July 2009).

[4] N. Destainville, *An alternative mechanism for the formation of specialized nano-domains (cluster phases) in biomembranes*, invited talk at the *Colloquium "Theoretical Physics of Biological Systems"* (Paris, France, 17-18 December 2009).

[5] J. Palmeri, *Brackish and seawater desalination using NF and RO membranes: transport theory, modeling, and process simulation*, invited 4-day Intensive Course *Middle East Desalination Research Center (MEDRC)* (Casablanca, Morocco, 2-5 February 2009).

[6] J. Palmeri, L. Schrive, and A. Deratani, *Modelisation des procedes de nanofiltration avec le logiciel NanoFlux: applications nucleaires*, invited talk at the *JournŐes Thematiques ÒMembranes et NucleaireÓ* (Marcoule, France, 15-16 January 2009).

[7] J. Palmeri, and M. Metaiche, *Optimization of Reverse Osmosis and Nanofiltration Desalination Systems*, invited talk at the *Microsoft-CNRS Chair Workshop: Optimization for Sustainable Development* (Palaiseau, France, 3 June 2009).

[8] P.-A. Cazade, J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Confinement of electrolyte solutions in nanopores*, oral presentation at the *7th International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids* (Kazimierz Dolny, Poland, 5-11 July 2009).

[9] P.-A. Cazade, J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Confinement d'une solution ionique dans une membrane de nanofiltration*, oral presentation at the *Journees Simulation Numerique 2009* (Paris, France, 11-12 Juin 2009).

[10] J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Study of ion transport through nanopores*, oral presentation at the *Euromembrane Conference 2009* (Montpellier, France, 6-10 September 2009).

[11] H. Saidani, N. Ben Amar, J. Palmeri, and A. Deratani , *Etude du comportement thermique des membranes organiques composites de nanofiltration*, oral presentation at the *Colloque Franco-Maghrebin sur les Membranes et Films Composites* (Monastir, Tunisie, 25-28 March 2009).

[12] L. Schrive, V. Bonhoure, J. Palmeri, and A. Deratani , *Nanofiltration of effluents containing heavy metals: nanoflux simulations as a descriptive and predictive tool for research and industry needs*, oral presentation at the *Euromembrane Conference 2009* (Montpellier, France, 6-10 September 2009).

[13] P.-A. Cazade, J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Dynamics of electrolyte solutions confined in nanopores*, poster presented at the *Diffusion Fundamentals III Conference* (Athens, Greece, 23-26 August 2009).

[14] J. Palmeri, *SIMONANOMEM (ANR-NANO-2007) SImulation and MOdelling of transport across polymeric NANOporous MEMbranes prepared by self-assembly of block copolymers*, poster presented at the *Journees Nationales en Nanosciences et Nanotechnologies (J3N)* (Toulouse, France, 21-23 October 2009).

[15] L. Schrive, V. Bonhoure, P. Viel, T. Le, A. Deratani, and J. Palmeri, *Combining nanofiltration and electrocapture for zero discharge perspective : Nanoflux simulation contribution*, poster presented at the *XIIeme congres de la SocietŐe Francaise de Genie des Procedes (SFGP2009)* (Marseille, France, 14-16 October 2009).

[16] C. Sire, *The statistical physics of Minimax*, invited talk at the *MECO35 – 35th Conference of the Middle European Cooperation in Statistical Physics* (Pont-à-Mousson, France, 15-19 March 2010).

[17] D. Dean, *Dynamical transitions for diffusion in random potentials*, invited talk at *Complex Dynamics of Fluids in Disordered and Crowded Environments* (CECAM, Lyon, France, 2010).

[18] D. Dean, *Forces induced by charge and dielectric disorder*, invited talk at *New Perspectives in Strongly Correlated Electrostatics in Soft Matter* (Aspen Center for Physics, USA, 2010).

[19] D. Dean, *Out of equilibrium fluctuation induced forces*, invited talk at *Fluctuation-induced Forces in Condensed Matter* (Dresden, Germany, 2010).

[20] D. Dean, *The nonequilibrium pseudo-Casimir effect*, invited talk at the *Workshop on Casimir forces* (Tenerife, Spain, 2010).

[21] S. Buyukdagli, M. Manghi, J. Palmeri, *Variational method for electrolytes confined in slit and cylindrical Pores*, poster at the *International Soft Matter Conference 2010* (Granada, Spain, 5-8 July 2010).

[22] N. Ben Amar, N. Kechaou, J. Palmeri, and A. Deratani, *Traitements membranaires des effluents textiles par NF/OI*, invited talk at the *2eme Journees Materiaux et Environnement* (MeknŔs, Maroc, 4-5 June 2010).

[23] J. Palmeri, N. Destainville, and M. Manghi, *Bubbles and Bending: how DNA's conformational fluctuations influence its thermal denaturation*, invited talk at the *MIBS Workshop - complex dynamics in biological systems, UPS* (Toulouse, France, 7-9 June 2010).

[24] N. Ben Amar, N. Kechaou, J. Palmeri, and A. Deratani , *Traitements membranaires des effluents textiles pour recyclage de l'eau*, oral presentation at the *Vième Congrès International, QPE-TVR 2010 - Qualité des Produits et de L'Environnement Traitement et Valorisation des Rejets et Effets sur la Santé Humaine* (Sousse, Tunisie, 9-11 April 2010).

[25] P.-A. Cazade, J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Confinement of electrolyte solutions in charged nanopores*, poster presented at the *4th International Workshop on Dynamics in Confinement* (Grenoble, France, 3Đ5 March 2010).

[26] P.-A. Cazade, J. Dweik, B. Coasne, F. Henn, and J. Palmeri, *Molecular simulation of ion-specific effects in confined electrolyte solutions using polarizable force fields*, poster presented at the *Frontiers in Water Biophysics Workshop* (Trieste, Italy, 23-26 May 2010).

[27] A. Deratani and J. Palmeri, *SIMONANOMEM (ANR-NANO-2007) SImulation and MOdelling of transport across polymeric NANOporous MEMbranes prepared by self-assembly of block copolymers*, poster presented at the *Journees Nationales en Nanosciences et Nanotechnologies (J3N)* (Lille, France, 8-10 November 2010).

[28] P.-H. Chavanis, *Kinetic theory of 2D point vortices*, invited talk at the *Meeting on "Models of Climate"* (Paris, France, 30-31 May 2011).

[29] C. Sire, *Theory of competitive systems*, invited talk at the conference *Challenge in Aperiodic Media* (Lyon, France, 28 February-4 March 2011).

[30] C. Sire, *The physics of poker tournaments*, invited talk at the *Young European Physicists Meeting* (Toulouse, 18-22 July 2011).

[31] C. Sire, *Theory of competitive systems*, invited talk at the *Atelier Modélisation des Systèmes Multi-agents* (Toulouse School of Economics, 26-27 September 2011).

[32] C. Sire, *Effective merging dynamics of two and three fluid vortices: Application to two-dimensional decaying turbulence*, invited talk at the *International Workshop on Long-range Interacting Systems* (Lyon, France, 17-19 October 2011).

[33] C. Sire, *Collapse and post-collapse dynamics of self-gravitating gas*, invited talk at the *Atelier limite champ moyen pour systèmes de particules auto-gravitantes, effets discrets* (Institut Dieudonné, Nice, 3-4 November 2011).

[34] D. Dean, *Diffusion in random potentials*, invited talk at *Search and Exploration* (Cargèse, France, 2011).

[35] D. Dean, *Out of equilibrium fluctuation induced forces*, invited talk at *Nonequilibrum Statistical Mechanics* (Nordita, Stockholm, Sweden, 2011).

[36] M. Manghi, *Stacked membranes and ions close to interfaces*, invited talk at the *Workshop on Membranes and Biolubrication* (Lyon, France, January 2011).

[37] M. Manghi, J. Palmeri, N. Destainville, *DNA bubbles and bending : how conformational fluctuations modify base pairing*, poster at the *European Biophysics Society Association 2011 Congress* (Budapest, Hungary, August 2011).

[38] N. Destainville, *Role of long-range protein-protein forces in the formation of membrane nanodomains*, invited talk at the *Workshop on "Imaging, Interpretation and Modeling in Modern Immunology"* (Banff, Canada, 10-15 April 2011).

[39] N. Destainville, *Role of long-range protein-protein forces in the formation and stability of membrane protein nano-domains*, contributed talk at the *8th European Biophysics Congress* (Budapest, Hungary, 23-27 August 2011).

[40] P.-H. Chavanis, *Kinetic theory of 2D point vortices*, invited talk at the *International Conference SigmaPhi2011 on "Statistical Physics"* (Larnaka, Cyprus, 11-15 July 2011).

[41] P.-H. Chavanis, *Kinetic theory of 2D point vortices*, invited talk at the *RIMS Camp-style Seminar on "Modern approach and developments to Onsager's theory on statistical vortices"* (Kyoto, Japan, 29-31 August 2011).

[42] P.-H. Chavanis, *New results on the Hamiltonian Mean Field model*, invited talk at the *Workshop on "Long-range interactions"* (Lyon, France, 17-19 September 2011).

[43] J. Palmeri, *Simulation and Modeling of the transport across Polymeric Nanoporous Membranes prepared by self assembly of block copolymers*, invited talk at the *Journées Nationales en Nanosciences et Nanotechnologies (J3N)* (Strasbourg, France, 7-9 November 2011).

[44] C. Sire, *Collapse dynamics in the Keller-Segel model of chemiotaxis*, invited talk at the *Workshop on Functional Inequalities and PDE in the Life Sciences* (Université Paris-Dauphine, France, 12-13 January 2012).

[45] C. Sire, *Synchronization In Long-range Interacting Systems*, invited talk at the *Workshop on Statistical Physics and Low Dimensional Systems* (Pont-à-Mousson, France, 29 May-1 June 2012).

[46] C. Sire, *Effective merging dynamics of two and three fluid vortices: Application to two-dimensional decaying turbulence*, invited talk at the *Workshop Vortex Theory Now – Frontiers of Mathematical Physics* (Osaka, Japan, 5-6 October 2012).

[47] M. Manghi, S. Buyukdagli, J. Palmeri, *Ionic capillary evaporation in weakly charged nanopores*, talk at the *ICREA Symposium Nanofluidics, Colloids and Membranes* (Barcelona, Spain, July 2012).

[48] S. Prolhac, *Fluctuations and large deviations in the one-dimensional Kardar-Parisi-Zhang universality class*, invited talk at the *Meeting of the GDR PHENIX* (Paris, France, November 2012).

[49] N. Destainville, *Quelques aspects de la modŐlisation physique des interactions et de la dynamique des protŐines membranaires*, invited talk at the *School "Microscopie fonctionnelle en biologie (MiFoBio 2012)* (Les-Sables-d'Olonne, France, 4-9 October 2012).

[50] P.-H. Chavanis, *Trapping of dust by coherent vortices in the solar nebula*, invited talk at the *Meeting on "Instabilities and Structures in Proto-Planetary disks"* (Marseille, France, 17-20 September 2012).

[51] P.-H. Chavanis, *Self-gravitating Brownian particles*, invited talk at the *Meeting on "Statistical Mechanics of Self-Gravitating Particles"* (Les Treilles, France, 22-27 October 2012).

[52] P.-H. Chavanis, *Statistical mechanics of self-gravitating fermions and bosons*, invited talk at the *IX Mexican School on Gravitation and Mathematical Physics on "Cosmology for the XXI Century: Inflation, Dark Matter and Dark Energy"* (Puerto Vallarta, Mexico, 3-7 December 2012).

[53] B. Coasne, J. Palmeri, A. Deratani, and D. Gigmes, *Simulation et Modelisation du Transport dans des Membranes Polymeriques preparees par Auto-Assemblage de Copolymeres*, invited talk at the *Colloque de l'action collective Membranes en Languedoc Roussillon - TRIMATEC* (Montpellier, France, 26 April 2012).

[54] B. Coasne, B. Siboulet, J.-F. Dufreche, P. Turq, P. Bonnaud, R. Pellenq, P. A. Cazade, L. Horvath, and J. Palmeri , *Adsorption and Dynamics of Ions Confined in Nanopores: from Simple Ions to Ionic Liquids*, oral presentation at the *Workshop Aging of Engineering Materials: a Computational Approach to Durability and Sustainability (CECAM)* (Zurich, Switzerland, 8-10 February 2012).

[55] R. Moliner-Salvador, A. Deratani, J. Palmeri, and E. Sanchez, *Use of nanofiltration membrane technology for ceramic industry wastewater treatment*, oral presentation at the *Conference QUALICER 2012* (Castellón, Spain, 13-14 February 2012).

[56] F. Sicard, *DNA denaturation bubble: Free-energy landscape and nucleation/closure rates*, poster at the *International Workshop on "DNA self-assembly: theory and experiment"* (Vienna, Austria, December 2013).

[57] C. Sire, *Mean-field theory for a realistic model for fish schools*, invited talk at the *International Workshop on Small Systems far from Equilibrium: Order, Correlations, and Fluctuations* (Dresden, Germany, 14-18 October 2013).

[58] M. Manghi, A. K. Dasanna, N. Destainville, J. Palmeri, *DNA twist and bending govern the denaturation bubble slow dynamics*, poster at the *International Soft Matter Conference 2013* (Rome, Italy, September 2013).

[59] P.-H. Chavanis, *Statistical mechanics of 2D turbulence*, invited talk at the *IUTAM Symposium on "Vortex Dynamics: Formation, Structure and Function"* (Fukuoka, Japan, 7-17 March 2013).

[60] P.-H. Chavanis, *Statistical mechanics of self-gravitating systems*, invited Lecture at the Institute Henri Poincaré during the *Workshop GRAVASCO on "N-body gravitational dynamical systems (from $N = 2$ to infinity)"* (Paris, France, 30 September-8 November 2013).

[61] N. Destainville, *Protein clusters in biomembranes*, contributed talk on organizers' solicitations at the *APS March Meeting* (Baltimore, USA, 18-22 March 2013).

[62] C. Ferreira Esmi, L. Schrive, Y. Barre, J. Palmeri, and A. Deratani, *A new environmentally friendly process for removing heavy metals from wastewater*, oral presentation at the *International Conference on Environmental Science and Technology - CEST 2013* (Athens, Greece, 5-7 September 2013).

[63] C. Sire, *Analytical results for a realistic model for fish schools*, invited talk at the *Workshop on Advances in Non Equilibrium Statistical Mechanics* (Galileo Galilei Institute for Theoretical Physics, Florence, Italy, 16-30 May 2014); Chairman of a session.

[64] M. Manghi, *Ionic transport in nanopores*, invited talk at the *Workshop Water depollution: from applications to fundamental, from physical-chemistry to processes* (Montpellier, France, March 2014).

[65] N. Destainville, *Role of long-range protein-protein in the formation, stability and specialization of bio-membrane nano-domains*, invited speaker at the *CECAM Workshop on "Simulation of bimolecular interactions with inorganic and organs surfaces as a challenge for future nanotechnologies"* (Toulouse, France, 24-26 March 2014).

[66] N. Destainville, *Organization of proteins breaking the up-down symmetry in membranes under tension*, invited talk at the *Interdisciplinary Workshop on "Membrane Dynamics"* (Paris, France, 24-26 March 2014).

[67] M. Manghi, *Closure dynamics of DNA denaturation bubble*, poster at the *Liquids 2014: 9th Liquid Matter Conference* (Lisbon, Portugal, July 2014).

[68] M. Manghi, *Statistical physics and mesoscopic models to describe DNA stretching under force*, invited talk at the *Inserm Workshop 231: Recent developments in single nucleic acid molecule approaches* (Bordeaux, France, October 2014).

6.4 Systèmes de Fermions Finis – Agrégats (Agrégats)

[1] E. Suraud, *Unité et diversité en physique: l'exemple des liquides quantiques*, invited talk at the *Humboldt Kolleg* (Paris, France, June 2009).

[2] E. Suraud, *Irradiation of organic molecules : a time dependent non adiabatic microscopic approach*, invited talk at the *International Conference RADAM 2009* (Frankfurt, Germany, June 2009).

[3] E. Suraud, *Towards the microscopic description of the irradiation of biomolecules* , invited talk at the *International workshop on Nuclear Theory IWNT28* (Rila, Bulgaria, June 2009).

[4] E. Suraud, *Irradiation of clusters and molecules*, invited talk at the *International Workshop Spin dynamics in metallic nanoparticles* (Barcelona, Spain, October 2009).

[5] E. Suraud, *TDDFT description of irradiation and the Self Interaction Problem* , invited talk at the *International workshop on TDDFT* (Benasque, Spain, January 2010).

[6] E. Suraud, *Towards the microscopic description of the irradiation of biomolecules*, invited talk at the *Workshop on irradiation dynamics* (Belfast, UK, June 2010).

[7] E. Suraud, *Interactions et incertitude(s) en physique*, invited talk at the *Humboldt Kolleg* (Evry, France, June 2010).

[8] E. Suraud, *Clusters and molecules in extreme light*, invited talk at the *International workshop on Nuclear Theory IWNT29* (Rila, Bulgaria, June 2010).

[9] E. Suraud, *Self Interaction Correction (SIC) in the time domain* , invited talk at the *International Conference Dubna Nano 2010* (Dubna, Russia, July 2010).

[10] E. Suraud, *Metal cluster dynamics through examples* , invited talk at the *Russian Confederation Nanophysics school* (Dubna, Russia, July 2010).

[11] E. Suraud, *Dynamics of irradiated clusters and molecules* , invited talk at the *International Conference DYSON 2010* (Roma, Italy, November 2010).

[12] E. Suraud, *Clusters and molecules in extreme light* , invited talk at the *Symposium in honour of Prof. Dr. Dr. h.c. Paul-Gerhard Reinhard* (Erlangen, Germany, June 10 2011).

[13] E. Suraud, *Towards Inclusion of Dissipation in Quantum Time Dependent Mean-field Theories* , invited talk at the *International workshop on Nuclear Theory IWNT30* (Rila, Bulgaria, June 2011).

[14] E. Suraud, *Clusters and molecules in extreme light* , invited talk at the *ISACC 2011 International Conference* (Berlin, Germany, July 2011).

[15] E. Suraud, *Self Interaction Correction (SIC) in the time domain* , invited talk at the *International Symposium on the 30 years of the Self Interaction* (Chester, UK, September 2011).

[16] E. Suraud, *Clusters and molecules in extreme light* , invited talk at the *International Conference on Correlation Effects CERF* (Rostock, Germany, September 2011).

[17] E. Suraud, *Dynamics of irradiation: From molecules to nano-objects and from material science to biology* , invited talk at the *International Conference on nano science* (Dalian, China, October 2011).

[18] E. Suraud, *Small fermionic systems : the common methods and challenges*, invited talk at the *Chinese Theoretical Nuclear Physics meeting* (Guilin, China, October 2011).

[19] E. Suraud, *Photoelectron Spectroscopy revisited* , invited talk at the *International Workshop on Condensed Theory, CMT34* (Pohang, Korea, November 2011).

[20] E. Suraud, *Towards Inclusion of Dissipation in TDDFT* , invited talk at the *International workshop on TDDFT* (Benasque, Spain, January 2012).

[21] E. Suraud, *Towards the microscopic description of the irradiation of biomolecules*, invited talk at the *International Conference on nanophysics* (Lanzarote, Spain, February 2012).

[22] E. Suraud, *Data collection on photon interactions with biomolecules and nanopartciles*, invited talk at the *International workshop on RADAM database, in relation to VAMDC* (Vienna, Austria, February 2012).

[23] E. Suraud, *Dynamics of irradiation: From molecules to nano-objects and from material science to biology* , invited talk at the *International conference on Nanoscience* (Omaha, USA, March 2012).

[24] E. Suraud, *Dynamics of irradiated clusters and molecules*, invited talk at the *International Symposium on quantum physics* (Linz, Austria, June 2012).

[25] E. Suraud, *Time resolved dynamics of clusters and molecules* , invited talk at the *International workshop on Nuclear Theory IWNT31* (Rila, Bulgaria, June 2012).

[26] E. Suraud, *Dynamics of irradiated clusters and molecules* , invited talk at the *International conference on cluster structure and dynamics* (Lausanne, Switzerland, July 2012).

[27] E. Suraud, *Irradiation dynamics of clusters and molecules* , invited talk at the *International Conference Dubna Nano 2012* (Dubna, Russia, July 2012).

[28] E. Suraud, *On electronic emission from irradiated clusters and nanostructures* , invited talk at the *International Conference o Mathematical modelling in physics, ICM2* (Budapest, Hungary, September 2012).

[29] E. Suraud, *On electronic emission from irradiated clusters and nanostructures* , invited talk at the *International Conference DYSON 2012* (Saint Petersburg, Russia, October 2012).

[30] E. Suraud, *Towards the microscopic description of the irradiation of biomolecules*, invited talk at the *International Conference on Nano Bio IBCT* (Sopot, Poland, May 2013).

[31] E. Suraud, *Dynamics of irradiation: From molecules to nano-objects and from material science to biology*, invited talk at the *International workshop on Ion interactions with materials at nano/micrometer scale* (Beijing, China, July 2013).

[32] E. Suraud, *Dynamics of irradiated clusters and molecules* , invited talk at the *International Conference ISACC 2013* (Wuhan, China, July 2013).

[33] E. Suraud, *Towards Inclusion of Dissipation in Quantum Time Dependent Mean-field Theories* , invited talk at the *Gordon Research Conference on TDDFT* (Biddeford, USA, August 2013).

[34] E. Suraud, *Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories* , invited talk at the *International Symposium on nuclear dynamics* (College Station, USA, August 2013).

[35] E. Suraud, *Dynamics of irradiation: From molecules to nano-objects and from material science to biology* , invited talk at the *International Conference on Mathematical modelling in physics, ICM2* (Prag, Czeck republic, September 2013).

[36] E. Suraud, *Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories* , invited talk at the *International Conference on Many Body theories, RPMBT17* (Rostock, Germany, September 2013).

[37] E. Suraud, *Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories* , invited talk at the *International workshop on TDDFT* (Benasque, Spain, January 2012).

[38] E. Suraud, invited talk at the *APS March meeting* (Denver, USA, March 2014).

[39] E. Suraud, , invited talk at the *International workshop on quantum dynamics in nanosystems* (Nashville, USA, March 2014).

[40] E. Suraud, *Clusters and molecules in extreme light* , invited talk at the *International Conference DYSON 2014* (Edimburgh, UK, May 2014).

[41] P. M. Dinh, *Dynamics of small organic molecules in strong electromagnetic fields*, invited talk at the *International workshop "Theory Days 2009 on Irradiation of Biomolecules"* (Toulouse, France, Dec. 6–9 2009).

[42] P. M. Dinh, *Chromophore effect in irradiated water clusters*, invited talk at the *Second World Conference on "Nanomedicine and Drug Delivery"* (Kottayam, India, March 11–13 2011).

[43] P. M. Dinh, *Surface plasmon resonances in real-space and real-time TDDFT studies*, invited talk at the *International Symposium on "Molecular Plasmonics 2011"* (Jena, Germany, May 19–21 2011).

[44] P. M. Dinh, *Chromophore effect in NaH_2O investigated by means of a real-time and real-space TDDFT study*, invited talk at the *Symposium in honour of Prof. Dr. Dr. h.c. Paul-Gerhard Reinhard* (Erlangen, Germany, June 10 2011).

[45] P. M. Dinh, *The self-interaction correction in (TD)DFT revisited*, invited talk at the *2011 general meeting of the GDR "CoDFT"* (Obernai, France, June 27–30 2011).

[46] P. M. Dinh, *Chromophore effect in irradiated water clusters : a TDDFT/MD study*, poster at the *6th International Symposium on Small Particles and Inorganic Clusters (ISSPIC-XVI)* (Louvain, Belgique, 8-13 juil. 2012).

[47] P. M. Dinh, *Les spectres de photoélectrons revisités par la TDDFT incluant SIC*, invited talk at the *2013 general meeting of the GDR "CoDFT"* (Lorient, France, May 21–24 2013).

[48] P. M. Dinh, *Dynamics of clusters and molecules in contact with an environment*, invited talk at the *International workshop on "ion interactions with materials at nano/micrometer scale"* (Beijing, China, July 16-18 2013).

[49] P. M. Dinh, *Les thérapies non invasives contre le cancer vues sous l'angle de la physique (théorique)*, invited talk at the *Toulouse meeting "Fête de la Science"* (Toulouse, France, Oct. 11 2013).

[50] P. M. Dinh, *The self-interaction correction in (TD)DFT revisited*, invited talk at the *International workshop on "Physics at the Falls : Common challenges in finite fermion systems"* (Buffalo, USA, Nov. 6–9 2013).

[51] P. M. Dinh, *Importance of low energy electrons in irradiated DNA damage and difficulties to address them theoretically*, invited talk at the *International workshop on "Atomic and Molecular Physics"* (Madrid, Spain, March 27–28 2014).

[52] P. M. Dinh, *Electronic dynamics controlled by an infrared pulse and an attopulse train and explored in means of TDDFT*, invited talk at the colloquium *PAMO-JSM 2014* organized by the French Society of Physics division "Physique Atomique, Moléculaire et Optique" and the "Journées de la Spectroscopie Moléculaire" (Reims, France, July 7–10 2014).

[53] P. Romaniello, G. Lani, and L. Reining, *Hubbard model: GW vs. exact solution*, poster at the *GDR-DFT++ 2009* (Dourdan, France, February 2009).

[54] P. Romaniello, G. Lani, and L. Reining, *Hubbard model: GW vs. exact solution*, poster at the *Young Researchers' Meeting 2009* (Berlin, Germany, June 2009).

[55] P. Romaniello, *Nonlinear optical properties of metal-dithiolenes*, invited talk at the *International Conference of Computational Methods in Sciences and Engineering 2009* (Rhodes, Greece, September 2009).

[56] P. Romaniello and L. Reining, *Beyond GW: local and nonlocal vertex corrections*, talk at the *XIVth Nanoquanta Workshop on Electronic Excitations* (Evora, Portugal, September 2009).

[57] P. Romaniello and L. Reining, *Beyond GW: local and nonlocal vertex corrections*, talk at the *Workshop "From Basic Concepts to Real Materials"* (Santa Barbara, USA, November 2009).

[58] P. Romaniello, F. Bechstedt and L. Reining, *Insights in the T-matrix formalism*, talk at the *APS March Meeting 2010* (Portland, USA, March 2010).

[59] P. Romaniello, *The Bethe-Salpeter equation and optical properties of many-body systems*, invited talk at the *Young Researchers' Meeting 2010* (Jyväskylä, Finland, June 2010).

[60] P. Romaniello, F. Bechstedt and L. Reining, *Insights in the T-matrix formalism*, poster at the *Psi-K 2010* (Berlin, Germany, September 2010).

[61] P. Romaniello and L. Reining, *Insights in the T-matrix formalism*, poster at the *XVth Nanoquanta Workshop on Electronic Excitations* (Berlin, Germany, October 2010).

[62] P. Romaniello, *DFT: insight from MBPT*, invited talk at the *workshop "Density Functional Theory: Fundamentals and Applications in Condensed Matter Physics"*, (Banff, Canada, January 2011).

[63] P. Romaniello, F. Bechstedt and L. Reining, *Insights in the T-matrix formalism*, talk at the *DPG March Meeting 2011* (Dresden, Germany, March 2011).

[64] P. Romaniello, F. Bechstedt and L. Reining, *Insights in the T-matrix formalism*, talk at the *XVIth Nanoquanta Workshop on Electronic Excitations* (Turin, Italy, October 2011).

[65] P. Romaniello, *Approximations for the 1-body Green's function*, invited lecture at the *Lectures on Many Body Perturbation Theory* (Juelich, Germany, February 2012).

[66] P. Romaniello, *Beyond the GW approximation: combining correlation channels*, talk at the *International Symposium and Workshop on Electron Correlations and Materials Properties of Alloys and Compounds* (Porto Heli, Greece, July 2012).

[67] P. Romaniello, G. Lani and L. Reining, *Determination of the one-body Green's function: freedom and constraints*, talk at the *XVIIth Nanoquanta Workshop on Electronic Excitations* (Coimbra, Portugal, October 2012).

[68] P. Romaniello, G. Lani and L. Reining, *Determination of the one-body Green's function: freedom and constraints*, talk at the *DPG March Meeting 2013* (Regensburg, Germany, March 2013).

[69] S. Di Sabatino, L. Reining and P. Romaniello, *RDMFT: insights from/for MBPT*, poster at the *XVIIth Nanoquanta Workshop on Electronic Excitations* (Luxembourg, Luxembourg, October 2012).

[70] S. Di Sabatino, L. Reining and P. Romaniello, *RDMFT: insights from/ MBPT*, poster at the *TDDFT Gordon Conference* (Biddeford, USA, August 2013).

[71] P. Romaniello, G. Lani and L. Reining, *Determination of the one-body Green's function: freedom and constraints*, talk at the *APS March Meeting 2014* (Denver, USA, March 2014).

[72] J. M. Escartin, *Insights into the surface hopping approach from a wave packet limit*, talk at the *XVIIth Nanoquanta Workshop on Electronic Excitations* (Coimbra, Portugal, October 2012).

[73] J. M. Escartin, *Exploring time-dependent current-density functional theory in real time*, talk at the *Theory Days on "Current-Density Functional Theory"* (Toulouse, France, November 2012).

[74] J. M. Escartin, *Exploring time-dependent current-density functional theory in real time*, talk at the *TD-DFT (Time-Dependent Density Functional Theory) internationale conférence* (Nantes, France, Apr. 23–26 2013).

[75] J. M. Escartin, *Time-dependent current-density functional theory: exploring the Vignale-Kohn functional in real time*, poster at the *CECAM workshop "Green's function methods: the next generation"* (Toulouse, France, June 2013).

[76] P. Wopperer, *Angular Distributions of photoelectrons from free Na clusters*, poster at the *Summer School "ATTOFEL"* (Heraklion, Greece, June 1–6 2011).

[77] P. Wopperer, *Angular Distributions of Photoelectrons from free Na Clusters and C_{60}*, talk at the *GDR "Agrégation, fragmentation et thermodynamique de systèmes moléculaires complexes isolés* (Mittelwihr, France, June 21–26 2011).

[78] P. Wopperer, *Photo-electron angular distributions and spectra from free, laser excited clusters*, talk at the international conference *Laser Micro and Nano Structuring* (Palaiseau, France, Dec. 10–12 2012).

[79] P. Wopperer, *On Electronic Photoemission from Irradiated C_{60}*, talk at the *7th International Conference on Quantum, Nano and Micro Technologies* (Barcelona, Spain, Aug. 25–31 2013).

[80] N. Slama, *Role of the variance in the description of an excited system* poster at the *9th ETSF Young Researchers' Meeting* (Brussels, Belgium, May 21–25 2012).

[81] N. Slama, *Role of the variance in the description of an excited system* poster at the International *CORINF PhD School* (Dresden, Germany, June 11–15 2012).

[82] N. Slama, *Dissipation in quantum mean field theories* poster at the International Workshop *"Green's function methods : the next generation"* (Toulouse, France, June 4–7 2013).

[83] N. Slama, *Dissipation in quantum mean field theories* talk at the International *XLIC-CORINF meeting* (Madrid, Spain, Nov. 11–15 2013).

[84] N. Slama, *Description of thermalization in quantum time dependent quantum mean field theories*, poster at the International PhD School *"Correlated Multi-electron dynamics in intense light Fields"* (Cargese, France, Apr. 28 – May 2 2014).

[85] C. Z. Gao, *Dynamics of proton collisions with small organic molecules at low energies*, invited talk at the *International workshop "Theory Days 2013 on Advances in Biomolecule Irradiation"* (Toulouse, France, Nov. 27–29 2013).

[86] C. Z. Gao, *Electron dynamics controlled by attosecond pulse train in presence of an infrared laser*, poster at the International PhD School *"Correlated Multi-electron dynamics in intense light Fields"* (Cargese, France, Apr. 28 – May 2 2014).

[87] S. Di Sabatino, L. Reining, and P. Romaniello, *RDMFT: insights from MBPT*, poster at the *CECAM workshop "Green's function methods: the next generation"* (Toulouse, France, June 2013).

[88] S. Di Sabatino, A. Berger, L. Reining, and P. Romaniello, *RDMFT: insights from MBPT*, poster at the *International school and workshop on TDDFT* (Benasque, Spain, January 2014).

[89] S. Di Sabatino, A. Berger, L. Reining, and P. Romaniello, *RDMFT ¡—¿ MBPT: mutual insight into electron correlation*, talk at the *ETSF Young Researchers' Meeting 2014* (Rome, Italy, May 2014).

[90] N. Raimbault, P. L. de Boeij, P. Romaniello, and J. A. Berger, *Magnetization in extended systems within TDCDFT*, talk at the *ETSF Young Researchers' Meeting 2013* (Budapest, Hungary, May 2013).

[91] N. Raimbault, P. L. de Boeij, P. Romaniello, and J. A. Berger, *Magnetization in extended systems within TDCDFT*, poster at the *CECAM workshop "Green's function methods: the next generation"* (Toulouse, France, June 2013).

[92] N.Raimbault,P. L. de Boeij, P. Romaniello, and J. A. Berger, *Magnetization in extended systems within TDCDFT*, poster at the *International school and workshop on TDDFT* (Benasque, Spain, January 2014).

[93] N. Raimbault, P. L. de Boeij, P. Romaniello, and J. A. Berger, *Magnetization in extended systems within TDCDFT*, talk at the *ETSF Young Researchers' Meeting 2014* (Rome, Italy, May 2014).

[94] L. Lacombe, *Probability of electron attachment on water molecules and ions calculated with a TDDFT approach* , poster at the International Conference on *Isolated Biomolecule and Biomolecular Interactions* (Porquerolles, France, May 19–23 2014).

7

Defended and ongoing PhD theses

7.1 Fermions Fortement Corrélés (FFC)

[1] D. Charrier, *Du magnétisme frustré aux fermions fortement corrélés : approches effectives et non perturbatives (From frustrated magnetism to strongly correlated fermions: effective and non-perturbative approaches)*, thèse de doctorat de l'Université de Toulouse (01/09/2006-17/09/2009); encadrant : P. Pujol.

[2] F. Trousselet, *Dopage de modèles de dimères quantiques: nouvelles phases exotiques (Doped quantum dimer models)*, thèse de doctorat de l'Université de Toulouse (01/09/2006-30/09/2009); encadrant : D. Poilblanc.

[3] D. Schwandt, *Approche liens de valence de la physique de basse énergie des systèmes antiferromagnétiques (Valence bond approach to the low-energy physics of antiferromagnets)*, thèse de doctorat de l'Université de Toulouse (01/09/2008-13/07/2011); encadrants : F. Alet et M. Mambrini.

[4] Y. Iqbal, *Liquide de spin dans des antiferro-aimants quantiques sur réseaux bidimensionnels frustrés (Spin liquids in quantum antiferromagnets on frustrated two-dimensional lattices)*, thèse de doctorat de l'Université de Toulouse (01/09/2009-24/09/2012); encadrants : D. Poilblanc.

[5] X. Plat, *Approches analytiques et numériques de systèmes antiferromagnétiques sous champ magnétique* (titre provisoire), thèse de doctorat de l'Université de Toulouse en cours (01/10/2011) ; encadrants : S. Capponi & P. Pujol.

[6] J.-P. Álvarez Zúñiga, *Études analytique et numérique de la transition superfluide - verre de Bose à deux dimensions* (titre provisoire), thèse de doctorat de l'Université de Toulouse en cours (01/10/2011) ; encadrant : N. Laflorencie.

[7] T. Picot, *Méthodes de Réseaux de Tenseurs (Tensor Networks) pour les systèmes de spins quantiques frustrés et les liquides de spins à 2 dimensions* (titre provisoire), thèse de doctorat de l'Université de Toulouse en cours (01/10/2012) ; encadrant : D. Poilblanc.

[8] M. Soni, *Modèles effectifs 1D et 2D des excitations à statistique fractionnaire non-Abelienne ("non-Abelian anyons") des phases avec ordre topologique* (titre provisoire), thèse de doctorat de l'Université de Toulouse en cours (01/10/2013) ; encadrant : D. Poilblanc.

[9] F. Bègue, *Phases exotiques, magnétisme quantique et isolants topologiques* (titre provisoire), thèse de doctorat de l'Université de Toulouse en cours (01/10/2012) ; encadrant : P. Pujol & R. Ramazashvili .

7.2 Cohérence Quantique (Quantware)

[1] L. Arnaud, *Statistique de l'interfÃ©rence quantique et circuits quantiques alÃ©atoires*, thèse de doctorat de l'Université de Toulouse (01/09/2006-17/12/2009); encadrant : D. Braun.

[2] B. Roubert, *Approche semi-classique de l'information quantique*, thèse de doctorat de l'Université de Toulouse (01/10/2007-28/09/2010); encadrant: D. Braun.

[3] M. Pasek, *Applications des méthodes du chaos quantique aux oscillations d'étoiles en rotation rapide*, thèse de doctorat de l'Université de Toulouse (01/11/2009-20/12/2012); encadrants: B. Georgeot & F. Lignières (IRAP-OMP).

[4] V. Kandiah, *Application of the Google matrix methods for characterization of directed networks* thèse de doctorat de l'Université de Toulouse en cours (01/10/2011) ; encadrants : B. Georgeot & D. L. Shepelyansky.

[5] F. Damon, *Chaos and cold atoms* thèse de doctorat de l'Université de Toulouse en cours (01/10/2012) ; encadrants : B. Georgeot & D. Guéry-Odelin (LCAR-IRSAMC).

7.3 Physique Statistique des Systèmes Complexes (PhyStat)

[1] C. Touya, *Diffusion dans des potentiels aléatoires non gaussiens (Diffusion in random non Gaussian potentials)*, thèse de doctorat de l'Université de Toulouse (01/09/2006-12/10/2009) ; encadrant : D. Dean.

[2] T. Portet, *Électroperméabilisation de systèmes modèles (Electropermeabilisation of model systems)*, thèse de doctorat de l'Université de Toulouse (01/09/2007-24/09/2010) ; encadrants : D. Dean & M.-P. Rols (IPBS). Prix jeune chercheur de la Fondation Bettencourt Schueller 2010.

[3] V. Démery, *Interactions induites par un environnement fluctuant (Interactions induced by a fluctuating environment)*, thèse de doctorat de l'Université de Toulouse (01/09/2009-15/06/2012) ; encadrant : D. Dean.

[4] A. K. Dasanna, *Fermeture de bulles de dénaturation de l'ADN couplée à l'élasticité de l'ADN (Closure of DNA denaturation bubbles coupled to DNA elasticity)*, thèse de doctorat de l'Université de Toulouse (01/10/2010-30/09/2013) ; encadrants : M. Manghi & N. Destainville.

[5] A. Brunet, *Étude par suivi de molécule unique de changements conformationnels de la molécule d'ADN et leur modélisation* (titre provisoire), thèse de doctorat de l'Université de Toulouse en cours (01/10/2012) ; encadrants : N. Destainville & C. Tardin (IPBS).

[6] G. Guéguen, *Mésophases lipidiques et interactions entre protéines dans les bio-membranes fluctuantes* (titre provisoire), thèse de doctorat de l'Université de Toulouse en cours (01/10/2013) ; encadrants : M. Manghi & N. Destainville.

7.4 Systèmes de Fermions Finis – Agrégats (Agrégats)

[1] J. Messud, *Théorie de la fonctionnelle de la densité dépendant du temps avec correction d'auto-interaction (Time-dependent Density Functional Theory with self-interaction correction)*, thèse de doctorat de l'Université de Toulouse (01/09/2006-28/09/2009); encadrant : E. Suraud.

[2] S. Vidal, *Mécanismes d'ionisation de systèmes libres en lumière extrême décrits par la théorie de la fonctionnelle de la densité dépendante du temps (Ionization mechanisms of free systems in extreme light described by the Time-Dependent Density Functional Theory)*, thèse de doctorat de l'Université de Toulouse (01/10/2008-07/12/2011); encadrant: P. M. Dinh.

[3] P. Wopperer, *Electron photoemission from sodium and carbon clusters*, thèse de doctorat de l'Université de Toulouse et de l'Université Erlangen-Nürnberg (01/09/2011-07/06/2014); encadrants: E. Suraud et P.-G. Reinhard (Erlangen).

[4] N. Slama, *Towards the inclusion of dissipation in electronic systems* thèse de doctorat de l'Université de Toulouse (01/01/2012-31/12/2014); encadrant: E. Suraud.

[5] N. Raimbault, *Magnetization in extended systems within time-dependent current-density functional theory* thèse de doctorat de l'Université de Toulouse (01/10/2012-30/09/2015); encadrant: P. Romaniello et A. Berger (LCPQ-IRSAMC).

[6] S. Di Sabatino, *Correlation in density matrix functional theory: new approximations from Green's function-based methods* thèse de doctorat de l'Université de Toulouse (01/10/2012-30/09/2015); encadrant: P. Romaniello.

[7] C. Z. Gao, *Laser irradiation of clusters and moelcules in FEL and atto regimes* thèse de doctorat de l'Université de Toulouse (01/10/2014-30/09/2017); encadrant: E. Suraud.

[8] L. Lacombe, *Compréhension microscopique des dommages causés à des molécules biologiques dans les thérapies contre le cancer (Microscopic understanding of damages to biological molecules in cancer therapies)* thèse de doctorat de l'Université de Toulouse (01/10/2014-30/09/2017); encadrant: P. M. Dinh.

8

Habilitations à Diriger des Recherches (HDR)

8.1 Fermions Fortement Corrélés (FFC)

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8.2 Cohérence Quantique (Quantware)

[1] B. Georgeot, *Applications du chaos quantique à l'information quantique et aux atomes froids*, Thèse d'habilitation à diriger des recherches, Université Paul Sabatier (19/03/2010).

8.3 Physique Statistique des Systèmes Complexes (PhyStat)

[1] M. Manghi, *Physique statistique d'objets biologiques et des électrolytes aux interfaces*, Thèse d'habilitation à diriger des recherches, Université Paul Sabatier (18/11/2010).

[2] P.-H. Chavanis, *Dynamique et thermodynamique des systèmes avec des interactions à longue portée*, Thèse d'habilitation à diriger des recherches, Université Paul Sabatier (23/12/2012).

8.4 Systèmes de Fermions Finis – Agrégats (Agrégats)

[1] P. M. Dinh, *Time-dependent density functional theory applied to molecules and clusters in contac with an environment*, Thèse d'habilitation à diriger des recherches, Université Paul Sabatier (07/12/2009).

9

Other realizations and achievements

This annex lists major contributions or achievements of the LPT scientists in various domains, including [a]:

- **Organization of conferences and schools**
- **Books as writers or editors**
- **Main achievements in education (responsible of a Master...)**
- **Popularization of science and diffusion of knowledge**
- **Prizes and honors**
- **Major administrative responsibilities**
- **Coordinator (or important partner) of major contracts (EU, ANR...)**
- **Author of commercial or major open source softwares**
- **...**

a. **Except for the two first items, most achievements are described in French**

9.1 Fermions Fortement Corrélés (FFC)

• **Organization of conferences and schools**

[1] F. Alet, organisation d'un mini-workshop "Quantum Magnetism", (Toulouse, France, July 2011).

[2] S. Capponi, membre du comité scientifique et co-organisateur du Mini-colloque «Matière condensée avec des atomes froids» durant le Congrès Général de la SFP (Bordeaux, 2011).

[3] S. Capponi, co-organisateur du colloque annuel de l'Institut Universitaire de France (Toulouse, 2013).

[4] S. Capponi, membre du collège scientifique de Physique de l'université Paul Sabatier Toulouse 3 (élu 2008-2013, réélu 2013-).

[5] N. Laflorencie, organiser of the international workshop "New Trends in Quantum Magnetism", (Orsay, June 1-3 2010).

[6] N. Laflorencie, member of the organising committee celebrating 100 years of superconductivity in 2011: "Supra 2011".

[7] N. Laflorencie, co-organiser of the international workshop "Quantum Disordered Systems", (Toulouse, June 24-27 2014).

[8] N. Laflorencie, D. Poilblanc and R. Ramazashvili, organisation et comité scientifique de *International Workshop "From Quantum Foundations to Quantum Fluids"* in the honor of Professor A. J. Leggett, Nobel Prize of Physics, Toulouse, April 4-6, 2012.

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

[10] D. Poilblanc, Member of Scientific Committee: Workshop "New Trends in Quantum Magnetism" (Orsay, June 1-3 2010).

[11] D. Poilblanc, Scientific adviser: International Workshop "Disentangling Quantum Many-body Systems: Computational and Conceptual Approaches" (Oct 11 - Dec 17, 2010), KITP & UC Santa Barbara (http://online.kitp.ucsb.edu/online/compqcm10/).

[12] D. Poilblanc, Organisation de: Symposium "Topological Quantum Information", Centro de Ciencias de Benasque Pedro Pascual (Espagne), 12-16 février 2013 (http://benasque.org/2013tqi/).

[13] D. Poilblanc, Organisation de: Workshop International "Topological Phases in Condensed Matter and Cold Atom Systems", Institut d'Etudes Supérieures de Cargèse (http://www.iesc.univ-corse.fr/), 24 juin – 6 juillet 2013, avec E. Ardonne (Université de Stockholm), N. Regnault (ENS) et M. Troyer (ETH Zürich).

[14] D. Poilblanc, Organisation de: CECAM School "Quantum spin liquids: from gauge theories to simulations", SISSA, Trieste, 9-20 septembre 2013, avec F. Becca (SISSA) et G. Misguich (CEA Saclay) (http://www.cecam.org/workshop-866.html).

[15] D. Poilblanc, Member of the Program Committee ("Quantum many-body physics"), XXVI IUPAP Conference on Computational Physics, CCP2014 August 11-14, 2014, Boston, Massachusetts, USA.

[16] D. Poilblanc, Organisation de: Workshop International "Analytical and numerical approaches to strongly correlated systems", Centro de Ciencias de Benasque Pedro Pascual (Espagne), 25 août – 12 septembre 2014 (http://benasque.org/general/cgi-bin/years.pl?ano=2014) avec R. Orus et J. Vidal.

[17] D. Poilblanc, Organisation de: Workshop International "Topological Phases in Condensed Matter and Cold Atom Systems" à l'Institut d'Etudes Supérieures de Cargèse (http://www.iesc.univ-corse.fr/), prévu du 31 août – 12 septembre 2015 avec Roderich Moessner (MPI-Dresden) et N. Regnault (ENS).

[18] P. Pujol, Organisation de : International school "Strong correlations in electronic systems" à l'Ecole de Physique des Houches, du 10 au 29 mai 2009 avec D. Cabra (La Plata) et A. Honecker (Gottingen).

[19] P. Pujol, Organisation de : International school "Strongly correlated electronic systems, beyond Fermi liquid theory" à l'Ecole de Physique des Houches, du 11 au 21 avril 2011 avec D. Cabra (La Plata) et A. Honecker (Gottingen).

- **Books as writers or editors**

[20] P. Pujol, co-rédacteur en chef du livre "Modern Theories of Many-Particle Systems in Condensed Matter Physics", Lecture Notes in Physics, Springer, avec D. Cabra (La Plata) et A. Honecker (Gottingen).

- **Main achievements in education (responsible of a Master or Bachelor program...)**

[21] S. Capponi, responsable du M1 physique de l'université Paul Sabatier (depuis 2012).

[22] P. Pujol, responsable de l'enseignement de la Physique 1, en première année de Licence de l'université Paul Sabatier (depuis 2010).

[23] P. Pujol, co-fondateur des parcours spéciaux en Licence de Physique, Chimie et mathématiques de l'université Paul Sabatier (en 2010-2011).

- **Popularization of science and diffusion of knowledge**

[24] D. Poilblanc, Vulgarisation: Conférence de presse "De la recherche à l'industrie : la supraconductivité prend son envol" (30 mars 2011, CNRS campus Michel-Ange); *Les supraconducteurs : de nouveaux défis conceptuels.*

[25] N. Laflorencie, popular science activity with high school pupils about superconductivity: experimental demonstrations of Meisner effect and levitation.

[26] P. Pujol, Plusieurs conférences de vulgarisation sur la mécanique quantique, et sur la supraconductivité, destinées à des élèves de classes de collége, de lycée et pour le grand public.

[27] F. Alet, parrainage d'une classe de 1ère S sur le thème du magnétisme et de la supraconductivité (Lycée Saint-Sernin, Toulouse, 2013-14)

- **Major administrative responsibilities and contract coordination**

[28] F. Alet, M. Mambrini, and S. Capponi, contrat ANR Jeunes Chercheurs : Q-BONDS "Corrélations Quantiques & Intrication dans les états Liens de Valence", (Janvier 2009-Septembre 2012).

[29] F. Alet, Responsable du contrat CEFIPRA (Centre Franco-Indien pour la Promotion de la Recherche Avancée) "Computational studies of frustrated quantum magnets", (Juin 2011-Mai 2014).

[30] F. Alet, membre du Comité National du CNRS, Section 06 (Septembre 2008-Août 2012).

[31] S. Capponi, membre du CNU 29e section (élu 2011-2015).

[32] S. Capponi, membre du bureau de la division «matière condensée» de la Société Française de Physique (élu 2009-2011).

[33] S. Capponi, membre du comité scientifique du GDR «physique mésoscopique» (2009-2013).

[34] N. Laflorencie, secretary of the local board of "Société Française de Physique" since 2012.

[35] N. Laflorencie, principal investigators of the *ANR Blanc International: Quapris "Quantum Phases of Random Interacting Systems"*, since January 2012.

[36] N. Laflorencie, elected member of "Conseil de la Faculté des Sciences et d'Ingénierie", Université Paul Sabatier, since 2013.

[37] D. Poilblanc, membre nommé du *Comité National du CNRS, Section 03*, (septembre 2012-janvier 2013).

[38] D. Poilblanc, Responsable programme BLANC ANR "Nouvelles phases quantiques et propriétés topologiques de systèmes corrélés de matière condensée" (12/2010 - 12/2015).

[39] D. Poilblanc, membre du comité scientifique du GDR "MICO" (2009-2015).

[40] P. Pujol, membre du CNU 29e section (élu 2006-2010).

[41] P. Pujol, président de la section locale Midi-Pyrénées de la Société Française de Physique (SFP) (depuis 2011).

[42] P. Pujol, membre élu du département de physique de l'université Paul Sabatier (depuis 2012)

[43] P. Pujol, membre nommé du groupe d'avancement et de primes (GAP) des départements de mathématiques et informatique de l'université Paul Sabatier (depuis 2014)

9.2 Cohérence Quantique (Quantware)

- **contract coordination**

[1] D.L. Shepelyansky: Principal Investigator for Toulouse node of EC IST FP6-015708 EuroSQIP project *European Superconducting Quantum Information Processor* (duration November 1, 2005 - April 30, 2010, 1 post-doc for 3 years, total funding of 150 keuro)

[2] D.L. Shepelyansky: Coordinator of EC FET Open project NADINE No 288956 *New tools and algorithms for directed network analysis* (duration 1 May 2012 - 30 April 2015, 1 post-doc for 2.5 years, total funding of network of 4 EC partners 1.22 Meuro, Toulouse node budget 322 keuro)

[3] D.L. Shepelyansky: Principal Investigator for LPT node of ANR PNANO project MICONANO *Microwave Control of Transport in Nanoscopic Structures* (nodes: LPN Paris, LPT Toulouse, CEA and LCMI Grenoble, coordinator: J.-C.Portal, LCMI Grenoble; duration December 1, 2005 - April 30, 2009; funding of 42 keuro)

[4] D.L. Shepelyansky: Principal Investigator for LPT node of ANR PNANO project NANOTERRA *NANOdetectors of microwave and TERahertz radiation based on RAtchet effect* (LPS Orsay, LPT Toulouse, LAAS Toulouse, LNCMI Grenoble (J.-C.Portal - coordinator), duration Jan 1, 2009 - Dec 31, 2012; 1.5 years of post-doc funding of 110 keuro)

[5] D.L. Shepelyansky: Principal Investigator for LPT node of France-Armenia collaboration *Classical and quantum chaos* grant CNRS/SCS No 24943 (Nerses Ananikyan is PI for Alikhanyan Nat. Sci. Lab., Yerevan, Armenia; duration Jan 1, 2012 - Dec 31, 2013; funding of 7 keuro)

[6] I. Nechita: Coordinator of the *PEPS ICQ project COGIT "Combinatoire et Géométrie pour l'InTrication"* .

[7] I. Nechita: Coordinator of the French team in the *ANR international project RMTQIT "Techniques de matrices aléatoires en theórie quantique de l'information"* (joint project with a team from Politechnica University, Timisoara, Romania).

[8] I. Nechita: Coordinator of the French team in the *Procope project "Random Matrix Theory and Free Probability"*(joint project with a team from Saarlandes University, Germany).

[9] I. Nechita: Member of the *ANR project OSQPI "Interactions entre espaces d'opérateurs et probabilités quantiques et leurs applications à l'information quantique"*.

[10] D. Braun Coordinator of three GDRI-471 French-Russian research projects, 2009-11

[11] D. Braun Coordinator of a DGA research project, "Semiclassical analysis of quantum algorithms", 2007-2010

[12] G. Lemarié, responsible of the *A01 international project SIKBEC* of the Université Paul Sabatier, involving N. Laflorencie (LPT), J. C. Garreau from PhLAM laboratory in Lille, D. Delande from LKB boratory in Paris, C. Castellani and L. Benfatto from Sapienza Università in Rome (Italy).

[13] G. Lemarié, head of the node in Toulouse of the
ANR project K-BEC Kick Rotor, in collaboration with P. Szriftgiser from PhLAM laboratory in Lille and D. Delande from LKB laboratory in Paris.

[14] B. Georgeot: Co-investigator of the Toulouse node of the *ANR project Siroco: SeIsmology, ROtation and COnvection with the COROT satellite* 2007-2012.

[15] B. Georgeot: Principal investigator of a *project PEPS from CNRS "multifractalité des fonctions d'onde quantiques"* for a collaboration between Toulouse, university of Créteil (J.M. Aubry, Mathématiques) l'University of Orsay (E. Bogomolny, O. Giraud), university of Liège (John Martin, Belgium) and the laboratory TANDAR at Buenos Aires (I. Garcia-Mata, Argentina)(7000 euros).

[16] B. Georgeot: Co-investigator of a *project funded by the University Paul Sabatier OMASYC "Ondes de Matière dans les systèmes complexes"* (collaboration with the experimental team of D. Guéry-Odelin, LCAR, Toulouse)(2011-2013) (17000 euros + two PhD fellowships)

[17] B. Georgeot: Principal investigator of a *project funded by the LABEX Next ENCOQUAM "Engineering of Complex Quantum Matter Waves"* (collaboration with the experimental team of D. Guéry-Odelin, LCAR, Toulouse)(2012-2015) (150000 euros)

[18] B. Georgeot: Co-investigator of a *project PICS from CNRS* for a collaboration between Toulouse, University of Orsay (E. Bogomolny, O. Giraud) and CONICET (I. Garcia-Mata, Argentina)(30000 euros).

- **editorial activities and reviewing**

[19] D.L. Shepelyansky: Editorial member of Physical Review E (duration 2011 - 2013, 2014 - 2016)

[20] D.L. Shepelyansky: Editor of Scholarpedia for Quantum Chaos (2008 - present)

[21] D.L. Shepelyansky: reviewer for EC FET Open proposals in 2008 - 2012.

- **conference organization**

[22] D.L. Shepelyansky: Organizer (with D.Donato) of Workshop *PageRank matrix days*, dedicated to 100 Anniversary of S.Ulam, 2 days in Dec 2009, LPT Toulouse (20 participants).

[23] D.L. Shepelyansky: Organizer (with G.Caldarelli, N.Litvak, T.Guhr) of Workshop *Spectral properties of complex networks*, at European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*), Trento Italy. 23-27 July 2012 (40 participants)

[24] D.L. Shepelyansky: Organizer (with P.Boldi, M.Santini, S.Vigna) of FET NADINE Workshop *Directed networks days*, LAW, U Milano, 13-14 July 2013 (20 participants).

[25] D.L. Shepelyansky: Organizer (with E.Kartashova, A.Pikovsky)) of Workshop *Weak Chaos and Weak Turbulence*, at MPI Complex Systems, Dresden, 3 - 7 February, 2014 (50 participants).

[26] D.L. Shepelyansky: Organizer (with A.Benczur, R.Palovics) of FET NADINE Workshop *Directed networks days*, Informatics Laboratory at the Computer and Automation Research Institute, Hungarian Academy of Sciences, Budapest 8 - 11 May, 2014 (20 participants).

[27] D.L. Shepelyansky: Organizer (with A.Benczur, A.Kaltenbrunner) of Session I of Summer School *Network analysis and applications* at École des sciencees avancées de Luchon, 21 June - 5 July, 2014 (50 participants).

[28] I. Nechita: Co-organizer of the second meeting of the "COGIT" CNRS PEPS-ICQ meeting in Toulouse, 13-15 November 2013.

[29] I. Nechita: Co-organizer of the first meeting of the "COGIT" CNRS PEPS-ICQ meeting in Rouen, 5-7 June 2013.

[30] I. Nechita: Co-organizer of the annual meeting of the Mathematics and Theoretical Physics departments at the Univeristy of Toulouse, 24th May 2013.

[31] I. Nechita: Co-organizer of the annual meeting of the Mathematics and Theoretical Physics departments at the Univeristy of Toulouse, 24th May 2012.

[32] I. Nechita: Co-organizer, wtih Stéphane Attal and Clément Pellegrini of the workshop Probabilistic Methods in Quantum Mechanics at the University of Lyon, 14-16 May 2012.

[33] I. Nechita: Co-organizer, wtih Stéphane Attal and Clément Pellegrini of the Open Quantum Systems and Quantum Information Theory workshop at the Univeristy of Toulouse, 16-18 November 2011.

[34] I. Nechita: Co-organizer of the annual meeting of the Mathematics and Theoretical Physics departments at the Univeristy of Toulouse, 4th April 2011.

[35] I. Nechita: Co-organizer, with Benoit Collins and Patrick Hayden, of the international workshop Random Matrix Techniques in Quantum Information Theory at the Perimeter Institute, 4-6 July 2010. Videos of the talks are available here.

[36] G. Lemarié, organizer, together with N. Laflorencie (LPT) and J. Billy (LCAR), of the *International Workshop "Quantum Disordered Systems: What's Next?"*, (Toulouse, France, 24-27 June 2014).

[37] B. Georgeot: Co-organizer of the conference *Colloquium of the quantum dynamics GDR* 8-10 february 2012, Toulouse, France.

- **Main achievements in education**

[38] D.L. Shepelyansky: launched with maire de Luchon Louis Ferré creation of École des sciencees avancées de Luchon in collaboration with NEXT, LPT, IRSAMC, Univ. P.Sabatier.

[39] D. Braun Coordinator (together with A. Bouchene at LCAR) of the master M2 "Physique de la matiére"

[40] K. Frahm Coordinator of the L3 "Physique"

- **Popularization of science and diffusion of knowledge**

[41] D. Braun Popular scientific lecture at the "Maison de la Philosophie", Toulouse, Feb. 2013 *La mécanique quantique : des fondements aux applications, et le boson de Higgs*

[42] D. Braun Two Popular scientific lectures at the "Fête d'IRSAMC", Toulouse, June 2012 *La crytpographie quantique*

[43] D. Braun Popular scientific lecture at the Café "Baton à palabres", Toulouse, Dec. 2011 *La mécanique quantique: fondements, applications, et implications philosophiques*

[44] D. Braun Popular scientific lecture at the "Maison de la Philosophie", Toulouse, Nov. 2011 *La mécanique quantique: fondements, applications, et implications philosophiques*

[45] D. Braun Popular scientific lecture for high-school teachers of physics in the framework of the continued education program of the "Académie de Toulouse", Jan. 2010 *La mécanique quantique: un voyage au monde microscopique*

[46] D. Braun Public popular scientific lectures at the "Fête de la Science", Toulouse Nov. 2009, Oct. 2010, Oct. 2011 *La mécanique quantique: des mystères aux applications*

[47] D. Braun Two popular scientific talks for middle- and high-school students during the "Fête de la Science", Nov. 2009, *La mécanique quantique: un voyage au monde microscopique*

[48] B. Georgeot: Co-redaction of a press release from CNRS on chaos in asteroseismology (2011).

[49] B. Georgeot: Co-redaction of a press release from CNRS on atom lasers (2012).

[50] B. Georgeot: The paper [84] was distinguished by the journal Europhysics Letters for having had more than 5000 downloads in 90 days.

[51] B. Georgeot: Co-redaction of a press release from CNRS on the network of the game of go (2012).

[52] B. Georgeot: participation in an interview on Radio France Internationale on the network of the game of go (2012).

[53] B. Georgeot: participation in an interview for the American Physical Society on the network of the game of go, released as a podcast(2014).

- **Prizes and honors**

[54] D. Braun Prize for best Ph.D. presentation of the Ecole Doctorale de Toulouse for Ph.D. student Ludovic Arnaud (1000 Euros for the Laboratoire de Physique Théorique), 2009

- **Major administrative responsabilities**

[55] D. Braun Member of the board of the European COST Action MP1006 "Fundamental Problems in Quantum Physics", 2011-2013

[56] D. Braun Member of the board of the French national research initiative (GdR) "Quantum Information from Foundations to Applications", 2010 - 2013

[57] K. Frahm: Member of the council of the department of physics, University Paul Sabatier (since 2012)

[58] B. Georgeot: Member of the board of the French national research initiative (GdR) "Dynamique quantique", (since 2009)

[59] B. Georgeot: Member of the scientific council of the UFR "Physique-Chimie-Automatique", University Paul Sabatier (2003-2010)

[60] B. Georgeot: Member of the scientific council of the University Paul Sabatier (since 2013)

[61] B. Georgeot: Director of the Fédération de recherche IRSAMC (FR 2568)(since 2013); as such, he is member of the executive committee of the LABEX NEXT, of the board of Directors of the pôle "Sciences de la matière".

9.3 Physique Statistique des Systèmes Complexes (PhyStat)

- **Organization of conferences and schools**

[1] D. Dean (au LPT jusqu'en décembre 2011) s'est fortement impliqué dans la gouvernance de l'Institut Henri Poincaré (IHP) : membre du *Comité de Programmation Scientifique* (CPS) de l'IHP, 2007-présent ; vice-président du CPS, 2009-2010 ; président du CPS, 2010-présent.

[2] P.-H. Chavanis a organisé la session *Self-gravitating systems* au XIIth Marcel Grossmann Meeting, à l'UNESCO, Paris (13-18 juillet 2009).

[3] P.-H. Chavanis a co-organisé le Workshop Systèmes de particules avec interactions à longue portée : limite continue et effets discrets, au Laboratoire Dieudonné, Nice (3-4 novembre 2011).

[4] C. Sire a initié (et coorganisé, certaines années) le mini-colloque annuel avec l'Institut de Mathématiques de Toulouse, organisé sur une journée au LPT ou à l'IMT depuis 2009 (3 intervenants de chaque laboratoire).

[5] M. Manghi a été membre du Comité d'organisation du Workshop Modeling complex dynamics in biological systems organisé par MIBS Toulouse les 7-9 juin 2010.

[6] En 2012, J. Palmeri a coorganisé la visite au LPT-Toulouse du Prof. A. J. Leggett, Prix Nobel et Prix Wolf 2003 (Professeur invité *Université Toulouse III-Paul Sabatier*, Toulouse, avril 2012). Il a été co-organisateur et chairman de la conférence internationale "From Quantum Foundations to Quantum Fluids" en l'honneur du Prof. A. J. Leggett, du 4 au 6 avril 2012, à *l'Université Toulouse III-Paul Sabatier*.

- **Main achievements in education (responsible of a Master or Bachelor program...)**

[7] M. Manghi est responsable pour la Physique du Master 1 Physique et Chimie pour le Vivant et la Santé (PCVS) créé en septembre 2011. Ce Master 1, unique en province, a pour objectif de former des étudiants en physico-chimie, matière molle et biophysique et aux outils chimiques pour le diagnostic et la thérapeutique.

[8] N. Destainville est responsable du Master 2 *Physique du vivant*, qui est un des deux M2 (avec Chimie-Santé) qui suivent le M1 PCVS précédent. Il a été dans, lors des 5 dernières années, responsable de plusieurs modules d'enseignement, dont le *module de stages du M1 de Physique*.

[9] M. Manghi est responsable de 3 modules d'enseignement, *Phénomènes hors-équilibre et processus irréversibles* (M2 Physique du Vivant), *Physique de la cellule* (M1 PCVS) et *Physique classique : ondes et mécanique* (L3 Physique).

[10] S. Prolhac est responsable du module d'enseignement, *Physique statistique* (L3 Physique).

[11] P.-H. Chavanis a donné un cours dans le cadre du Workshop GRAVASCO: N-body gravitational dynamical systems (from $N = 2$ to infinity...), à l'Institut Henri Poincaré (IHP), Paris (10-11 octobre 2013).

- **Popularization of science and diffusion of knowledge**

[12] J. Palmeri (au LPT jusqu'en septembre 2012) a développé *Nanoflux*, un logiciel commercial de simulation pour la nanofiltration (voir aussi la news sur le site web de l'UPS ; aussi présenté dans le Journal du CNRS), qui a accumulé plus de 60 k€ de licences achetées par différents acteurs de la chimie et de l'industrie pharmaceutique.

[13] J. Palmeri, et al., *Projet SIMONANOMEM*, Cahier Numéro 3 de l'ANR *Calcul haute performance* (Janvier 2010).

[14] L. Cailloce, J. Palmeri, *Un logiciel qui simule la filtration de l'eau*, Journal du CNRS **255**, 34 (2011) (rédigé par un journaliste du journal).

[15] L. Cailloce, J. Palmeri, *Nanofiltration Simulation Software*, CNRS International Magazine **21**, 32 (2011) (rédigé par un journaliste du journal).

[16] C. Sire réalise une douzaine d'interventions par an dans le domaine de la vulgarisation scientifique (collèges/lycées, festivals, associations, milieu médical, médias...). Les présentations, résumés, et programme sont disponibles sur cette page consacrée entièrement à la vulgarisation.

- **Prizes and honors**

[17] T. Portet a reçu le prix jeune chercheur de la Fondation Bettencourt Schueller 2010 pour sa thèse réalisée au LPT et à l'IPBS : *Électroperméabilisation de systèmes modèles (Electropermeabilisation of model systems)* (01/09/2007-24/09/2010) ; encadrants : D. Dean & M.-P. Rols (IPBS).

[18] C. Sire a été nommé Outstanding Referee of the American Physical Society à compter de 2012.

- **Major administrative responsibilities and contract coordination**

[19] C. Sire a été un contributeur et rédacteur majeur du projet de Laboratoire d'Excellence (LABEX) NEXT, mais aussi du projet d'IDEX Toulouse, tous les deux couronnés de succès.

[20] Outre la direction du LPT, C. Sire est membre du bureau et du comité exécutif du LABEX NEXT, membre du conseil scientifique et de gouvernance du LABEX CIMI (maths-informatique, Toulouse), membre du bureau de la Fédération IRSAMC, membre du Conseil de l'École doctorale Sciences de la Matière. Il a présidé le comité d'évaluation AERES du LPTM de Cergy-Pontoise, en novembre 2013.

[21] M. Manghi est membre élu du Collège Scientifique (Rang B, Section 29) *Physique et Sciences de l'Univers* et du *Groupe d'Avancement C* (Rang B, Maîtres de Conférences) de l'Université Paul Sabatier (2013-2017).

[22] De 2009 à 2013, N. Destainville a été membre élu du même Collége Scientifique *Physique et Sciences de l'Univers*.

[23] De 2008 à 2012, N. Destainville a été membre élu des sections 02 et CID 43 (interfaces de la Biologie) du *Comité National de la Recherche Scientifique* du CNRS.

[24] Depuis 2012, N. Destainville est membre élu du Conseil d'Administration *l'Université Toulouse III-Paul Sabatier* et en est également Vice-Président Délégué aux Personnels et au Dialogue Social.

[25] De 2008 à 2012, J. Palmeri a été coordinateur du projet ANR-NANO-2007 SIMONANOMEM : *SImulation and MOdelling of transport across polymeric NANOporous MEMbranes prepared by self-assembly of block copolymers*, impliquant quatre partenaires différents.

9.4 Systèmes de Fermions Finis – Agrégats (Agrégats)

- **Organization of conferences and schools**

[1] P. M. Dinh et E. Suraud: organisateurs de la conférence internationale *"Theory Days 2009 on the Irradiation of Biomolecules"* (Toulouse, 2–4 déc. 2009).

[2] P. Romaniello: organisatrice des *"CECAM (Ile de France) discussion meetings on Correlation"* (Palaiseau, France, biannuelle depuis 2010).

[3] P. M. Dinh, X. Marie, Ll. Serra et E. Suraud: organisateurs de la conférence internationale *"Theory Days 2010 on Quantum Dots et Wires"* (Toulouse, 17–19 nov. 2010).

[4] P. M. Dinh, P. Romaniello, E. Suraud et V. Véniard: organisateurs de la conférence internationale *"Theory Days 2011 on Stochastic et Dissipative Effects"* (Toulouse, 28–30 nov. 2011).

[5] P. M. Dinh and E. Suraud: membres du comité d'organisation de la conférence *"E2PHY : Physique de l'Espace"* (Toulouse, 28–31 août 2012).

[6] L. Calmels, P. M. Dinh, P. Romaniello, T. Saue et E. Suraud: organisateurs de la conférence internationale *"Theory Days 2012 on Time-Dependent Current Density Functional Theory"* (Toulouse, 28–30 nov. 2012).

[7] P. M. Dinh and E. Suraud: membres du comité d'organisation des *"Journées annuelles de l'Institut Universitaire de France"* (Toulouse, 2–4 Avril 2013).

[8] A. Berger, L. Reining et P. Romaniello: organisateurs de la conférence internationale CECAM *"Green's function methods: the next generation"* (Toulouse, 4–7 juin 2013).

[9] J. P. Champeaux, P. M. Dinh, P. Moretto-Capelle, P. Romaniello et E. Suraud: organisateurs de la conférence internationale *"Theory Days 2013 on Advances in Biomolecule Irradiation"* (Toulouse, 27–29 nov. 2013).

[10] A. Berger, P. M. Dinh, S. Kuemmel, P. Romaniello et E. Suraud: organisateurs de la conférence internationale *"Theory Days 2014 on Self-Interaction Correction"* (Toulouse, 26–28 nov. 2014).

[11] E. Krotscheck, S. A. Chin, et E. Suraud: organisateurs de la conférence internationale *"Common challenges in finite fermion systems"* (Buffalo, USA, 6-9 nov. 2014).

- **Books**

[12] J. Maruhn, P.-G. Reinhard, et E. Suraud: auteurs du livre *"Simple models of many fermions systems"* (Springer, 2010).

[13] P. M. Dinh, P.-G. Reinhard, et E. Suraud: auteurs du livre *"Introduction to cluster science"* (Wiley-VCH, 2013).

- **Popularization of science and diffusion of knowledge**

[14] P. M. Dinh: "Novélisée 2012", Festival "La Novela" (Toulouse 5–21 oct. 2012), interview réalisée pour la soirée des Novélisés.

- **Prizes and honors**

[15] E. Suraud: Professeur Associé de physique, State University New York, University at Buffalo, NY, USA, depuis 2013.

[16] E. Suraud: membre senior 2010 de l'Institut Universitaire de France.

[17] P. M. Dinh: membre junior 2012 de l'Institut Universitaire de France.

[18] P. Romaniello: Prime d'excellence scientifique CNRS 2011.

- **Major administrative responsibilities and contract coordination**

[19] E. Suraud: Président du comité scientifique SIMI4 (maintenant CES32) "Physics of dense et dilute matter" de l'Agence Nationale de la Recherche, depuis 2013.

[20] E. Suraud: Membre correspondant de European Academy of Sciences, Arts and Letters, depuis 2014.

[21] E. Suraud: Membre de *International Advisory Committee of the annual Condensed Matter Theory Workshops*, depuis 2004 (dernière édition en 2011, prochaine édition en suspens).

[22] E. Suraud: Membre de *Technical Program Committee of IARIA-ICQNM* depuis 2013.

[23] E. Suraud: Chargé de mission au CNRS-USAR pour la physique, en relation avec l'ANR, de 2007 à fin 2010, puis directement respondsable de l'ANR en 2011.

[24] E. Suraud: Membre du *Comité de Sélection du Prix Thibaud*.

[25] E. Suraud: Président du GAP (commission des promotions) des Professeurs de l'Université de Paul Sabatier depuis 2012.

[26] E. Suraud: Membre du *Bureau Éditorial de "European Journal of Physics Special Topics"* depuis 2009.

[27] E. Suraud: Membre de *Editorial advisory board of Versita (now part of deGruyter) open access books*, depuis 2012.

[28] P. Romaniello: Research Team Leader (since 2010) and member of the Steering Committee (since 2013) of the *European Theoretical Spectroscopy Facility*.

[29] P. M. Dinh et E. Suraud: partenaires du financement ANR-10-BLAN-0411 "COLDIRR" (Irradiation of Cold Molecular Nanosystems, 2009-2013), porté par Prof. M. Farizon, IPNL.

[30] P. M. Dinh et E. Suraud: partenaires du financement ANR-10-BLAN-0428 "MUSES" (Multiscale Electron Dynamics, 2010-2014), porté par Dr. F. Lépine, ILM Lyon.

[31] P. M. Dinh et E. Suraud: partenaires du financement ANR-11-IS04-0003 PWTELEMAN (Beijing-Wuxi-Toulouse-Erlangen-Le Mans, collaboration on Time dependent Electronic dynamics in Molecules et Nanosystems, 2011-2014), porté par Prof. F. Calvayrac, LPEC Le Mans.

[32] P. M. Dinh et E. Suraud: partenaires du financement ANR-13-BS04-0007 LASCAR (Étude expérimentale et théorique de l'interaction d'une impulsion ultracourte avec un nanocone de carbone): porté par Dr. B. Châtel, LCAR, Toulouse.

[33] E. Suraud: partenaire du réseau européen ITN CORINF (2011-2014), porté par Profs. M. Ivanov et O. Smirnova (Berlin).

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