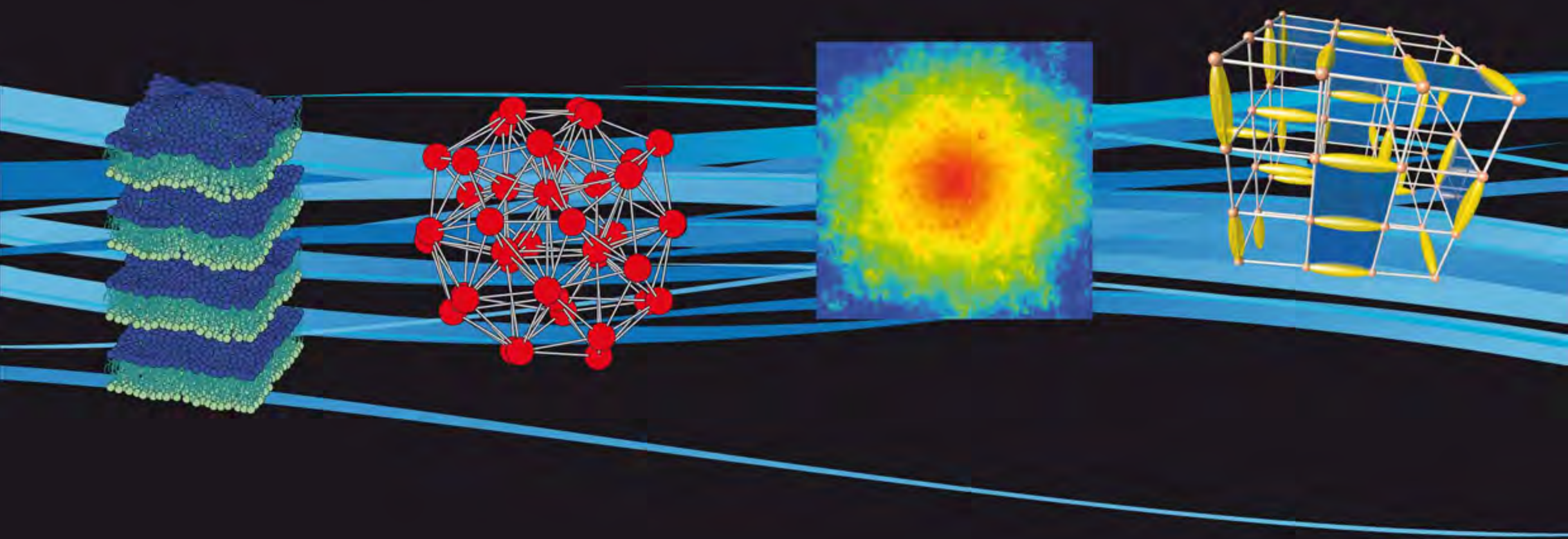
Université de Toulouse

Laboratoire de Physique Théorique



UMR 5152 CNRS & Université Toulouse III

Scientific Project

Projet Scientifique

2011-2014

Contents

1

Projet 2011-2014 du LPT (French version)

Dans ce chapitre, nous exposons le projet 2011-2014 du Laboratoire de Physique Théorique **sans pour autant aborder en détail les projets scientifiques des quatre équipes du LPT, qui seront développés au Chapitre 3. Nous présentons ici l'évolution attendue du laboratoire concernant son personnel permanent et son organisation, sa relation étroite avec la Fédération IRSAMC, et le développement de nouveaux axes scientifiques généraux. Ce chapitre se conclut par l'auto-analyse du LPT.**

1.1 Organisation et évolution du LPT

Les quatre équipes du LPT

Au cours du prochain *contrat quadriennal* 2011-2014, le LPT continuera à être structuré en quatre équipes :

❍ FFC : Fermions Fortement Corrélés ; *Strongly Correlated Fermions* (Directeur : Didier Poilblanc)

❍ Quantware : Information et Chaos Quantiques ; *Quantum Information and Chaos* (Directeur : Dima Shepelyansky)

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

❍ Agrégats : Systèmes de Fermions Finis – Agrégats ; *Finite Fermionic Systems – Clusters* (Directeur : Éric Suraud)

Évolution du personnel permanent

Revaz Ramazashvili a été sélectionné par le jury de la Section 06 du CNRS (physique de la matière condensée) au concours CR1, et doit prendre ses fonctions au LPT en octobre 2009.

Le LPT devrait obtenir un poste de professeur en Section CNU 29 à l'UPS, avec un *comité de sélection* prévu en mai 2010. La description du poste concerne trois thèmes de recherche à la frontière entre les activités scientifiques des quatre équipes du LPT.

Pour raisons personnelles, Olivier Giraud devrait rejoindre le Laboratoire de Physique Théorique et Modèles Statistiques (UMR 8626 Orsay) à la mi-2010. Le LPT lui adresse tous ses vœux de réussite dans son nouveau laboratoire, et espère que ses collaborations fructueuses avec les chercheurs du LPT ne seront pas trop affectées par son départ. En juin 2009, l'équipe Quantware a obtenu un financement CNRS *PEPS-Physique Théorique et ses Interactions*, afin, notamment, de contribuer à financer les futurs séjours d'Olivier Giraud à Toulouse.

Robert Fleckinger, professeur émérite UPS depuis son départ à la retraite en décembre 2006, et qui a joué un rôle déterminant dans la création du GPT en 1991, ne devrait pas prolonger son éméritat au-delà de 2010.

Au 1er janvier 2010, l'enseignant-chercheur actif le plus âgé du LPT aura 50 ans, et l'agent CNRS le plus âgé (en incluant le personnel technique) aura 53 ans. Il est donc évident que le LPT ne devrait pas enregistrer de départ à la retraite avant longtemps. Les priorités de recrutement du LPT sont décrites dans la section suivante, à la suite des principaux objectifs scientifiques du laboratoire.

Organisation du LPT

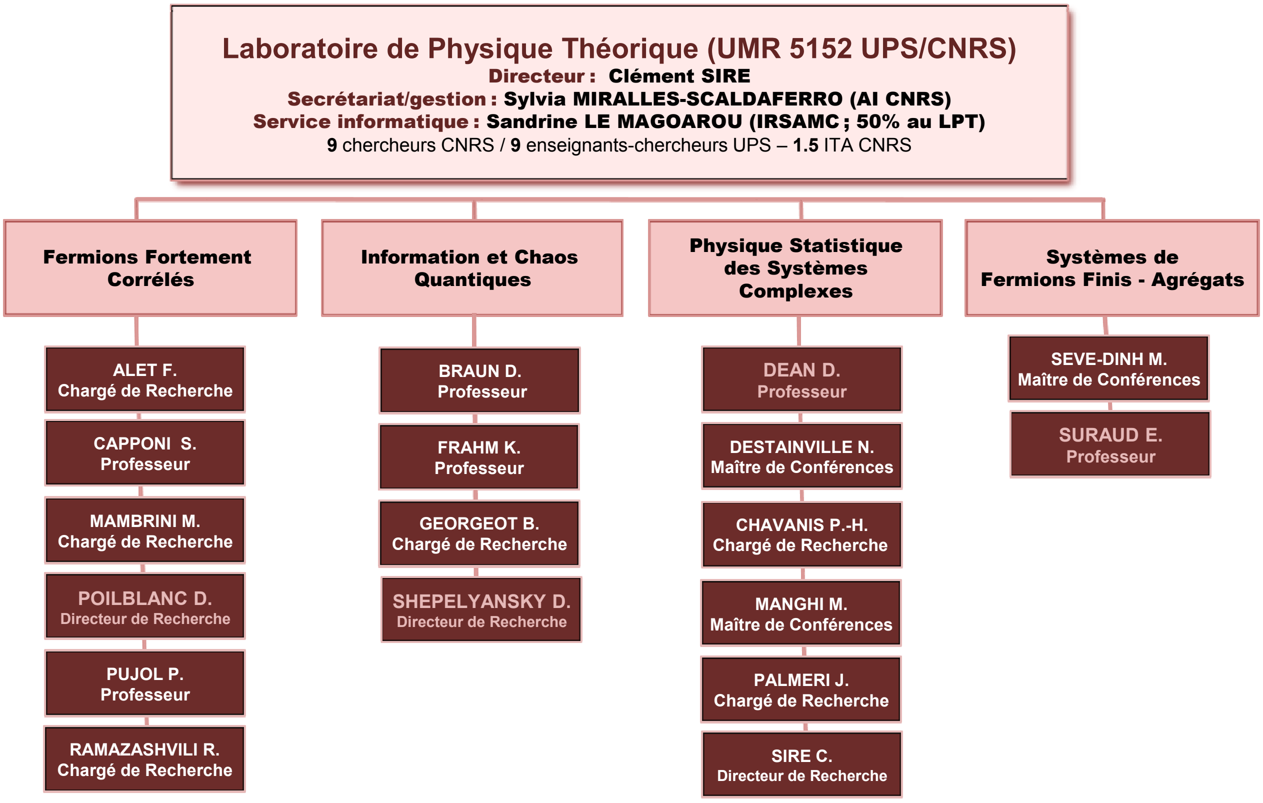


Tableau 1.1 : Organigramme du LPT attendu au 01/01/2011. Les noms des directeurs d'équipe sont indiqués en rouge.

- **Directeur du LPT :** C. Sire (représentant du LPT au *Bureau de l'IRSAMC*)
- **Gestion et administration :** S. Miralles-Scaldaferro
- **Formation permanente :** S. Miralles-Scaldaferro
- **Technicienne informatique, AE (CNRS) et CSSI (CNRS & UPS) :** S. Le Magoarou
- **Webmaster :** F. Alet
- **Communication :** S. Miralles-Scaldaferro et C. Sire
- **Séminaire LPT :** par période de 2 ans (P. Pujol en 2009-2010)
- **Hygiène et sécurité :** B. Georgeot

Clément Sire, l'actuel directeur du LPT, devrait poursuivre sa mission à la tête du laboratoire pendant la période 2011-2014, avec le soutien de l'ensemble du personnel permanent du LPT.

La ventilation des chercheurs CNRS et des enseignants-chercheurs UPS entre les quatre équipes du LPT, ainsi que leurs tâches respectives au sein du laboratoire, sont présentées dans l'organigramme de la Tab. 1.1 et en Tab. 1.2.

NOM & Prénom	Poste	Commentaires	CNRS
ALET Fabien	CR2 - 10/2005	—	06
CAPPONI Sylvain	PR2 - 10/2000	HDR ; PEDR ; ANR ; Promu 10/2008	06
CHAVANIS Pierre-Henri	CR1 - 10/1998	Promu 10/2001	02
BRAUN Daniel	PR2 - 10/2004	HDR ; PEDR ; CNRS	02
DEAN David	PR1 - 10/1998	HDR ; PEDR ; IUF 2007 ; CNRS ; Promu 10/2006	02/05
DESTAINVILLE Nicolas	MCF - 10/1998	HDR ; PEDR ; CNRS	02/05
FRAHM Klaus	PR2 - 10/1997	HDR ; CNRS ; Promu 02/2000	02
GEORGEOT Bertrand	CR1 - 10/1996	Promu 10/2000 ; HDR prévue en 2009-2010	02
MAMBRINI Matthieu	CR1 - 10/2002	Promu 10/2007	06
MANGHI Manoel	MCF - 01/2004	HDR prévue en 2009-2010 ; CNRS	05/02
PALMERI John	CR1 - 09/2006	HDR ; Promu 10/1998	05
POILBLANC Didier	DR1 - 07/1992	HDR ; Promu 10/2007	06
PUJOL Pierre	PR2 - 10/2006	HDR ; PEDR	06/02
RAMAZASHVILI Revaz	CR1 - 10/2009	—	06
SÈVE-DINH Mai	MCF - 10/2003	HDR prévue en 12/2009	05/04
SHEPELYANSKY Dima	DR1 - 10/1992	HDR ; Promu 10/2004	02
SIRE Clément	DR2 - 10/1991	HDR ; Promu 10/2005	02
SURAUD Éric	PREX - 10/1992	HDR ; PEDR ; IUF 1994 ; CNRS ; Promu 10/2007	04/05
SCALDAFERRO Sylvia	AI - 10/1991	Gestion et Administration du LPT	—
LE MAGOAROU Sandrine	AI - 10/2006	Tech. informatique (IRSAMC ; 50% at LPT)	—

Tableau 1.2 : *Personnel permanent du LPT attendu au 01/01/2011. La seconde colonne indique le poste actuel et la date de recrutement au LPT. La troisième colonne précise : HDR, PEDR, IUF, Délégation CNRS, décharge de service financée par l'ANR, et la date de la dernière promotion. La dernière colonne indique la ou les Section(s) CNRS d'affiliation.*

Finances

Comme illustré au Chapitre 2 du rapport scientifique du LPT, les ressources financières globales du laboratoire (~ 500 k€/an en 2007-2009) proviennent aujourd'hui essentiellement de contrats à court ou moyen terme avec l'ANR, l'Union Européenne, le CNRS, l'Université Paul Sabatier (UPS), et d'autres institutions. Par la même occasion, la part des crédits annuels CNRS et MESR/UPS s'est établie à moins de 15 % du budget total du LPT au cours de cette période (contre presque 100 %, il y a encore cinq ans). Cette situation traduit l'évolution du mode de financement de la recherche française, marqué par la création de l'ANR en 2005, et illustre aussi la capacité des chercheurs du LPT à obtenir des financements externes.

En tenant compte de l'augmentation attendue de la part des *programmes blancs* de l'ANR dans sa dotation totale, et de la reconnaissance de la qualité des recherches menées au laboratoire, le LPT est confiant que ses futurs projets scientifiques trouveront un financement approprié, notamment en ce qui concerne le recrutement de postdoctorants. Cependant, le LPT, comme la plupart des laboratoires français, s'inquiète de la baisse des crédits annuels, qui ont atteint un niveau qui met en danger le financement de moyens mutualisés (séminaires, missions, invitations de visiteurs, ordinateurs, dépenses courantes...). Cet état de fait nécessitera certainement une participation des porteurs de contrats, si la situation venait encore à se dégrader. Le LPT regrette ainsi que le CNRS (qui gère les contrats du LPT, notamment ceux impliquant l'ANR) ait récemment décidé de prélever la part de 4 % de ses contrats qui était censée couvrir les frais des laboratoires induits par leur bonne réalisation (un postdoctorant « coûte effectivement de l'argent » à un laboratoire).

Concernant les investissements futurs du laboratoire, le LPT s'attachera à maintenir l'excellent niveau de ses infrastructures informatiques (grappe de calcul, serveurs et terminaux), afin de placer ses chercheurs dans les meilleures conditions de travail possibles.

Hygiène et sécurité

Les membres du LPT n'étant pas particulièrement soumis à des risques découlant de leur activité professionnelle, le LPT continuera à appliquer les mesures présentées dans la section 1.6 de la partie bilan de ce rapport. Un nouveau membre du LPT devrait rapidement suivre une formation aux gestes de premiers secours.

Par ailleurs, le bâtiment principal de l'IRSAMC (hors LPCNO à l'INSA Toulouse) fait partie des priorités de rénovation du *plan Campus* de l'UPS (première tranche de travaux).

Le LPT et la Fédération IRSAMC

En janvier 2008, les quatre laboratoires de l'IRSAMC ont étudié l'éventualité de leur fusion complète ou partielle en une grande *Unité Mixte de Recherche (UMR)* [1]. Après de nombreux débats, les chercheurs du LPT ont dans leur très large majorité exprimé leurs réticences à une telle fusion, une position par ailleurs présentée à la direction de l'*Institut de Physique* du CNRS et au *Conseil Scientifique* de l'UPS, dans un document téléchargeable ici. Les arguments principaux à l'encontre d'une fusion concernant le LPT sont résumés ci-dessous :

❍ De nombreux thèmes scientifiques actuellement développés au LPT, un laboratoire pluridisciplinaire, risqueraient de devenir marginaux dans une UMR de plus de 100 chercheurs permanents et 25 techniciens, travaillant principalement en physique atomique, nanophysique et nanochimie, et en chimie théorique. On peut effectivement douter que ces thèmes resteraient des priorités de la politique scientifique d'une telle UMR. Certains membres du LPT ont ouvertement exprimé la possibilité de quitter l'institut en cas de fusion.

❍ De la même manière, les priorités de financement d'un laboratoire théorique (visiteurs pour un à trois mois, postdocs, moyens de calcul...) ne sont pas forcément de la même nature et du même coût que celles d'un laboratoire ayant une forte composante expérimentale.

❍ Le LPT constitue un exemple rare d'une implantation récente et réussie de physiciens théoriciens en province. La dynamique et la visibilité scientifique indéniable du LPT, acquise au fil du temps, pâtiraient certainement d'une fusion, qui serait d'ailleurs peu cohérente avec l'obtention en 2003 du statut d'UMR auprès du CNRS et de l'UPS. Ceci concerne à la fois la place du LPT dans la communauté, notamment française, de physique théorique, mais aussi la place de ses chercheurs dans les communautés scientifiques très diverses dans lesquelles ils travaillent.

❍ Le LPT collabore déjà avec six laboratoire toulousains, et espère que les échanges amorcés récemment avec le LCAR, l'IMT, le CEMES, le LCC, le LAAS, et des laboratoires d'écologie et de biologie, conduiront à de nouvelles collaborations concrètes. Les chercheurs du LPT sont intimement convaincus que ce sont des intérêts scientifiques communs, plutôt que des liens administratifs, qui constituent le ciment d'échanges et de collaborations scientifiques futurs.

❍ De part sa taille modeste, le management du LPT est efficace, transparent, réactif, et implique l'ensemble de son personnel permanent. Le fait que la fusion des quatre laboratoires engendrerait

1. En 2009, la Fédération IRSAMC comprend environ 100 chercheurs CNRS et enseignants-chercheurs UPS, 25 techniciens CNRS et UPS, et 55 thésards et postdoctorants.

un institut qui dépendrait de 7 Sections du CNRS, 4 Directeurs Scientifiques Adjoints, l'*Institut de Physique* et l'*Institut de Chimie* du CNRS, l'UPS, et l'INSA de Toulouse, compliquerait nettement son management et sa gestion.

❍ Le CNRS et l'UPS n'ont pas exprimé de réels arguments scientifiques afin de motiver une telle fusion.

❍ Le LPCNO, un laboratoire créé en 2007, est aussi très réticent à l'idée d'une fusion, pour des raisons souvent assez proches de celles du LPT.

Cependant, le LPT et les trois autres laboratoires de l'IRSAMC s'accordent sur le fait que l'IRSAMC est destiné à devenir l'interlocuteur privilégié de nos tutelles, et notamment de l'UPS, qui semble d'ailleurs se satisfaire de cette approche.

L'IRSAMC mutualise déjà de nombreux services communs : l'équipe de techniciens informatiques, les serveurs mail et Web et le réseau, la salle des grappes de calcul (en 2009-2010), la bibliothèque IRSAMC, les ateliers de mécanique et d'électronique, le séminaire général IRSAMC... De plus, les gestionnaires du LPT et du LCPQ assurent une permanence en cas d'absence de l'une d'entre elles. Enfin, l'IRSAMC gère en commun les bourses de thèse MESR allouées par l'*École doctorale Sciences de la Matière* (depuis 2007), et soumet une liste classée de ses priorités de recrutements MCF/PR à l'*UFR Physique-Chimie-Automatique* (liste classée établie pour la première fois en mai 2009).

La très bonne ambiance qui règne au sein de l'IRSAMC, et notamment entre ses cinq directeurs, illustrée par l'organisation annuelle des *Journées de l'IRSAMC* (dernière édition organisée du 2 au 4 juin 2009, à Najac) et de *La Fête de la Science*, facilite clairement cette mutualisation partielle de nos ressources et une politique scientifique commune en matière de postes UPS et de bourses doctorales MESR/UPS.

1.2 Objectifs scientifiques généraux et priorités de recrutement

Sans entrer dans le détail des projets scientifiques des quatre équipes du LPT, qui seront développés au Chapitre 3, nous présentons ci-dessous des objectifs scientifiques généraux et les priorités de recrutement du LPT.

Objectifs scientifiques généraux

Pluridisciplinarité et nouvelles collaborations

Comme abondamment illustré dans le bilan scientifique 2005-2009 du LPT, la **pluridisciplinarité** est l'un des principaux moteurs de l'activité scientifique du laboratoire. Les physiciens du LPT collaborent et partagent des contrats avec de nombreux laboratoires expérimentaux et théoriques, dans des domaines très variés : physique de la matière condensée et mésoscopique, physique de la matière molle, biophysique et biologie, physique atomique et des agrégats, astrophysique, mathématiques,... Le LPT fera évidemment son possible pour poursuivre cette politique scientifique pluridisciplinaire au cours des prochaines années. En particulier, le campus toulousain offre de nombreuses opportunités afin de développer activement cette politique :

❍ Les équipes FFC et Quantware ont entamé des échanges encourageants avec le nouveau groupe Atomes Froids du Laboratoire Collisions Agrégats Réactivité – LCAR, groupe dirigé par D. Guéry-Odelin (le dispositif expérimental est en cours de déménagement/montage, en provenance de l'ENS Paris). Leur intérêt commun réside dans la relation évidente entre réseaux de basse dimension d'atomes corrélés, et les modèles théoriques de la physique de la matière condensée, ainsi que l'intrication, la cohérence, et l'information quantiques.

❍ L'équipe FFC a récemment entamé une collaboration avec le groupe Fermions Fortement Corrélés du Laboratoire National des Champs Magnétiques Intenses – LNCMI (Toulouse) et interagit aussi avec la branche grenobloise du LNCMI. Le recrutement au LPT de R. Ramazashvili en octobre 2009, qui collabore déjà avec le LNCMI (Grenoble), devrait contribuer à solidifier les liens entre le LPT et le LNCMI.

❍ L'équipe Quantware étudie les possibilités d'implémentations expérimentales du fruit de ses travaux dans plusieurs domaines. En particulier, des contacts ont été initiés avec le Laboratoire de Chimie de Coordination – LCC et le Centre d'Élaboration de Matériaux et d'Études Structurales – CEMES, tous les deux à Toulouse. De plus, l'équipe Quantware partage un nouveau projet ANR-PNANO avec le LNCMI et le Laboratoire d'Analyse et d'Architecture des Systèmes – LAAS (Toulouse), sur le transport à l'échelle nanométrique.

❍ L'équipe PhyStat a développé depuis plusieurs années des collaborations avec des laboratoires de biologie à Toulouse et ailleurs et continuera dans cette voie. En particulier, il participe activement à un nouveau *réseau de biologie systémique* (créé en mai 2009) sur le campus toulousain, qui implique aussi l'Institut de Mathématiques de Toulouse – IMT et plusieurs laboratoires d'écologie ou de biologie (premier colloque organisé le 18 juin 2009), et qui a pour principale vocation d'encourager les collaborations dans ce domaine.

❍ Bien qu'il y ait déjà quelques collaborations entre physiciens du LPT (particulièrement dans l'équipe PhyStat) et mathématiciens de l'IMT, ces deux laboratoires ont récemment entamé une série d'opérations afin d'affirmer leurs liens. En plus d'échanges de séminaires en 2009 (ayant notamment conduit à un atelier commun « dimères »), le LPT et l'IMT ont organisé un mini-colloque d'une journée, le 12 juin 2009 (trois interventions de chaque laboratoire ; trois équipes du LPT représentées), afin de faciliter les interactions entre nos deux communautés, et idéalement, de motiver des collaborations futures.

Développer les interactions entre les quatre équipes du LPT

Malgré la vigueur et la diversité de l'activité scientifique des chercheurs du LPT, qui a conduit à de nombreuses collaborations locales, nationales et internationales, et bien que les physiciens du LPT collaborent largement entre eux (voir le Chapitre 9 du bilan scientifique du LPT ; chaque permanent du LPT a publié au moins un article avec l'un de ses collègues en 2007 et en 2008), on peut déplorer qu'il n'y ait eu qu'une poignée de publications inter-équipes lors de ces quatre dernières années. Bien sûr, ceci est une conséquence directe du large spectre de sujets étudiés et de méthodes analytiques et numériques utilisées au LPT, et reflète sans doute la cohérence des équipes telles qu'elles ont été formées, il y a une douzaine d'années. Notons que le séminaire hebdomadaire du LPT, qui suit le *lunch meeting* (un moyen efficace de s'assurer que tout le monde y participe !), permet à l'ensemble des personnels permanents et non permanents du LPT de rester informé des sujets scientifiques d'importance pour leurs collègues travaillant dans d'autres domaines. Cette *culture générale* est essentielle en physique théorique, où de nombreux mécanismes physiques et méthodes d'un domaine sont amenés tôt ou tard à s'appliquer dans d'autres communautés.

Ceci étant dit, le développement de projets scientifiques inter-équipes est très certainement une priorité scientifique du LPT. Trois axes thématiques sont actuellement explorés, et le LPT reste confiant que d'autres émergeront d'eux-mêmes dans un futur proche :

❍ ***Information quantique, intrication en matière condensée, atomes froids :*** les équipes FFC et Quantware ont déjà collaboré dans ce domaine, mais on peut attendre que cette collaboration se développe encore, notamment dans le domaine des atomes froids, avec notamment l'interaction prometteuse avec le nouveau groupe Atomes Froids du LCAR.

❍ ***Systèmes biologiques :*** l'équipe PhyStat, et plus récemment l'équipe Agrégats partagent des intérêts communs en biophysique, bien qu'à des échelles spatiales et temporelles très différentes (échelle *statistique vs* échelle *microscopique*). Il est cependant courant dans d'autres domaines (comme en physique de la matière condensée où l'équipe FFC applique ce genre d'approches) d'obtenir des modèles statistiques effectifs – et notamment leurs paramètres effectifs – à partir d'une étude microscopique.

❍ ***Hamiltoniens quantiques en physique classique hors d'équilibre :*** de nombreux systèmes hors d'équilibre, conduisant souvent à des transitions de phase dynamiques, sont associés à des hamiltoniens quantiques, généralement non hermitiens. L'expertise de l'équipe FFC en simulations numériques quantiques devrait répondre à l'intérêt de l'équipe PhyStat pour la physique hors d'équilibre.

Priorité de recrutement au CNRS et à l'UPS

En conformité avec l'évolution récente du personnel permanent du LPT, avec les objectifs généraux exposés ci-dessus, et avec les projets scientifiques des quatre équipes du LPT (voir le Chapitre 3), le laboratoire a identifié ses priorités de recrutement pour les prochaines années, qui sont présentées par ordre de priorité :

❍ L'équipe Quantware pourrait pâtir des départs programmés d'O. Giraud (CR2 CNRS) et de R. Fleckinger (PR Émérite UPS) en 2010. Étant donné le degré de reconnaissance et la qualité de l'activité de cette équipe, et le fait qu'elle inclut déjà 1 DR1 et 2 PR2, la première priorité du LPT est le recrutement d'un jeune chercheur au niveau CR2 CNRS ou MCF UPS au sein de l'équipe Quantware. Un profil scientifique possible pourrait être, soit similaire à celui d'O. Giraud (méthodes analytiques et aspects mathématiques de l'information quantique), soit concerner les interactions entre l'information quantique et la physique de la matière condensée, la physique mésoscopique, et la physique atomique.

❍ Un priorité du même ordre d'importance concerne le recrutement d'un jeune chercheur au niveau CR2 CNRS dans l'équipe Agrégats, en Section 05 du CNRS (ou plus hypothétiquement, en Section 04 ou 02). Malgré son intense activité scientifique, cette équipe reste sous-critique en taille et consiste en deux enseignants-chercheurs UPS, auxquels incombent de lourdes tâches et responsabilités d'enseignement. Idéalement, le LPT souhaiterait donc l'embauche d'un CR2 CNRS ayant des intérêts marqués en biophysique, de manière à motiver des collaborations entre les équipes Agrégats et PhyStat.

❍ Les équipes FFC et PhyStat ont certainement atteint une taille critique. Cependant, le LPT se doit d'encourager des candidatures au CNRS, préparées par ces deux équipes, de chercheurs talentueux au niveau CR2 ou CR1 (Sections 02 et 06). Concernant l'équipe PhyStat, des candidats de haut niveau ayant notamment des compétences en théorie statistique des champs appliquée aux systèmes désordonnés, hors d'équilibre, ou à longue portée intéresseraient certainement le LPT. Concernant l'équipe FFC, des candidats affichant des compétences dans des méthodes numériques non représentées au LPT (comme la DMFT), ou en phénoménologie et théorie quantique des champs seraient fortement appréciés. Alternativement, le LPT serait certainement intéressé par des candidats dont l'activité se situerait à l'interface entre ces deux équipes, afin de dynamiser leurs interactions.

Par ailleurs, le LPT est très attentif à la promotion de ses talentueux MCF à l'UPS [2] (deux MCF du LPT devraient passer leur HDR en 2009-2010). Pour la première fois depuis 2000, un MCF au LPT a été promu professeur au 2008. Malgré le fait assez regrettable qui veut que le système universitaire français n'ait pas de disposition officielle afin de promouvoir ses meilleurs MCF, le LPT veillera à une évolution satisfaisante de la carrière de ses MCF les plus méritants.

Finalement, avec deux techniciennes CNRS travaillant actuellement au LPT, qui remplissent parfaitement leurs tâches respectives, le LPT considère que ses besoins en matière de personnel technique sont satisfaits.

2. la promotion des CR1 CNRS vers le corps des DR2 reste de la seule responsabilité du *Comité National de la Recherche Scientifique* du CNRS.

1.3 Auto-analyse du LPT

Comme requis par l'AERES, le LPT évalue ci-dessous, le plus objectivement possible, ses forces, ses opportunités de développement, mais aussi ses faiblesses, et les risques de nature à contrarier la bonne réalisation de son projet. Cette « auto-analyse » est bien sûr principalement basée sur les éléments présentés dans le *Bilan scientifique* 2005-2009 du LPT, auquel nous faisons amplement référence, et auquel nous renvoyons aussi le lecteur.

❍ Spécificités du LPT à Toulouse :

- Grâce en particulier au soutien du CNRS et de l'UPS, le LPT constitue incontestablement l'une des rares implantations récentes et réussies de physiciens théoriciens en province. Il est bon de rappeler qu'en 1991, à l'arrivée des premiers membres du futur LPT et de l'IRSAMC, la physique fondamentale était un domaine clairement sous-représenté à Toulouse (le Groupe de Physique théorique était d'ailleurs alors hébergé par le LPQ, un laboratoire de chimie théorique). Nos chercheurs ont donc dû « faire leur trou », dans des conditions parfois difficiles au début, et la reconnaissance par le CNRS et l'UPS du LPT en tant qu'UMR en 2003 est le résultat d'un pari scientifique qui était très loin d'être gagné d'avance.
- Le LPT s'est parfaitement adapté au paysage scientifique du campus toulousain et a su ainsi développer des collaborations avec de nombreuses équipes locales, notamment expérimentales, dans des domaines scientifiques très variés, une situation que le présent projet du LPT devrait encore affirmer davantage. De plus, les membres du LPT assurent de nombreuses responsabilités à l'UPS (voir Chapitre 4.2) et participent donc très largement à la vie scientifique, à l'enseignement, et à l'administration de la recherche sur le site toulousain.
- Le LPT à Toulouse, est éloigné géographiquement des centres traditionnels de la physique théorique française, dominée par la concentration importante en Île-de-France, en région Rhône-Alpes, voire à Marseille et Montpellier (physique mathématique et des particules non représentées au LPT). Cet état de fait ne facilite pas les collaborations françaises, et prive le LPT de l'afflux de visiteurs étrangers de courte durée qui irrigue notamment la région parisienne. Le LPT se doit donc de poursuivre une politique agressive (et malheureusement aussi coûteuse) d'invitations (séminaires, visites courtes de collaborateurs, visiteurs pour 1 à 3 mois...) afin de combler les désavantages de son isolement géographique dans sa communauté. Il est cependant clair que le LPT a aussi su tirer de nombreux bénéfices de la présence d'une communauté scientifique toulousaine forte et diverse, et nous osons penser que l'inverse est aussi vrai.

❍ Production scientifique :

- Quantitativement et qualitativement, la production scientifique du LPT (300 publications et prépublications, plus de 200 interventions en conférences internationales, un logiciel commercial et deux batteries de codes *Open Source* développés...) le place clairement au niveau de ses meilleurs homologues français. L'introduction du Chapitre 9 du bilan scientifique présente quelques données qui devraient parfaitement illustrer ce point, et le fait que les quatre équipes du LPT interviennent et sont reconnues dans des communautés scientifiques très diverses.
- L'activité des chercheurs du LPT engendre de nombreux actes de diffusion de l'information scientifique, incluant l'organisation de 14 conférences ou écoles thématiques, et des opérations diverses de vulgarisation scientifique (voir les Chapitres 4.3 & 4.4).

❍ Collaborations scientifiques :

- L'introduction du Chapitre 9 et les rapports et projets scientifiques du LPT illustrent amplement l'effort réalisé ces dernières années afin de développer des collaborations locales, nationales, et internationales (plus de 200 collaborateurs dans 130 institutions), et cela dans des communautés scientifiques très diverses : physique de la matière condensée et mésoscopique, physique de la matière molle, biophysique et biologie, physique atomique et des agrégats, astrophysique, mathématiques,... En particulier, le LPT dispose aujourd'hui de tous les éléments pour intervenir de façon décisive dans des sujets aussi porteurs que les relations entre information quantique et physique de la matière condensée, ou la biophysique de l'ADN et de la cellule.

- Comme déjà mentionné plus haut, le LPT poursuit une politique agressive d'invitations de chercheurs pour des périodes courtes ou moyennes (1 à 3 mois), ces dernières permettant, spécialement dans notre communauté de physique théorique, de conduire à bien ou d'avancer un projet de manière décisive.
- On peut regretter qu'il n'y ait eu qu'une poignée de publications inter-équipes lors de ces quatre dernières années, malgré le nombre important de publications impliquant plusieurs membres du LPT au sein de chacune de ses équipes (voir le Chapitre 9). Le développement de projets scientifiques inter-équipes constitue une priorité scientifique du LPT, exprimée ouvertement en Section 1.2 du présent projet scientifique 2011-2014.

❍ **Pluridisciplinarité :**

- Comme devrait l'illustrer amplement les rapports scientifiques de ses quatre équipes, l'une des grandes originalités du LPT, et qui le distingue de nombreux laboratoires de physique théorique français, est sa véritable pluridisciplinarité, et sa collaboration et le partage de contrats avec des groupes expérimentaux et théoriques dans des domaines très variés. Cette pluridisciplinarité et la qualité scientifique du LPT constituent des attraits certains pour les jeunes postdocs et chercheurs sur le marché du travail.
- Cette pluridisciplinarité est donc l'une des grands forces du laboratoire, mais est aussi, paradoxalement, un facteur potentiellement fragilisant. En effet, le bon développement de chaque thème scientifique repose sur peu de chercheurs et serait fortement affecté par le départ de l'un d'eux pour raisons diverses (rapprochement familial, opportunité salariale à l'étranger,...). Par ailleurs, cette place particulière du LPT dans le paysage de la physique théorique française a pu, par le passé, nuire à la reconnaissance, en terme d'avancement de carrière, de certains de ses membres, notamment au CNRS (l'exemple de F. Mila est évoqué plus bas). Il incombe donc aux tutelles du LPT, le CNRS et l'UPS, de continuer à encourager notre approche pluridisciplinaire qui a conduit à des résultats scientifiques de tout premier plan, en reconnaissant la particularité et l'originalité de la politique scientifique du LPT.

❍ **Personnel permanent :**

- Le LPT est clairement un laboratoire « jeune » (voir le Chapitre 1.2) et international (6, et bientôt 7 permanents possédant un passeport étranger) dont tous les chercheurs et enseignants-chercheurs sont « publiants ». Il doit être noté que la proportion de 50 % d'enseignants-chercheurs au LPT est supérieure à celle observée en moyenne dans les laboratoires de physique théorique de la région parisienne. Au regard de la production scientifique du LPT, et des lourdes responsabilités d'enseignement qui leur incombent, cela ne fait qu'ajouter au mérite des enseignants-chercheurs du LPT, qui sont d'ailleurs récompensés par un taux important de PEDR (6 sur 9), de délégations au CNRS, et par l'IUF (un membre junior, un ex membre senior, un autre ex membre senior ayant depuis quitté le LPT ; voir aussi le Chapitre 1.2).
- Il a déjà été noté que les membres du LPT sont fortement impliqués dans l'administration locale de la recherche et de l'enseignement. Il en va de même au niveau national, où ils occupent des responsabilités importantes au CNRS et à l'ANR, et interviennent comme experts auprès de nombreuses institutions françaises et étrangères (voir la fin du Chapitre 4.2).
- Le LPT se doit de mentionner la grande qualité de son personnel technique (gestion/administration et informatique), qui place les chercheurs du LPT dans les meilleures conditions de travail possibles dans ce domaine.

- Le taux d'encadrement de la physique à l'UPS empêche actuellement nos chercheurs CNRS d'enseigner à l'UPS, si ce n'est à titre purement gratuit (5 sur 9 le font, jugeant de l'importance de rester au contact de l'enseignement et des étudiants). Cet état de fait est très regrettable, notamment dans le cadre des dispositions récentes visant à améliorer la carrière des chercheurs CNRS, en l'échange de 64 h d'enseignement à l'université. Inversement, les possibilités de décharges d'enseignements à l'UPS, pour nos enseignants-chercheurs les plus impliqués dans la recherche, sont presque inexistantes. Le LPT attend donc une politique plus volontariste de l'UPS sur ce point, afin d'éviter que certains de nos membres soient attirés par des universités menant une politique plus agressive de décharges d'enseignements et de cours alloués aux chercheurs CNRS.
- Le prochain départ à la retraite d'un enseignant-chercheur UPS au LPT ne devrait pas intervenir avant quinze ans. La politique des postes de l'UPS étant principalement menée sur la base de « postes vacants », il conviendra de veiller à ce que ce laboratoire, aujourd'hui uniformément « jeune », ne devienne pas uniformément « vieux ». Nous espérons donc que l'UPS continuera à soutenir le LPT sur la base de son excellence scientifique, comme elle l'a fait jusqu'ici.
- Même si le départ de certains membres d'un laboratoire fait partie de son évolution naturelle, le LPT a connu plusieurs départs dommageables au cours de son histoire, qui le pénalisent d'autant plus qu'il reste un laboratoire de taille modeste, et donc fragile : Frédéric Mila (au LPT de 1993 à 2000 ; titulaire de la *Chaire de Théorie de la Matière Condensée* à l'EPF Lausanne), Erik Sørensen (au LPT de 1996 à 2001 ; *full professor* à McMaster University, Canada), Satya Majumdar (au LPT de 1999 à 2004 ; DR2 LPTMS Orsay), et Olivier Giraud (au LPT de 2005 à 2010 ; CR2 au LPTMS Orsay). Ces départs sont soit liés à l'obtention d'un poste extrêmement attractif financièrement/scientifiquement (F. Mila, E. Sørensen), soit aux difficultés rencontrées par le partenaire du chercheur à trouver un travail satisfaisant à Toulouse (S. Majumdar, O. Giraud), soit à un avancement de carrière peu en rapport avec l'excellence internationalement reconnue du chercheur concerné (F. Mila). À noter que F. Mila (*Chaire Pierre de Fermat* à l'UPS en 2008) et S. Majumdar continuent à publier régulièrement avec les chercheurs du LPT, et que nous sommes confiants qu'O. Giraud poursuivra sa collaboration fructueuse avec l'équipe Quantware.
- Pour nuancer ce dernier point, indiquons que LPT peut ouvertement se féliciter d'avoir su attirer en France de brillants chercheurs étrangers, en poste au laboratoire, ou ailleurs (S. Majumdar, au LPT de 1999 à 2004 ; *prix Langevin* de la SFP en 2005 ; un chercheur extrêmement prolifique, maintenant au LPTMS Orsay).

○ Personnel non permanent :

- Grâce à la capacité de ses chercheurs à trouver des financements externes, un signe implicite de la qualité de leur activité scientifique, le LPT héberge de nombreux postdoctorants (10 en 2007-2009 ; voir le Chapitre 4.1), un objectif déclaré de son précédent projet scientifique, et un fait qui confirme l'attractivité du laboratoire auprès des jeunes chercheurs étrangers. Le LPT se félicite que la qualité de la formation qu'il dispense à ses étudiants en thèse et postdoctorants contribue à leur excellente insertion dans le marché du travail, en France et à l'étranger, dans les meilleurs laboratoires de nos communautés scientifiques, ou dans le secteur privé (voir le Chapitre 4.1).
- Comme de nombreux laboratoires de « sciences dures », en France et dans la plupart des pays occidentaux, le LPT s'inquiète de la difficulté croissante à trouver des étudiants désirant réaliser une thèse de doctorat en recherche fondamentale. En particulier, la filière du M2 Recherche *Physique de la Matière* de l'UPS est de plus en plus fragilisée par la baisse du nombre d'étudiants. Le LPT anticipe donc le fait qu'il devra attirer une grande majorité d'étudiants extérieurs à Toulouse pour continuer à former des thésards : les 3 étudiants commençant leur thèse au LPT, en septembre 2009, viennent de l'École Polytechnique (Palaiseau), de l'université du Maine, et de l'Indian Institute of Technology in Madras (Inde), confirmant l'attractivité scientifique du LPT. La concentration de laboratoires de physique théorique offerte aux étudiants de la région parisienne,

et parfois leur frilosité à venir travailler en province, nous obligent à redoubler d'efforts dans ce domaine : à la rentrée 2009-2010, l'IRSAMC éditera une plaquette de ses sujets de thèses, qui présentera aussi ses quatre laboratoires, et qui sera très largement distribuée à travers la France et auprès de nos principaux collaborateurs à l'étranger.

❍ **Ressources financières :**

- Les chercheurs du LPT se sont parfaitement adaptés à l'évolution du mode de financement de la recherche française. Le grand nombre de contrats (notamment 7 ANR et 2 contrats européens actifs en 2007-2009 ; voir Chapitre 2) témoignent implicitement de la reconnaissance et de la qualité des recherches menées au LPT.
- La situation géographique du LPT implique des dépenses importantes en missions pour ses propres chercheurs, mais aussi pour ses invités de courte durée ou moyenne (voir Tab. 2.1 & 2.2 du Chapitre 2). La baisse continuelle des crédits annuels du CNRS (23 k€ en 2009) est un frein à cette politique d'invitations, même si les contrats peuvent en partie prendre le relais dans ce domaine. Cependant, la faiblesse des crédits annuels limite les dépenses concernant des postes mutualisés au sein du laboratoire.

❍ **Management du LPT :**

- Le LPT a atteint une taille critique qui reste toutefois très raisonnable. Ceci rend son management efficace, réactif et transparent, et assure aussi une bonne communication entre ses membres, qui, même quand ils ne collaborent pas ensemble, sont parfaitement conscients des problématiques majeures étudiées par leurs collègues. La publication régulière sur notre site Web de brèves scientifiques permet d'ailleurs de contribuer à diffuser l'information scientifique en interne et en externe. Ce mode de fonctionnement, avec notamment le court *lunch meeting* précédant le séminaire hebdomadaire, est très apprécié par les membres du LPT.
- Le LPT et l'IRSAMC ne peuvent que se réjouir de la très bonne ambiance qui règne au sein de l'institut, qui se traduit par l'organisation d'opérations communes (*Journées de l'IRSAMC*, *La Fête de la Science*), et permet la gestion mutualisée de nombreux moyens, dont les postes UPS, et les bourses doctorales MESR/UPS (voir le Chapitre 1.4).

2

LPT project 2011-2014 (version en anglais)

In this chapter, we describe the general project of the LABORATOIRE DE PHYSIQUE THÉORIQUE **without entering into the details of the scientific projects of the four LPT groups, which are presented in Chapter 3. We hence focus on the expected evolution of the LPT with regards to its permanent staff and organization, and in particular its relationship with the Fédération IRSAMC, and the development of novel general scientific axes. As required by the AERES, this chapter ends with a self-analysis of the LPT.**

2.1 Organization and evolution of the LPT

The four LPT groups

During the next *contrat quadriennal* 2011-2014, the LPT will remain structured into its current four groups:

- FFC: Fermions Fortement Corrélés; *Strongly Correlated Fermions* (Head: Didier POILBLANC)
- QUANTWARE: Information et Chaos Quantiques; *Quantum Information and Chaos* (Head: Dima SHEPELYANSKY)
- PHYSTAT: Physique Statistique des Systèmes Complexes; *Statistical Physics of Complex Systems* (Head: David DEAN)
- AGRÉGATS: Systèmes de Fermions Finis – Agrégats; *Finite Fermionic Systems – Clusters* (Head: Éric SURAUD)

Evolution of LPT permanent staff

Revaz RAMAZASHVILI was selected by the CNRS Section 06 (condensed matter physics) in the CR1 competition, and will start working at the LPT in October 2009.

The LPT should obtain a professor position at UPS, starting October 2010 (hiring committee expected around May 2010). The quite general job profile concerns scientific themes at the frontier between the activities of the four LPT groups.

For personal reasons, Olivier GIRAUD is expected to join LABORATOIRE DE PHYSIQUE THÉORIQUE ET MODÈLES STATISTIQUES (UMR 8626; Orsay) in mid 2010. The LPT wishes him good luck in his new laboratory, and is confident that his collaborations with LPT scientists will not be too affected by his departure. The QUANTWARE has obtained a CNRS grant *PEPS-Physique Théorique et ses Interactions* in June 2009, in particular to help finance O. GIRAUD's future visits to the LPT.

Robert Fleckinger, Emeritus professor since his retirement in 12/2006 – a founding member of the GPT in 1991 – is not expected to extend his *éméritat* after 2010.

Considering that the oldest active member of the LPT (including the administrative staff) is 53 for the CNRS and 50 for the UPS (as of 01/01/2010), the LPT does not expect any retirement among its permanent staff during the next *contrat quadriennal*. The recruitment priorities of the LPT are presented in the next section along with its main general scientific objectives.

Organization of the LPT

The expected affiliation of CNRS researchers and UPS enseignants-chercheurs to the four LPT groups is described in the organization diagram of Tab. 2.1 and in Tab. 2.2. The different administrative tasks assumed by LPT members are also listed below.

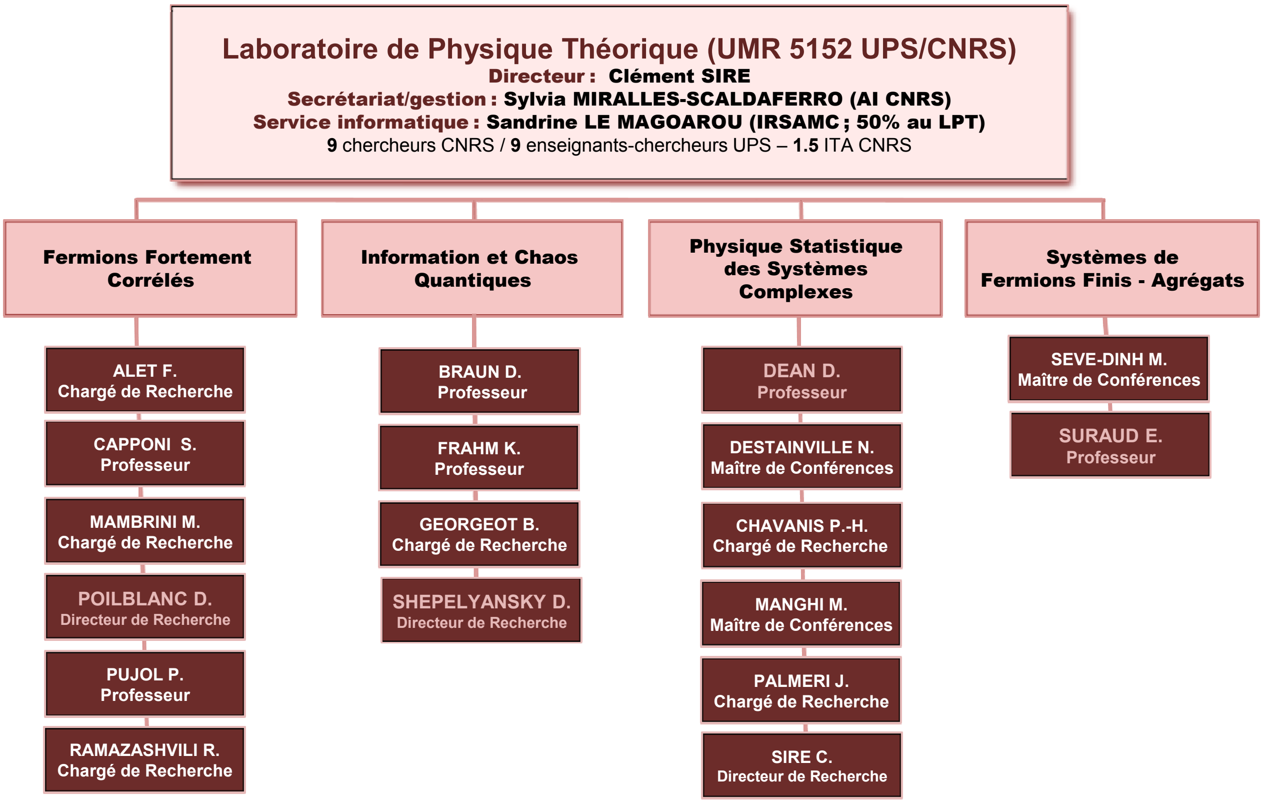


Table 2.1 : Expected organization diagram of the LPT as on 01/01/2011. Group leader names are in light red.

- ❍ **Head of LPT:** C. Sire (LPT representative at *Bureau de l'IRSAMC*)
- ❍ **Secretary and administration:** S. Miralles-Scaldaferro
- ❍ **Training program:** S. Miralles-Scaldaferro
- ❍ **Computer technician, AE (CNRS), and CSSI (CNRS & UPS):** S. Le Magoarou
- ❍ **Webmaster:** F. Alet
- ❍ **Communication:** S. Miralles-Scaldaferro and C. Sire
- ❍ **LPT seminar:** 2 years turnover (P. Pujol in 2009-2010)
- ❍ **Hygiene and security:** B. Georgeot

NAME & First name	Position	Comments	CNRS
ALET Fabien	CR2 - 10/2005	—	06
CAPPONI Sylvain	PR2 - 10/2000	HDR; PEDR; ANR; Promoted 10/2008	06
CHAVANIS Pierre-Henri	CR1 - 10/1998	Promoted 10/2001	02
BRAUN Daniel	PR2 - 10/2004	HDR; PEDR; CNRS	02
DEAN David	PR1 - 10/1998	HDR; PEDR; IUF 2007; CNRS; Promoted 10/2006	02/05
DESTAINVILLE Nicolas	MCF - 10/1998	HDR; PEDR; CNRS	02/05
FRAHM Klaus	PR2 - 10/1997	HDR; CNRS; Promoted 02/2000	02
GEORGEOT Bertrand	CR1 - 10/1996	Promoted 10/2000; HDR expected in 2009-2010	02
MAMBRINI Matthieu	CR1 - 10/2002	Promoted 10/2007	06
MANGHI Manoel	MCF - 01/2004	HDR expected in 2009-2010; CNRS	05/02
PALMERI John	CR1 - 09/2006	HDR; Promoted 10/1998	05
POILBLANC Didier	DR1 - 07/1992	HDR; Promoted 10/2007	06
PUJOL Pierre	PR2 - 10/2006	HDR; PEDR	06/02
RAMAZASHVILI Revaz	CR1 - 10/2009	—	06
SÈVE-DINH Mai	MCF - 10/2003	HDR expected in 12/2009	05/04
SHEPELYANSKY Dima	DR1 - 10/1992	HDR; Promoted 10/2004	02
SIRE Clément	DR2 - 10/1991	HDR; Promoted 10/2005	02
SURAUD Éric	PREX - 10/1992	HDR; PEDR; IUF 1994; CNRS; Promoted 10/2007	04/05
SCALDAFERRO Sylvia	AI - 10/1991	Secretary and Administration of LPT	—
LE MAGOAROU Sandrine	AI - 10/2006	Computer technician (IRSAMC ; 50% at LPT)	—

Table 2.2 : *Expected permanent staff of the LPT as on January 2011. The second column indicates the position currently held and the hiring date at the LPT. The third column provides additional information: HDR, PEDR, IUF, Délégation CNRS, ANR teaching dispensation, and date of promotion to the current position. The last column shows the CNRS Section(s) of affiliation.*

With the full support of the LPT permanent staff, Clément Sire, the current director of the LPT, should retain the direction of the LPT during the period 2011-2014.

Finances

As illustrated in Chapter 2 of the LPT scientific report, the overall financial resources of the laboratory (∼ 500 k€/year in 2007-2009) now come essentially from short or medium term contracts with the ANR, the EU, the CNRS, the Université Paul Sabatier (UPS), and other institutions. In this time, the proportion of funding coming from the CNRS and MESR/UPS has fallen to below 15 % of the LPT's total budget (from almost 100 %, just five years ago). This situation reflects the evolution of the funding of the French research system, notably by the creation of the ANR in 2005, but also illustrates the high success rate of LPT scientists in obtaining external financial resources.

Given the expected increase of the share of the *programmes blancs* of the ANR (programs open to any scientific theme), and the recognition of the high quality of the four LPT groups' scientific activity, the LPT is confident that its future scientific projects will find adequate funding, in particular with regards to the hiring of postdocs. However, the LPT considers that the continuous decrease in its annual funding from CNRS and MESR/UPS (as experienced by all laboratories in France) has reached a critical threshold and that it will become more and more difficult to finance mutualized services (seminars, missions, general expenses, computers...) without demanding a financial contribution from contract holders. It is also regrettable that the CNRS (which manages the LPT's non-MESR/UPS resources, including ANR grants) has recently decided to keep the 4 %

overhead fraction of all ANR contracts, which was initially supposed to cover the expenses incurred by the laboratory in relation to these contracts (for example the real costs associated with hosting a postdoc).

As for future investments, the LPT will keep on investing in its computer infrastructure (cluster, servers, and terminals) via its own resources and contracts, in order to maintain the excellent conditions currently offered by the LPT in this domain.

Hygiene and security

The members of LPT are not particularly exposed to risks related to their professional activity, and the LPT will continue to apply the prescriptions presented in the Section 1.6 of the scientific report. In particular, a new LPT member will participate in the next UPS first aid training.

Finally, one should mention that the main IRSAMC building (excluding the LPCNO at INSA Toulouse) should belong to the first wave of the renovation program of the UPS *plan Campus*.

The LPT and the Fédération IRSAMC

Despite some discussions within the institute, initiated by the four laboratories in January 2008, there is no current plan to regroup the four laboratories of the IRSAMC into one big *Unité Mixte de Recherche (UMR)*[1]. The main arguments of the LPT against a merger of the four laboratories have been exposed in a document approved by the entire LPT permanent staff (which can be downloaded here; in French) and was also addressed to the *Institut de Physique* of CNRS and to the *Conseil Scientifique* de l'UPS. These arguments are summarized below:

❍ Many scientific themes currently developed at the LPT, a multidisciplinary laboratory, would be marginal in a big UMR of more than 100 permanent researchers and 25 technicians mainly working in atomic physics, nanophysics and chemistry, and theoretical chemistry. It is difficult to imagine that such LPT themes would remain priorities of the scientific policy of a much bigger institute. Some LPT scientists have openly expressed their intention to leave the institute in the case of such a merger.

❍ Furthermore, the funding priorities of a theoretical laboratory (short term and 1-3 month visitors, postdocs, computers...) are clearly not of the same nature and cost of those of a mainly experimental institute.

❍ The scientific visibility of the LPT, a rare example of a recent and successful establishment of theoretical physicists in the French "province", would be clearly affected by a merger, and would be inconsistent with the decision to recognize the LPT as an *Unité Mixte de Recherche* by CNRS and UPS, in 2003. This issue not only concerns the position of the LPT in the general theoretical physics community, but also the position of our researchers in the very diverse communities in which they work.

❍ The LPT already collaborates with six laboratories in Toulouse, and hopes that current discussions with the Cold Atoms group of the LCAR, mathematicians at the IMT, biologists in various laboratories, and other laboratories (CEMES, LAAS, LCC) will lead to even more local collaborations. LPT scientists are convinced that common scientific interests rather than administrative links are the best cement for fruitful exchanges and collaborations.

❍ Thanks to the moderate size of the laboratory, its current management is efficient, transparent, reactive, and involves all the permanent staff. The fact that a merged institute would depend on at least 7 CNRS Sections, 4 Directeurs Scientifiques Adjoints, the *Institut de Physique* and the *Institut de Chimie* of the CNRS, the UPS, and the INSA Toulouse, would certainly greatly complicate its management.

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

❍ The CNRS and UPS have not expressed any real scientific argument to motivate such a merger.

❍ The LPCNO, a laboratory created in 2007, is also reluctant to merge, for reasons quite similar to those of the LPT.

However, the LPT and the three other laboratories of the IRSAMC acknowledge that the IRSAMC is clearly destined to become the preferred contact organization of the UPS for matters common to our four laboratories, a situation which seems to satisfy the UPS.

The IRSAMC already mutualizes several services: the pool of computer technicians, computer network, mail and web servers, a computer room (projected for 2009-2010), the IRSAMC library, the IRSAMC joint seminar... Moreover, the secretaries of the LPT and the LCPQ are able to share administrative duties of the two laboratories, so that in the absence of one, the other can assume her colleague's responsibilities. In addition, from 2007 on, the IRSAMC has managed internally its PhD fellowships obtained from the MESR/UPS, through the *École doctorale Sciences de la Matière*, and submits a classed list, according to its scientific priorities, of its demands for MCF/PR positions to the *UFR Physique-Chimie-Automatique* (the first such IRSAMC classed list was sent to the UPS in May 2009).

The positive and friendly atmosphere within the IRSAMC (and in particular between the five directors), illustrated by the yearly organization of *Les Journées de l'IRSAMC* (last session organized at Najac; 2-4 June 2009) and *La Fête de la Science*, certainly facilitates this pooling of resources.

2.2 General scientific objectives and recruitment priorities

Without entering into the details of the specific scientific projects of the four LPT groups, which are presented in Chapter 3, we list below some general scientific objectives and the recruitment priorities of the LPT.

General scientific objectives

Multidisciplinarity and new collaborations

As illustrated in the 2005-2009 scientific report, **Multidisciplinarity** is a vital and inspiring motor of the scientific activity of the LPT. LPT researchers already collaborate and share contracts with experimentalists and theorists working in many fields: condensed matter and mesoscopic physics, soft-condensed matter physics, biophysics and biology, cluster and atomic physics, astrophysics, mathematics... It is clear that the LPT will do its best to pursue its multidisciplinary scientific policy in the future. In particular, the Toulouse campus offers many opportunities to initiate new collaborations, and the LPT certainly expects to see developments in this direction over the next few years:

❍ The FFC and Quantware groups have started promising discussions with the new Cold atoms group of the Laboratoire Collisions Agrégats Réactivité – LCAR, headed by D. Guéry-Odelin (the main experimental set-up is to be moved/remounted from ENS Paris in 2009). Their common interest lies in the obvious connection to low-dimensional lattices of (correlated) atoms, mimicking models of condensed matter physics, and to the entanglement/coherence/quantum information aspects of cold atomic systems.

❍ The FFC group has started a collaboration with the Strongly Correlated Fermions group at the Laboratoire National des Champs Magnétiques Intenses – LNCMI (Toulouse) and also interacts with the Grenoble branch of the LNCMI. The recruitment at the LPT of R. Ramazashvili in October 2009, who already works with the LNCMI (Grenoble), is expected to further strengthen the link between the LPT and the LNCMI.

❍ The Quantware group is investigating experimental implementations of their quantum information work. In particular, contacts will be pursued with experimentalists at the Laboratoire de Chimie de Coordination – LCC and the Centre d'Élaboration de Matériaux et d'Études Structurales – CEMES, both in Toulouse. In addition, the Quantware group shares a new ANR-PNANO project with the LNCMI and the Laboratoire d'Analyse et d'Architecture des Systèmes – LAAS (Toulouse), on transport at the nanoscale.

❍ The PhyStat group has already strong collaborations with biology laboratories in Toulouse and elsewhere and certainly expects to develop more of them. In particular, it actively participates in a new *systemic biology network* on the Toulouse campus (created in May 2009), also involving the Institut de Mathématiques de Toulouse – IMT and several ecology and biology laboratories (first workshop organized on 18 June 2009), which is meant to lead to new interdisciplinary collaborations in this field.

❍ Although there have already been occasional collaborations between some LPT physicists, notably in the PhyStat group, and mathematicians from the IMT, both laboratories have very recently initiated a series of operations in order to strengthen their interactions. In addition to shared seminars in 2009 (leading to a new collaboration concretized by a working group on dimers involving the FFC group), the LPT and the IMT have organized a one-day mini-colloquium on June 12th 2009 (three talks from each laboratory; involving three LPT groups) in order to facilitate exchanges between both our communities and, hopefully, initiate further collaborations. The LPT will certainly work toward a stronger interaction between LPT physicists and IMT mathematicians in the near future.

Developing the interactions between the four LPT groups

Despite their intense and diverse scientific activity resulting in many local, national, and international collaborations, and although researchers at the LPT do strongly interact together (see Chapter 9 of LPT scientific project; each LPT researcher published at least one paper with a LPT colleague in 2007 and 2008), there have only been a handful of inter-group publications during the last four years. Obviously, this is essentially a consequence of the wide range of domains of study and of analytical and numerical methods used at the LPT, and it certainly reflects the coherence of the current composition of the LPT groups. Note that the LPT seminar, which follows the *lunch meeting* (an efficient way of making sure that everybody attends the seminar!), ensures that all LPT permanent and non-permanent staff keep abreast of problems of interest to their colleagues in other fields. This “common culture” is essential in theoretical physics, where physical mechanisms or methods from one domain sooner or later prove useful in other fields.

Hence, it is a clear scientific priority for the LPT to develop common projects between our four groups. Three directions are currently being explored and we are confident that others will soon emerge:

❍ ***Quantum information, entanglement in condensed matter, cold atoms:*** the FFC and Quantware groups have already collaborated in this domain, and one can expect this collaboration to develop further, especially in the field of cold atoms, studied experimentally by the corresponding group at the LCAR.

❍ ***Biophysical systems:*** the PhyStat group, and more recently the Agrégats group have common interests in biological systems, albeit at a different scale (“statistical” scale *vs* microscopic scale). However, a common approach is often to obtain effective statistical models, and more specifically, their effective parameters starting from a more microscopic treatment (an approach also quite common in condensed matter physics and already used in the FFC group).

❍ ***Quantum Hamiltonians in classical out of equilibrium physics:*** many out of equilibrium systems (often exhibiting dynamical phase transitions) can be associated with a generally non-Hermitian quantum operator. The strong expertise of the FFC group in advanced quantum numerical methods should be of interest to the PhyStat group in the context of out of equilibrium statistical physics.

Recruitment priorities at the CNRS and the UPS

In accordance with the recent evolution of the LPT permanent staff, with LPT's general scientific objectives presented above, and with the scientific projects of the four LPT groups developed in Chapter 3, the laboratory has identified its main recruitment objectives for the next few years, which are listed below in order of priority:

❍ The Quantware group will certainly suffer from the expected departure of O. Giraud (CR2 CNRS) and R. Fleckinger (PR Émérite UPS) in 2010. Considering the high level of recognition of this group, and the fact that it already includes three senior scientists, the highest priority of LPT is the hiring of a young researcher at the CR2 CNRS or MCF UPS level in the Quantware group. His/her possible profile could be either similar to that of O. Giraud (analytical methods and mathematical aspects of quantum information), or could concern the interactions between quantum information and condensed matter/mesoscopic/atomic physics.

❍ An equally major priority concerns the hiring of a young researcher at the CR2 CNRS level in the Agrégats group in Section 05 of the CNRS (or less likely, in Section 04 or 02). Despite its intense scientific activity, this group is still subcritical in size and consists of two enseignants-chercheurs with heavy teaching duties. Ideally, the LPT wishes to hire a young CR2 CNRS scientist with interest in biophysical systems, in order to foster interactions between the Agrégats and PhyStat groups.

❍ The FFC and PhyStat groups have certainly reached a critical size. However, the LPT will certainly encourage the application to the CNRS of talented French and foreign scientists at the CR2/CR1 level (Sections 02 and 06). Concerning the PhyStat group, talented candidates with skills in statistical field theory in the field of disordered/long range systems would be welcomed. Concerning the FFC group, candidates with skills in advanced numerical methods not represented at LPT (for instance DMFT), or with interest in phenomenology or quantum field theory would certainly be of great interest. Alternatively, any candidate developing an activity at the interface between these two groups would be valuable in order to foster collaborations between the two groups.

In addition, the LPT is very concerned with the career evolution of its talented MCF UPS researchers [2] (two MCF at LPT are expected to defend their HDR thesis in 2009-2010). For the first time since 2000, a MCF at the LPT was appointed Professor in 2008. Despite the regrettable fact that the French university system has no official means to guarantee the promotion of talented MCF (other than via hiring competitions open to internal *and* external candidates), the LPT will do its best to assure the career advancement of the best of our MCF.

Finally, hosting two CNRS technicians who perfectly fulfill their tasks, the LPT does not feel the need for any recruitment in this domain.

2.3 Self-analysis of the LPT

In this section, and as requested by the AERES, the LPT evaluates as objectively as possible its strengths, its opportunities for development, but also its weaknesses and the external issues which could hamper the LPT project. This "self-analysis" is of course mostly based on the LPT's *Scientific Report* 2005-2009, to which we shall constantly refer.

❍ The LPT in the context of the Toulouse campus

- Thanks in particular to the support given by the CNRS and UPS, the LPT is a clear example of a rare recent and successful operation to create a theoretical physics laboratory in *province*. When the first members of the then GPT (Groupe de Physique Théorique) and IRSAMC arrived in Toulouse, fundamental physics was clearly under-represented locally (indeed the GPT was first set up in the LPQ, a theoretical chemistry laboratory). At its inception, the GPT group

2. The promotion of CR1 CNRS researchers to DR2 is the sole responsibility of the *Comité National de la Recherche Scientifique* of the CNRS.

had to establish its scientific identity and reputation under conditions which were sometimes difficult. The recognition, in 2003, by the CNRS and UPS of the group as an *Unité Mixte de Recherche* (independent laboratory) is a testament to the success of a scientific project which, at the beginning, was far from a sure bet.

- The LPT has extremely well established itself within the scientific structure of the Toulouse campus and has initiated collaborations with a wide variety of local laboratories and teams, notably experimental ones, and in a wide variety of subjects. A large component of our present proposal is based on tightening and extending scientific collaborations at the local level. Members of the LPT have taken on local administrative responsibilities in the UPS (see Chapter 4.2) and the LPT is thus very active in the scientific, teaching and administrative life of the Toulouse campus.
- Most theoretical physics laboratories in France are concentrated in the Paris and Lyon area along with sizable laboratories in Marseille and Montpellier, which are centers of mathematical and particles physics (subjects which are not really present at the LPT). The LPT is very active in inviting people for seminars, short and medium term visits (of 1-3 months) in order to compensate for our relative geographic isolation, although these external invitations consume a substantial proportion of our budget (see Chapter 2.1). Fortunately, we have been able to benefit from the presence of the strong and varied scientific community of Toulouse, and we are confident in turn that the LPT is similarly appreciated by our local colleagues.

❍ Scientific research and production

- In terms of quantity and quality, the scientific production of the LPT (300 publications and preprints along with more than 200 conference presentations and the development of one commercial and two *Open Source* softwares) is clearly at a level comparable to the best of French theoretical physics laboratories. Chapter 9 of the scientific report highlights a few statistics which justify this assertion and also shows the extent to which the four groups comprising the LPT are recognized in their respective, and very diverse, scientific communities.
- The LPT has been highly involved in scientific communication, notably the organization of 14 conferences or specialized schools along with activities of scientific popularization for the general public (see Chapters 4.3 & 4.4).

❍ Scientific collaborations

- The introduction to Chapter 9 and the scientific project of the LPT shows the full extent of our efforts over the last few years to develop collaborations at the local, national, and international level covering a wide range of themes: hard and soft condensed matter, mesoscopic physics, biophysics and biology, atomic and cluster physics, astrophysics, mathematics... In particular, the LPT is now in a position to make important contributions in a number of emerging and extremely promising areas, such as the interplay between condensed matter physics and quantum information and the biophysics of DNA and the cell.
- As mentioned above, the LPT has an active policy of inviting researchers for short, medium (1 to 3 months) and long term (postdocs) visits. In theoretical physics such visits are vital to making progress and completing ongoing collaborations.
- Despite the large number of joint publications between members of the same group, it is regrettable that there have only been a handful of publications as a result of collaborations between different groups (see Chapter 9). The development of projects between groups will be a priority, as stated in Section 1.2 of this scientific project for 2011-2014.

❍ Interdisciplinary research

- As clearly demonstrated in the scientific reports of the four LPT groups, one of the distinguishing characteristics of the LPT, which sets it apart from most other French theoretical physics laboratories, is its degree of interdisciplinary research and collaboration and joint research contracts with experimental groups in a wide variety of areas. The interdisciplinary nature and quality of research carried out at the LPT makes it an attractive option for postdocs and young researchers.
- The interdisciplinary nature of the LPT's research is a force but also, in some respects, a potential weakness of the laboratory. The fact that the LPT has developed a wide range of scientific activities while being of modest size means that the groups are, with respect to many leading groups in the same disciplines elsewhere in France, relatively small. The research capacity and global visibility of a group can thus be strongly affected by the departure of even a single researcher (for family reasons, or for more attractive salaries and working conditions abroad). The relatively small size of our groups means that there is also a risk that some of our CNRS researchers could – and have in the past, in one notable example – suffer from a lack of recognition in terms of career advancement. We hope that the CNRS and UPS will continue to encourage our policy of maintaining a diverse research base and that, in the future, the laboratory will be able to maintain and achieve groups with the critical size necessary for optimal scientific visibility.

❍ Permanent staff

- The LPT is clearly a laboratory which is young (see Chapter 1.2) and international (6, and soon 7, LPT members hold a foreign passport). All of its CNRS and UPS staff are scientifically active (as defined by the publication criteria applied by the AERES). It should be noted that more than half of the laboratory members are university academics, a proportion which is significantly higher than in most theoretical physics laboratories in the Paris area. The level of scientific production of the university academics is especially impressive when one takes into account both their heavy teaching loads and the teaching and administrative responsibilities held by them. The quality of the UPS academics is attested to by the fact that 6 out of 9 benefit from the PEDR, and their success in obtaining delegations to the CNRS and becoming IUF fellows (a current junior member, an ex-senior member, and an ex-senior member who has since left the laboratory; see also Chapter 1.2).
- As well as being actively involved in teaching and scientific administration at the UPS, LPT members are also very active at the national level. They have held responsibilities in the CNRS and ANR and are experts for a variety of scientific institutions both in France and abroad (see the end of Chapter 4.2).
- The LPT must mention the high quality of its technical staff – secretarial/administrative and computer system technicians – which means that the LPT researchers have excellent working conditions in these areas.
- The low (according to UPS) student to university staff ratio in physics means that physics academics have difficulty obtaining their full teaching load (192 h/year) and that our CNRS researchers have difficulty teaching at the UPS, even if it is done for free (5 out 9 do teach in these conditions, given the importance of keeping in touch with teaching and students). This state of affairs is regrettable, notably in the context of measures recently taken to improve the salaries of CNRS researchers in exchange for 64 h/year of teaching. In addition, teaching dispensation for our UPS academics most active in research are practically nonexistent. The LPT would like to see a more flexible policy by the UPS with regards to both teaching dispensation for university academics and possibilities for CNRS researchers to teach. This would limit the possibility that certain of our members be attracted to other universities which might actively exploit these new measures in order to attract the best researchers.

- The next retirement by an LPT UPS academic is not expected within the next fifteen years. As the recruitment policy of the UPS is strongly based on the creation of positions to fill vacancies, UPS recruitments at LPT risk drying out. Today, we have a laboratory quite uniformly "young". However, if younger people are not recruited at a regular rate, the LPT risks becoming a uniformly "old" laboratory. We hope that the UPS will continue to provide the LPT with positions based on the criteria of scientific excellence, as has to date been the case.
- Even though the departure of certain members of a laboratory constitutes a natural part of its evolution, and mobility is clearly a positive point, the LPT has suffered from its fair share of departures. Departures particularly weaken laboratories of modest size as there is always the risk that once a laboratory becomes too small its members will simply leave for larger more stable structures. Departures include Frédéric Mila (at the LPT from 1993 to 2000; and now holding the *Chaire de Théorie de la Matière Condensée* at the EPF Lausanne), Erik Sørensen (at the LPT from 1996 to 2001; *full professor* at McMaster University, Canada), Satya Majumdar (at the LPT from 1999 to 2004; DR2 LPTMS Orsay), and Olivier Giraud (at the LPT from 2005 to 2010; CR2 at the LPTMS Orsay). Some of these departures have been motivated by job propositions abroad that are more attractive financially, scientifically or in terms of working conditions (F. Mila, E. Sørensen). Another reason is a purely personal one, as the partners of LPT members were sometimes unable to find satisfactory employment in Toulouse (S. Majumdar, O. Giraud). It should be noted that F. Mila (who held a visiting *Chaire Pierre de Fermat* at the UPS in 2008) and S. Majumdar still publish with LPT members on a regular basis. We are moreover confident that O. Giraud will continue his fruitful collaboration with the Quantware group.
- To qualify this last point, it should be noted that the LPT has been able to attract to France internationally renowned foreign researchers, now working at LPT, or elsewhere (*e.g.* S. Majumdar, at the LPT from 1999 to 2004; *Prix Langevin* of the SFP in 2005; an extremely prolific researcher, now at the LPTMS Orsay).

❍ Non-permanent staff

- Due to the high success rate of LPT researchers in finding funding, the LPT hosts a relatively large number of postdocs (10 over the period 2007-2009; see Chapter 4.1). This increase in the number of postdocs was stated as a goal in our previous scientific report and testifies to the attractiveness of the LPT to young foreign researchers. The LPT is highly satisfied with the training it provides to its postdocs and PhD students and this success is reflected by the fact that many go on to take up permanent positions in excellent research laboratories or accept stable positions in the private sector, both in France and abroad (see Chapter 4.1).
- Like many hard science laboratories in France and the rest of the western world, the LPT is worried by the increasing difficultly in finding students who wish to do a PhD in fundamental research. In particular the Master (Research) *Physique de la Matière* at the UPS must increasingly recruit students form outside Toulouse in order to retain its current level of student numbers. The LPT anticipates that it will increasingly have to attract PhD students from outside Toulouse, although we already have recruited a fair number of external candidates in the past. In fact, the three students starting their PhD in September 2009 come from the École Polytechnique (Palaiseau), the Université du Maine and the Indian Institute of Technology in Madras (India), confirming the scientific attractiveness of our laboratory. Given the large number of theoretical physics laboratories in the Paris area, and sometimes the reluctance of Parisian students to leave Paris, we will increase our efforts to attract students from the Paris area and elsewhere. At the beginning of 2009-2010, IRSAMC will produce a brochure of thesis subjects which will also shortly describe the research activities of its component laboratories. This document will be widely circulated across France and sent to our main foreign collaborators.

❍ Financial resources

- The LPT researchers have adapted well to the evolution of research funding in France. The large number of contracts obtained (notably 7 ANR contracts and 2 European contracts under progress in 2007-2009; see Chapter 2) implicitly testifies to the recognition of the quality of the laboratory's scientific activity.
- The geographical location of the LPT means that we incur substantial traveling expenses, both for the visits of our members and to invite people for short term visits (see Tab. 2.1 & 2.2 of Chapter 2). The continual cuts in the recurrent annual CNRS funding (which was 23 k€ in 2009) hampers our flexibility and ability to invite researchers as the research contracts have highly targeted budgets and thus can only partially replace CNRS funds for this use. The reduction in recurrent funding also presents us with difficulties regarding the financing of resources shared by the whole laboratory.

❍ Management of the LPT

- The LPT has reached a critical size but is still small enough to be managed in a straightforward, reactive and transparent manner, with good lines of communication between all members both at the interior and exterior of the different research groups. The LPT seminar and the publication of recent scientific highlights on our web site contributes to the diffusion of scientific results both inside and outside the laboratory, and specifically ensures that all LPT members are well informed of the research activities of their colleagues. This light and flexible management structure, notably with a short informative *lunch meeting* before the weekly seminar, is greatly appreciated by the members of the LPT
- The LPT and IRSAMC benefit from the extremely good collegial atmosphere within the institute, which facilitates many joint activities and projects (*Les Journées de l'IRSAMC*, *La Fête de la Science*), and allows the joint management of many resources, in particular positions at the UPS, and MESR/UPS PhD grants (see Chapter 1.4).

3

Research project of the four LPT groups

In this chapter, the four LPT groups present their project for the period 2011-2014, focusing on the scientific aspects of the LPT project.

3.1 Équipe Fermions Fortement Corrélés (FFC)

The combination of analytical and numerical approaches has led to remarkable progress in understanding the general features of collective states of quantum systems constituted by bosonic or spin degrees of freedom. However, there are a number of important outstanding problems that have for decades resisted solutions, most prominently the many fermions problem. Other examples include quantum spin systems with frustrating interactions that can suppress any type of ordering (giving rise to spin liquid behavior, topological order in two-dimensional systems, or out-of-equilibrium quantum systems). Remarkably, these open problems are not only of theoretical importance but also deeply relevant for today's experimental issues. Amongst many experimental realizations, we will highlight three particular topics in the rest of this project description: novel developments in high temperature superconductors, cold atomic gases and frustrated spin compounds. We first describe several middle-term projects, and finish with longer-terms perspectives for our group.

Quantum Correlations & Entanglement in valence bond states

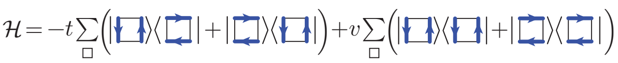
At low temperature, quantum fluctuations in frustrated antiferromagnetic (AF) spin systems are strong enough to prevent long range magnetic ordering and generate unconventional and only partially understood states of matter, such as Valence Bond Crystals or Spin Liquids. These states are deep inside the quantum regime and can not be apprehended on semi-classical grounds. Moreover, they provide genuine examples of macroscopic quantum objects characterized by both substantial entanglement and unusual magnetic correlations. In that respect, they lie at a crossing point between modern issues in condensed matter physics and quantum information theory.

Using new approaches based on Valence Bond (VB) states, we aim to investigate these unconventional low-energy states emerging from realistic spin or effective dimer models. We also plan to study the connection with quantum information theory using these methods, which could benefit from the expertise of the Quantware group in this domain.

Generalized Quantum Dimer Models

The most widely studied effective model in quantum magnetism are quantum dimer models (QDMs) as a good compromise between simplicity and richness of their phase diagrams. One essential caveat is that these models do not retain the original spin degrees of freedom, therefore missing all magnetic phases.

SU(2) QDM. A first attempt to bring back the spins into QDMs is by considering SU(2) Quantum Dimer Models :



Note the similarity with the celebrated QDMs, but dimers are here real singlets formed by spins 1/2, and no longer hardcore objects. This makes a huge difference, as now the full quantum mechanics of VB states (non-orthogonality of dimer configurations) must be taken into account. This type of model can be studied with recently developped Quantum Monte Carlo (QMC) techniques in the VB basis[1].

Generalized QDM. Another approach is the extension of the QDM derivation scheme to include more accurately the non-orthogonality effects. Formally, the projection of the Heisenberg Hamiltonian in the nearest neighbors VB states manifold *and* the rigorous orthogonalization of the VB basis can be performed in one step defining an effective Hamiltonian $H_{\text{eff}} = \mathcal{O}^{-1/2}\mathcal{H}\mathcal{O}^{-1/2}$. Both $\mathcal{O}$ and $\mathcal{H}$ can be developed according to the hierarchical structure of $\mathcal{O}$. Such an expansion generates a Generalized QDM that includes not only standard QDM processes but also resonance effects on larger loops. These new QDMs can be studied with Exact Diagonalization (ED) or QMC in some cases.

Open questions. Besides the standard questions inherent to the QDMs (phase diagram, crystalline phases), we can now address several issues that are absent within the traditional QDMs: (i) Can antiferromagnetic correlations destroy crystalline VB states? (ii) Can novel types of quantum spin liquids be found in SU(2) QDMs, similarly to the Z_2 spin liquid found with usual QDMs on non-bipartite lattices? (iii) At or close to Rokhsar-Kivelson points on bipartite lattices, can a new gapped U(1) spin liquid be stabilized? (iv) Can novel exotic excitations emerge on top of these spin liquids? If the gauge symmetry of the underlying field theoretical description of the liquid phase is more complicated than U(1), it is possible that non-abelian anyons are the lowest-lying excitations of the system. This is particularly appealing in view of the key role played by non-abelian statistics in topological quantum computation (see below).

Realistic models in the short-range VB basis

The most efficient numerical methods (QMC and DMRG) are not available for direct simulations of $d > 1$ frustrated magnets and almost all firmly established results come either from few exact results or by ED studies. Despite of its key assets, this method has to deal with the exponential growth of Hilbert space with system size.

One interesting approach to push limits starts from a phenomenological observation: not all singlet states are relevant for describing the low-energy sector of frustrated AF, and essentially all the physics can be captured using the Short Range VB basis (SRVB). Although it is no more exact and cannot reproduce magnetically ordered states, such an approximation is particularly optimized for *strongly* frustrated phases (such as Spin Liquids).

The price to pay is of course the intrinsic complexity of the VB basis directly related to its non-orthogonality: one has to solve a generalized eigenvalue problem, for which no iterative method à la Lanczos was available until now. The situation is likely to change dramatically in the next month thanks to a new algorithm called MAPL (see inset 3.1) that could allow to simulate few millions of SRVB states! This breakthrough in accessible system sizes will certainly allow to tackle many important topics, such as: (i) The nature of the spin 1/2 kagome AF which is still highly debated (VB liquid, VB crystal with a large unit cell,. . .). Moreover, the issue concerning the existence of a finite spin-gap for this model could be investigated by probing the confinement of spinons. (ii) Three-dimensional frustrated AF are notoriously out of reach of numerical calculation. Such computations would nevertheless be precious to describe various compounds. Typically, the first non-trivial hyperkagome cluster has 96 sites, clearly a huge quantum system. But, using a massive parallel computer, we are confident in its feasibility.

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

MAPL is a generalization proposed by M. Mambrini and collaborators of a recent *iterative algorithm* (APL) to the generalized eigenvalue problem. Successful preliminary results show that this new implementation will allow to solve generalized eigenvalue problem for large non-sparse matrices involved in VB calculations. From a technical point of view, the time-consuming part of the calculation concerns matrix-vector multiplication, which can be easily parallelized on supercomputers. Moreover, the use of symmetries can be efficiently implemented by using large vectors, so that large memory is equally needed.

Insert 3.1 : MAPL.

Entanglement and fidelity in quantum magnets

We propose to compute the first results on entanglement properties of interacting spin models for $d > 1$. We have defined a new measure of entanglement through the VB entropy that counts the number of singlets shared between two subsystems. Recently, this measure has allowed us for the first time to compute entanglement properties of various phases (magnetically ordered or not) in $2d$ [2]. Our results were obtained thanks to large-scale VB QMC simulations. Therefore, a direct extension of our work would be to study $3d$ cases, where no results have been presented so far.

We also plan to compute the behavior of the VB entropy in all relevant $1d$ phases, where the usual von Neumann entropy is available. Since we will consider frustrated models, QMC simulations cannot be used. We have just performed a first analytical step to circumvent this problem by expressing the VB entropy as a certain projection of the ground-state, which allows computations with the recently developed matrix-product states version of the DMRG algorithm.

Another topic which we wish to develop further is the fidelity approach to detect quantum phase transitions without any knowledge of the phases [3]. The basic idea is that ground-states are getting more and more orthogonal close to a quantum critical point. We have very recently made a technical breakthrough by developing novel QMC techniques to compute fidelity. We wish to apply them to several quantum spin systems in order to check the validity of this procedure. In particular, there are several basic issues (such as a finite size scaling theory for instance) that are still open in the fidelity approach.

Correlated fermions in two dimensions

Fermionic mean-field theories and Variational Monte Carlo techniques

Quantum AF on frustrated lattices cannot be simulated efficiently with QMC. However, based on Variational Monte Carlo (VMC) and Green Function MC techniques, S. Sorella and collaborators [4] have proposed that the Heisenberg model on the anisotropic triangular lattice could exhibit a spin liquid state with fermionic spinon excitations. The Dirac spin liquid phase with algebraic correlations proposed for the Heisenberg quantum on the kagome lattice also involves fermionic degree of freedom. "Renormalized Mean-Field Theories" [5] based on a *fermionic* representation of the SU(2) spins and using Gutzwiller approximation to deal with the local constraints can be constructed and have proven to be quite successful. Such methods can be readily extended to finite doping and can serve as a guide for more complex stochastic VMC computations based on fermionic trial wavefunctions. We plan to apply such methods to the case of Heisenberg or $t-J$ models on frustrated lattices with possible candidate ground states exhibiting exotic *fermionic* excitations. A PhD thesis funded by CNRS will be devoted to this topic starting September 2009. Interestingly, such an approach offers a *unified framework* to describe on a same footing the competition between various exotic phases from spin liquids, RVB phases, valence bond solids, supersolids, etc.

Inhomogeneities in cuprate superconductors

The experimental observation of charge inhomogeneities in cuprate superconductors have made recent tremendous progress with Scanning Tunneling Spectroscopy (STS) and with the syn-

2. F. Alet *et al.*, Phys. Rev. Lett. **99**, 117204 (2007).
3. S.-J. Gu, arXiv:0811.3127.
4. S. Yunoki and S. Sorella, Phys. Rev. B **74**, 014408 (2006).
5. P.W. Anderson, *et al.*, J. Phys. Condens. Matter **16**, R755-R769 (2004).

thesis of ultra-pure single crystals. The latter have also enabled the observation of quantum oscillations, giving crucial informations on the Fermi surface and its possible recombinations. Recently we have investigated the formation of superconducting stripes in $2d$ cuprates [6]. With Javier Almeida, post-doc funded by the UPS, we plan to investigate the conditions of stability of these exotic orders by using Mean-field, VMC or DMRG approaches. The role of the coupling to the lattice or to dynamical phonons will be of particular interest. This work will be done in collaboration with the LNCMI.

Itinerant bosons or fermions on frustrated geometries with ice-rule constraints

Correlated fermions (or bosons) moving on frustrated lattices like kagome or pyrochlore lattices at special commensurate densities are of particular interest. Indeed, strong interactions can stabilize a new type of Mott insulator where remaining (charge and spin) degrees of freedom can lead to exotic behaviors.

These ideas can be simply illustrated starting from an extended Hubbard model on the checkerboard lattice [7]. In fact, this can easily be extended to a wide class of frustrated lattices constituted of arrays of corner sharing units [8]. When the nearest-neighbor repulsion is dominant (classical limit), a ground state manifold is defined by an "ice rule" constraint and, hence, is highly degenerate. The kinetic energy introduces dynamics within this manifold and an interesting correspondance with the physics of the (undoped) QDM (or the quantum loop model [9]) can be drawn. Fulde *et al.* [10] have suggested that, due to the constraint, such models should exhibit fractional $Q = e/2$ charge excitations. Pioneering work has been performed in our group [11] to study the phase diagrams of such models. In fact, a number of exotic Valence Bond Crystals (VBC) have been found as ground state candidates.

We plan to pursue the investigation of this class of realistic models which we believe, are a gold mine to discover exotic behaviors. We wish to better take advantage of the rich connections with the QDM discussed above. Also understanding the exotic nature of the insulator-superfluid / insulator-metal transition that occurs when the Coulomb repulsion is reduced (*i.e.* when the ice-rule constraint is soften) hence allowing for "ice-rule defects" to propagate, is also one of our goals. Whether such defects are confined in pairs or deconfined should also play a crucial role in the zero-temperature phase transition. This project should ultimately suggest completely new routes to investigate metal-insulator transitions in correlated fermionic materials or bosonic insulator-superfluid transitions in frustrated quantum magnets. This project is part of the new ANR of D. Poilblanc and collaborators involving the hiring of a new post-doc.

Topological States and non-Abelian anyons

Anyons are excitations, or pseudo-particles, whose statistical properties interpolate between Bose-Einstein and Fermi-Dirac statistics. They were first studied in the 80's in the context of low-dimensional field theories and discussed in the context of high-temperature superconductivity. Anyons also appear in $2d$ topological quantum liquids such as the Fractional Quantum Hall state [12]. From a more mathematical point of view, particle statistics can be seen as the effect on the wave function when particles are transported around each other, which can be represented by drawing their world-lines which are the paths they trace out in space-time. These world-lines braid around each other and the set of all possible braidings is a group, acting on the space of states of the system. Different types of statistics correspond to different representations, often non-Abelian, of the braid group.

Initiated by M. Freedman (1986 Fields Medallist) pioneering work on $1d$ models of *in-*

6. M. Raczkowski, M. Capello, D. Poilblanc, R. Frésard, and A.M. Oleś, Phys. Rev. B **76**, 140505 (2007).
7. D. Poilblanc, K. Penc, and N. Shannon, Phys. Rev. B **75**, 220503 (2007).
8. F. Pollmann, J. J. Betouras, K. Shtengel, and P. Fulde, Phys. Rev. Lett. **97**, 170407 (2006).
9. N. Shannon, G. Misguich, and K. Penc, Phys. Rev. B **69**, 220403(R) (2004).
10. P. Fulde, K. Penc, and N. Shannon, Annalen der Physik, **11**, 892 (2002).
11. D. Poilblanc, Phys. Rev. B **76**, 115104 (2007).
12. G. Moore and N. Read, Nucl. Phys. B **360**, 362 (1991); N. Read and E. Rezayi, Phys. Rev. B **59**, 8084 (1999); For an experimental search of non-Abelian particles, see J.B. Miller *et al.*, Nature Physics **3**, 561 (2007).

teracting non-Abelian Fibonacci anyons [13] has been performed at *Station Q*, UC Santa Barbara. A large collaboration involving M. Troyer (ETH-Zürich), S. Trebst and others at *Station Q*, and D. Poilblanc in our group, has started to extend these investigations to quasi-1d systems (ladders) with the ultimate goal of approaching the 2d limit. We anticipate a vast program extending over the next three years which should have important implications in the field of *quantum computing*.

Strong correlations in multicomponent fermionic cold atoms

From recent progress in cold atom experiments, it appears feasible to build artificial "solids" that realize almost perfect toy models of strongly correlated systems. At low temperature, quantum effects start to play an important role and all the remarkable phases of solid-state physics should be observed. However, ultracold atomic systems possess a major distinction with respect to their solid state analogues: the atom total angular momentum F can be non-zero for bosons or larger than 1/2 for fermions. We expect that, when these $2F+1$ states remain quasi-degenerate, there is a possibility to form new states of matter, such as molecular superfluidity or exotic Mott phases.

Following some of our recent works, we plan to tackle these problems with state-of-the-art analytical and numerical techniques in order to clarify the rich phase diagrams, both the nature of the phases as well as the quantum phase transitions between them. On the other hand, given that realistic experiments are in progress (for instance, a condensate of 3 species of Lithium has been realized), we also plan to provide realistic predictions by taking into account the effects of finite temperature (which represents an additional complexity and challenge), of the trapping potential, or of the anisotropic scattering lengths.

Our second task will be dedicated to the commensurability effects in low-dimensional cold atomic quantum gases. Indeed, strong correlations are responsible for the occurrence of a so-called Mott transition into an incompressible state. Although it has been observed for bosonic systems for some time, the fermionic case has only been reached recently [14].

Note that a new cold atom experimental group headed by D. Guéry-Odelin has arrived at the LCAR so that we expect some collaboration on related topics.

Future directions

Many of the outstanding problems cited above and the continuing search for new quantum states of matter have made it obvious that the established methods despite their successes are not capable of solving all problems without major breakthroughs. Over the past few years a number of novel algorithms have been developed that significantly extend the applicability of the well-established techniques that we routinely use such as QMC methods or DMRG approach. We would like to highlight two recent developments that we foresee to have a great potential.

First, a new class of diagrammatic, continuous-time QMC methods bears the potential to study several lattice fermionic models (as well as non-equilibrium quantum problems) [15]. This is of particular interest as these QMC methods can also be used as impurity solvers in a Dynamical Mean Field Theory approach. Also, in a remarkable interplay between quantum information theory and computational condensed matter physics, the recent introduction of 2d tensor product states and of the related multiscale entanglement renormalization ansatz (MERA) [16] have allowed very recently the first "DMRG-like" simulations of frustrated quantum spin systems and fermionic models [17]. These perspectives of using these quantum information-related methods make a natural connection with the recent interest we have developed for these approaches. Naturally, these topics could involve a collaboration with the Quantware group.

13. S. Trebst, E. Ardonne, A. Feiguin, D. A. Huse, A. W. W. Ludwig, and M. Troyer, Phys. Rev. Lett. **101**, 050401 (2008).
14. R. Jördens, N. Strohmaier, K. Günter, H. Moritz, and T. Esslinger, Nature **455**, 204 (2008).
15. A. N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein, Phys. Rev. B **72**, 035122 (2005); P. Werner *et al.*, Phys. Rev. Lett. **97**, 076405 (2006); P. Werner, T. Oka, and A. J. Millis, Phys. Rev. B **79**, 035320 (2009).
16. G. Evenbly and G. Vidal, Phys. Rev. Lett. **102**, 180406 (2009).
17. G. Evenbly and G. Vidal, arxiv:0904.3383; P. Corboz *et al.*, arXiv:0904.4151; C. Kraus *et al.* arxiv:0904.4667.

Finally, another aspect which would be of great interest to develop in our group deals with the direct connection to the experiments, for instance through a collaboration with LNCMI on high-temperature superconductors. This line of research will also benefit from our future hiring of R. Ramazashvili (CR1, CNRS, starting 10/2009) who already interacts with the Grenoble branch of LNCMI.

3.2 Équipe Information et Chaos Quantiques (Quantware)

The Quantware group has accumulated internationally recognized expertise in classical and quantum chaos, nonlinear dynamics, random and complex matrices, mesoscopic physics and quantum transport at nanoscale, many-body quantum systems with interactions and disorder, and quantum computation and information. This expertise in various domains of physics allows to develop new approaches and investigation methods for a wide variety of physical problems, and will be used in our research plan for the next four years.

Quantum Computing

The research in quantum information and quantum computing will be developed along several lines. At the most fundamental level, the study of the quantum resources will further expand both our knowledge of their role in quantum information, as well as be useful in the conception of new quantum procedures. The most important such quantum resources, namely entanglement and interference (the quantitative study of this resource was pioneered in our group), will be studied together in several quantum processes to compare their respective roles during the different phases of the process. In particular, the detailed study, both numerical and analytical, of these resources in families of quantum algorithms performing the same task with various levels of efficiency will enable to elucidate further how specific parts of the algorithms are sensitive to a destruction of a certain amount of these resources (*e.g.* through the presence of imperfections or decoherence), and therefore establish their relative importance. We will also continue our research on quantum non-locality.

Such works will also be used in order to probe new quantum algorithms, for example based on the recent concept of quantum walks, which can be performed on quantum complex networks such as those already studied by the group. A particular emphasis will be put on optimization of algorithms to small quantum computers such as those being built through different implementations, enabling to envision their realization in experimental systems. The study of quantum algorithms in presence of realistic imperfections will also be continued.

An important part of this effort will be devoted to specific implementations of quantum computers on physical systems, were experiments are being done throughout the world. The properties of superconducting qubit in presence of decoherence will be investigated by the method of quantum trajectories. In parallel, the quantum synchronization of two or more qubits with a microwave resonator will be studied in details, keeping close links with advances of experimental groups at NEC, Saclay, Grenoble, ETH Zurich, Yale. This research line will be done in close links with the EC project "EuroSQIP" which regroups the major European teams in this field (the project is operating until April 30, 2010).

In parallel, new possible implementations will be studied, including a proposal made in the group for using triangular arrays of atoms on surfaces as a protected logical qubit, or using bistable molecules to implement qubits.

At last, we will investigate the use of decoherence to perform precision measurements. The development of quantum information theory has lead to new and important developments in other areas of physics, notably in the domain of precision measurements (quantum enhanced measurements). Moreover, using information theoretical concepts, fundamental quantum mechanical bounds have been developed for the precision of different kinds of measurements, such as phase shifts in an interferometer. These measurements are primers for many important applications, both scientific and technological, such as improvement of frequency standards, gravitational wave detection, navigation, remote sensing, or the measurement of very small magnetic fields. So far these bounds were developed for unitary quantum mechanical evolution. Recently we have shown that, surprisingly, non-unitary (i.e. dissipative or decoherent) quantum evolution may in certain cases lead to better precision. This opens up a new research field, where decoherence is used intentionally in a quantum mechanical system in order to improve measurement sensitivities. This new field will be thoroughly investigated over the next few years.

The questions in these fields are inter-related, and we are convinced that understanding the fundamental limitations of quantum information processing and quantum enhanced measurements will have significant long-term impact, both in science and society.

Transport at nanoscale

We will keep on investigating the ratchet transport induced by microwave and terahertz radiation in asymmetric nanostructures. Recently we showed that electron-electron interactions give an important contribution to the directionality properties of this transport. This effect should be further studied in order to interpret experiments performed at LNCMI Grenoble in the group of J-C Portal and at LPS Orsay in the group of H. Bouchiat. We will also develop theoretical studies of microwave-induced zero-resistance states experimentally observed and described by R. G. Mani *et al.* (*Nature*, 2002) and M. A. Zudov *et al.* (*Phys. Rev. Lett*, 2003). These studies could lead to development of new types of detectors for radiation in the terahertz range. This research will be done in collaboration with the other partners of the ANR-PNANO project *NANOTERRA* (LNCMI Grenoble, LPS Orsay, LAAS Toulouse). This research line will be developed in collaboration with the Russian Academy of Sciences (Budker Institute of Nuclear Physics and Institute of Semiconductor Physics, Novosibirsk).

Nonlinearity, Anderson localization and transport in Bose-Einstein condensates and photonic lattices

Anderson localization has been studied widely in the past fifty years, and the group has internationally recognized expertise on this subject. In connection with recent experiments in Bose-Einstein condensates and photonic lattices, the question of the effects of nonlinearity on the localization process has gained new actuality. The group will pursue work in this direction, with the aim to precisely elucidate this problem through numerical and analytical work. It will be investigated both in the context of disordered systems, and also for the problem of dynamical localization, in which quantum chaotic dynamics localizes a wave-packet in the absence of disorder. Both types of systems can be investigated through Bose-Einstein condensates in optical potential, and our results should be useful to experiments performed, for instance, in the group of A. Aspect in Paris. The theory developed could also be applied to experiments with nonlinear photonic lattices performed by the group of Y. Silberberg at Weizmann Institute (Israel).

These studies will also allow to explore new phenomena concerning transport in Bose-Einstein condensates in optical lattices. In particular, we plan to explore the effects of nonlinearity on time-reversal of matter waves (which was recently proposed by the group using Bose-Einstein condensates), on chaos assisted tunneling (observed by the Raizen group, using cold atoms), and on the properties of fractal wave functions, which we think can be obtained in such systems.

Applications to astrophysics

A collaboration with astrophysicists of the Observatoire Midi-Pyrénées in Toulouse enabled to show that acoustic oscillation modes of rapidly rotating stars can be divided into subspectra of chaotic and regular modes. Such oscillation frequencies are now observed with unprecedented precision through the space missions COROT and KEPLER. Work in this direction will be pursued along two axes. First, detailed numerical and analytical studies will also allow to precisely relate the properties of the subspectra to astrophysical quantities. Second, through confrontation with observed spectra, we will try to extract such information from the frequencies of real stars, in order to confirm the theory and to apply it to get insight on the star interior. This project will be performed in the framework of the ANR program SIROCO which coordinates scientists working on the COROT observations, and will involve a new PhD student, starting in September 2009.

In parallel, investigation of synchronization effects and their relation with the enormous sharpness of edges in Saturn rings will be continued in collaboration with physicists and astrophysicists from the University of Potsdam (Germany).

Quantum and classical chaos

A line of research will concern fundamental studies of systems displaying classical and quantum chaos. New models with continuous chaotic time flows will be investigated. We will also study the properties of Poincaré recurrences in systems with divided phase space where sticking near critical invariant curves leads to very slow decay of correlations and recurrences. For systems displaying quantum chaos, we will investigate the properties of non-unitary operators, characterized by emergence of fractal Weyl laws. In addition, the study of systems characterized by multifractal wave functions should lead to a better understanding of their links with specific spectral statistics.

Delocalization transition for the Google matrix

Recent results obtained by the group opened new prospects for investigation of Google-type matrices and directional networks, with potential important applications to information classification and retrieval in complex databases. The expertise of the group in complex systems, random matrices and localization properties will allow to develop new tools and obtain new results in this important field of research. The first results indicate existence of a delocalization transition in the Google matrix. Above the transition point, the classification and retrieval of information through Google-type algorithms becomes inefficient. This effect was established in the frame of a well-known network model (Albert-Barabasi model). It is important to study other types of network to understand the properties of this transition and conditions under which it takes place.

Summary

Its accumulated expertise allows the Quantware group to develop new research lines in various areas of physics, including theory of chaos, complex systems, quantum computers, transport at nanoscale, information retrieval, and astrophysics. While the theoretical research is strong enough, we think that the Quantware group should enhance its links to experimental groups in Toulouse, France, and abroad. The enhancement of such links will be an important strategic part of the future research program. First steps are already done *e.g.*, in the framework of the ANR projects *MICONANO* and *NANOTERRA*, which allowed to establish close contacts with experimental groups in Grenoble and Orsay, and at Institute for Semiconductor Physics (Novosibirsk, Russia), and they will be continued. We also plan to enhance contacts with cold atoms groups such as the ones of D. Guéry-Odelin (LCAR) in Toulouse, J.-C. Garreau in Lille, and similar groups in the world. In parallel, we are investigating experimental implementations of our quantum information work, where in particular contacts will be pursued with experimentalists at the Laboratoire de Chimie de Coordination – LCC and the Centre d'Élaboration de Matériaux et d'Études Structurales – CEMES, both in Toulouse.

The study of nonlinear effects and chaos in astrophysics should lead to close interaction with astronomical observations, *e.g.*, from the CASSINI and COROT missions. We will also maintain our close and fruitful contacts with research groups at the Russian Academy of Science, especially in Novosibirsk, with whom we share a long-term collaboration.

Another activity we want to increase is collaboration with other teams of the LPT. In particular there are points of convergence between the studies of our team and the subjects investigated by the FFC group, and some joint works have been made in the past few years (see *e.g.*, F. Alet, D. Braun, and G. Misguich, *Physical Review Letters* **101**, 248901 (2008)). Common areas of interest include condensed matter and mesoscopic physics but also cold atom experiments.

Within the last five years, the number of permanent scientists working in the Quantware group increased from four to six members (recruitment of D. Braun in 10/2004 and O. Giraud in 10/2005). However, R. Fleckinger has retired in 12/2006 (and will not extend his *éméritat* beyond 2010) and O. Giraud is leaving Toulouse for LPTMS Orsay in 2010, for purely personal reasons, although he will certainly continue to strongly interact with the Quantware group. Hence, the proper realization of the many promising scientific projects of the Quantware group would certainly benefit from the hiring of a young researcher at the CNRS (CR level) or the UPS (MCF level).

3.3 Équipe Physique Statistique des Systèmes Complexes (PhyStat)

In this section, we present the research project of the PhyStat group. This project is structured along the same three main themes developed in the scientific report, although it should be clear below that the frontier between these apparently distinct subjects is often very thin.

Soft condensed matter and biophysics

Effects of polarizability in confined electrolytic systems: surfaces and nanopores

Over the past few years, extensive molecular dynamical simulations, and more recently, experimental studies of ion/water systems near interfaces or in confined geometries have shown that the conventional view of ion behavior is inadequate. This conventional view, based on the pioneering work of Debye, Huckel, and Onsager in the early part of the last century, fails to account adequately for ion specificity and therefore cannot explain the **apparent propensity** of large highly polarizable anions, such as Br^- and I^-, to accumulate at water interfaces.

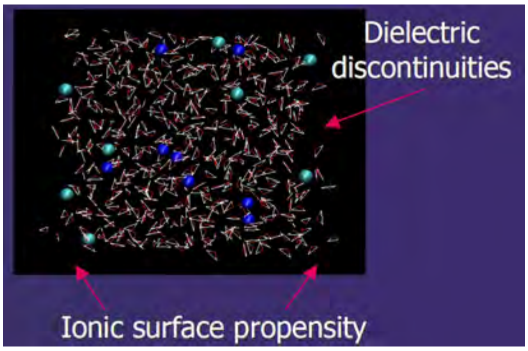


Figure 3.1 : *Snapshot of a water/vapor interface containing NaI (MD simulations).*

The impact of this unexpected ionic behavior in confined aqueous environments on a large number of important phenomena in physics, chemistry, biology, and engineering is enormous. Our theoretical work in this area will be aimed at elucidating the role of the various interactions at play near surfaces and in neutral and charged nanopores. We are especially interested in understanding the role of ionic polarizability and entropic hydrophobic effects due to the finite ion size. Our goal is to extend equilibrium and transport theories beyond the usual continuum (mean field) approaches, down to the nanoscale. We intend to use powerful statistical field theory techniques that allow one to go beyond mean field theory and test our approach by comparing its predictions with the results of lower level classical molecular dynamical simulations.

Physical mechanisms of membrane organization

To extend our previous work on the organization of membrane proteins, a key step will be to take into account effects arising from the large variety of membrane proteins present in living cells. One of our goals is to show how, via inter-protein interactions, micro-reactors composed of specific proteins type could be organized in specific domains. We wish to understand, in terms of inter-protein interactions (both physical and chemical), how the formation of organized regions with certain functionalities can be achieved thermodynamically. In order to play a biological role, such organized regions must exist on time scales of a few minutes and it is thus important to understand the stability and metastability of these regions. At the level of specific inter-protein interactions, we also plan to study the role of the interactions induced via the lipids present in the membrane. The fact that biological membranes have lipid compositions which are typically close to a continuous phase transition means that long range critical Casimir type interactions should be present between proteins (due to their direct interactions with lipids). Tendencies of proteins to wet or de-wet with certain lipids could lead to the formation of protein clusters rich in specific lipid types – such clusters are often invoked by biologists and are called **lipid rafts**. This idea of lipid-mediated interaction has been invoked in the literature but not studied systematically or in any great detail. An interesting physical challenge arising in this study will be to incorporate the effect of non-equilibrium processes, such as lipid recycling, on induced interactions.

Electropermeabilization

The widely accepted theory in the electropermeabilization community is that the electric field induces the formation of pores, as it locally increases the surface tension thus enabling the system to overcome the line tension of the pores – it is essentially a modification of theories developed to explain soap film rupture in the 1950s. Recent experimental work in Toulouse has indeed clearly demonstrated the formation of pores in artificial vesicles. One component of our research project is to try and understand the dynamics of pore formation and also tubule and vesicle formation which have also been observed. The existing theories of pore dynamics in electropermeabilization are restricted to planar membranes. However, pore dynamics has been studied in a number of other contexts (for example where pores are formed by a mechanically induced tension) for spherical vesicles. We aim to develop a theory specific to the experiments on artificial vesicles in order to better understand the observed phenomena. Another understanding of electropermeabilization comes from the purely microscopic studies that can be achieved by numerical simulations. Recent work has shown that very thin water filled pores can be formed when electric fields are applied across membranes in molecular dynamics simulations. The problem with these simulations is that due to the complexity of the composition (lipids plus water) the simulations can only be run over short time and length scales, which casts doubt on their relevance to the real physical system. Notably, the fields necessary to induce pore formation are an order of magnitude larger than those seen to induce electropermeabilization in experiments. A major part of our program will be to develop a **coarse-grained model** which can be used to explain the phenomenon of electropermeabilization. The idea is to develop a coarse-grained theory where lipids are described not only by director and concentration fields (as in liquid crystals), but also a electric dipole field which couples to the applied field – the idea being to investigate how the coupling of the electric field to the dipole field via its coupling to the director and concentration fields, could induce a phase transition where the corresponding nucleation phenomenon could describe the pores.

Models for DNA

We are interested in applying our DNA model, which takes into account the coupling between base-pair states and the whole DNA chain conformation, and which was first developed to describe DNA denaturation, to several problems investigated in recent experiments. First, it has been shown that the lifetimes of denaturation bubbles are very long (on the order of several μs). Our goal is to extend our model to the study of bubble closing dynamics in order to see whether the whole chain dynamics influence the base-pair ones. If so, this coupling could explain the long closing times. The force-induced transition, observed in force experiments on stretched DNA, will also be studied with our model, using variational methods. Our ongoing collaboration with experimentalists at the IPBS will continue. Our aim is to model dsDNA in the Tethered Particle Motion experimental setup in order to analyze experiments on **single DNA denaturation** and DNA/protein complexation. In this context, the proper inclusion of the dissociation equilibrium dsDNA $\rightleftharpoons$ 2ssDNA in the modeling of dsDNA denaturation, taking into account base-pair translational entropy, is central, especially for short DNA. Moreover, the influence of spatial constraints on the local DNA base-pair states, *e.g.* when wrapped around a protein, will be taken into account within a complete study of DNA/protein complexation.

Stochastic processes and disordered systems

Effects of disorder on the Casimir effect

Recent ultrahigh sensitivity experiments on Casimir (zero temperature and ideally polarizable surfaces) and van der Waals (finite temperature and non-ideally polarizable surfaces) interactions between surfaces *in vacuo* have accentuated the need for accurate assessment of the possible electrostatic contribution to the total interactions between surfaces bearing disordered charge distribution. This surface charge distribution can be of various origins. In the so-called patch effect, the variation of the local crystallographic axes of the exposed metallic surface of a clean polycrystalline sample can lead to the variation of the local surface potential. These variations are of course sample specific and depend heavily on the method of preparation of the samples. The electrostatic forces due to this surface potential disorder can not be eliminated by grounding the two interacting surfaces. A similar type of surface charge disorder can be expected also for amorphous films deposited on crystalline substrates. Surface annealing of these films can produce grain structure of an extent that can be larger then the thickness of the deposited surface film. In addition, adsorption of various contaminants, whose concentration can not be controlled and is in general not known in any of the experiments, can influence the nature and type of the surface charge disorder and again contribute to the total interaction between the bounding surfaces. We will use the LPT's combined expertise in **fluctuation induced interactions and disordered systems** to investigate theoretically the effects of charge disorder, both surface and volume, in the currently used experimental systems. For van der Waals or thermal Casimir interactions, we plan to further investigate the effects of dielectric disorder, as well as to try to take into account the fact that the surfaces in the experiments are not perfectly flat.

Diffusion in random media and dynamical phase transitions

In many mean field spin glass models, one can identify the presence of a dynamical transition even in the absence of a thermodynamic one. This is done via the marginality condition which relies on the identification of the proliferation of metastable states. The dynamical transition is thus encoded in the static energy landscape. An interesting question which is still hotly debated is whether this mean-field like scenario is relevant to finite dimensional systems. Recently, we have identified a number of situations for overdamped Langevin particles where a dynamical phase transition occurs. However, these overdamped systems can be seen as the adiabatic limit of systems with **potentially richer dynamics**, for example dipoles in random electric fields and partially damped Newtonian dynamics of a particle in a random potential. As well as establishing the location of the dynamical transition (between normal and abnormal subdiffusion), we plan to investigate how one can determine the anomalous exponents in the low temperature regime.

In general, dynamical phase transitions also arise naturally in reaction-diffusion models for which the effect of disorder is poorly understood. The evolution operator of a reaction-diffusion system can be also generally seen as a – possibly non-Hermitian – quantum operator. The low-lying excitation spectrum of this operator provides crucial information about the nature of the dynamical phase transition, and we expect to benefit from the expertise of the FFC group in the numerical study of **quantum Hamiltonians** to elucidate some puzzling dynamical phase transitions (PC, PCPD...), and the role of disorder in directed percolation (DP). Lanczos diagonalization and DMRG appear as well adapted methods in this context, especially for one-dimensional systems.

Theory of signals and physics and society

Physicists are now more than ever involved in the study of complex systems which do not belong to the traditional realm of their field. In particular, the tools and methods of statistical physics are well adapted to the study of a large variety of complex systems arising in the human or natural world (finance, organization of human or animal societies, phyllotaxis, theory of competition in sports or economics...). For instance, and as illustrated in the companion scientific report, the theory of competition naturally involves the theory of extreme events, the theory of persistence of random processes, and the theory of traveling wave fronts. In collaboration with our colleagues S. N. Majumdar, (LPTMS Orsay), S. Redner and P. Krapivsky (Boston University), the latter two having spent respectively 1 and 3 months at LPT in 2009, we expect to apply these techniques further and develop new models in order to understand and describe quantitatively **competitive situations** arising both in sporting competitions and in human and animal societies. The former have the appealing property of being truly isolated systems contrary, for instance, to most financial systems.

The analysis of the large amount of statistical data available in many complex systems (sports, finance, genetics, neurobiology...) requires the development of advanced statistical tools. The recent advances in the theory of persistence presented in the scientific report provide such a valuable tool which allows the exploration of subtle non-Markovian aspects of general signals (probability to remain below a given threshold, statistics of extrema...). The exploitation of these results is in progress and should find a first application in a collaboration with biophysicists at Cold Spring Harbor Laboratory involved in the analysis of neurobiological signals and imaging. In addition, the PhyStat group actively participates in the recent organization of a systemic biology activity group in Toulouse, also involving the Institut de Mathématiques de Toulouse (IMT) and ecology and biology laboratories (the first workshop is on 18 June 2009). The PhyStat group was naturally solicited to participate in this project and its organization thanks to its well established and successful collaborations with biologists and its expertise in the theory of signals. We hope that this will motivate new collaborations between the PhyStat group and other scientist involved in this project. In addition, starting in 2009, LPT and IMT have organized a series of seminars and a mini-colloquium (12 June 2009) in order to share their methods (and their applications) in the field of probability and statistics and, hopefully, encourage future collaborations.

The statistical physics of optimization problems

The traveling salesman problem (TSP) is perhaps the most famous optimization problem. Given a set of N points randomly distributed in a region of space, one can ask what is the shortest route visiting each point once and what is the average length of this optimal path. Recently, we developed statistical mechanics techniques to compute the optimal path for the maximal TSP problem where the path length should be maximized. However, this method does not work for the minimal TSP. We have developed a field theory to analyze problems such as the TSP and the related matching problem. This field theory is currently under analysis and we intend to pursue this line of attack to see if we can solve the problem of computing the expected length of the optimal path. Many optimization problems have a graph structure in their underlying geometry. Mathematically, they are specified by values at the graph nodes and on the edges. For instance, one may want to maximize the flow of a certain commodity about the graph. An important algorithm for solving these sorts of problems is the MAXCUT algorithm. Intriguingly, there are classes of problems which are generically "easy" and others that are "hard". An interesting example of a MAXCUT type problem is the problem of **sports elimination numbers**. The problem is simple to describe: imagine a sports league halfway through the season; your team has been losing but you want to see if it is still possible for them to win the league. One way to do this is to enumerate all the possible outcomes although this will take a lot of computing time for large leagues. We plan to study this type of problem using techniques from disordered systems (replica theory) in order to understand when these types of problem become "hard". Extreme value statistics, persistence, and the theory of traveling wave fronts are also expected to play a significant role in this domain.

Dynamics and thermodynamics of systems with long-range interactions

The dynamics and thermodynamics of systems with long-range interactions are very rich topics with ramifications in different areas such as astrophysics, hydrodynamics, biology... Furthermore, from a theoretical point of view, the statistical mechanics of systems with long-range interactions poses new and challenging questions. In particular, they present unusual properties compared to systems with short-range interactions, such as negative specific heats, non equivalence of statistical ensembles, self-organization, non-Boltzmannian quasi stationary states (QSS), fast collisionless relaxation, slow collisional relaxation... It is therefore of interest to develop this topic at a general level, considering both conceptual issues and applications. The development of the analogies (and differences) between the different systems has already proven to be very fruitful. In addition to pursuing this study of certain systems mentioned in our scientific report, we list below three new directions of research which will be developed in the future.

Kinetic theories

The statistical equilibrium states of systems with long-range interactions are now relatively well understood and the different types of phase transitions that they can undergo have been described thoroughly. However, less is known concerning the kinetic theories that describe the **relaxation of the system** towards these equilibrium states. One direction of research is to develop kinetic theories appropriate to systems with long-range interactions. A first step is to derive the kinetic equations from first principles, while a second step consists in solving these equations numerically and, when possible, analytically. This project has already been initiated in the past. However, two interesting problems will be given particular scrutiny in the future. One concerns the problem of evaporation of stars from self-gravitating systems like globular clusters. With M. Lemou (Université de Rennes), we aim to develop new analytical methods to tackle this problem. One interest of this approach over previous ones is to obtain non-perturbative results. Another interesting issue concerns the influence of the rotation on the kinetic theory of a self-gravitating system. This project will be developed in the case of rotating self-gravitating Brownian particles where the kinetic theory is simpler.

Fluctuations

Most studies of chemotaxis rely on the Keller-Segel model which consists of two coupled partial differential equations (a Fokker-Planck equation coupled to the Poisson equation). In particular, this model completely ignores the **influence of fluctuations** which can be important when the number of particles is not too large (which is the case for bacterial populations in biology) or when one is close to a critical point. If we take into account fluctuations, the standard Keller-Segel model is replaced by a Fokker-Planck equation with a stochastic term and the fluctuations can trigger the transition from one metastable state to the other. This is somewhat similar to the evolution of a Brownian particle in a double-well potential except that the evolution of the particle is replaced here by the evolution of a field.

Decaying 2D turbulence

Two-dimensional turbulence is known to self-organize spontaneously into coherent structures (vortices) that dominate the dynamics. In a simplified model, the vortices evolve according to Hamiltonian equations punctuated by some merging events when two like-sign vortices come in contact with each other. As a result, the number of vortices decreases with time while their size increases. Numerical simulations and experiments suggest that the evolution is self-similar and that the vortex number decreases as $N \sim t^{-\xi}$ with $\xi \simeq 0.7$. P. H. Chavanis and C. Sire have developed a theory according to which the scaling regime is reached on much larger timescales than those achieved numerically or experimentally. In this asymptotic regime, the scaling exponent is expected to be $\xi = 1$. This can be understood schematically by considering three-body interactions involving a ballistic dipole encountering a standing monopole, a process which should be the most relevant at low vortex density, *i.e.* late time. However, it might be useful to develop an **effective two-body interaction process** to justify an effective exponent closer to 0.7 in the first regime. It would also be of interest to develop a kinetic theory of vortex aggregation (similar to the Smoluchowski coagulation equation) in order to predict the distribution of sizes. More generally, these methods could be applied to other systems experiencing a similar "decay" dynamics such as self-gravitating Brownian particles and biological populations.

3.4 Équipe Systèmes de Fermions Finis – Agrégats (Agrégats)

The Agrégats group has developed several theories in the realm of violent dynamical scenarios in irradiated free metal clusters, from fully quantum to mostly classical approaches. These methods have been recently extended to the case of organic molecules and to the case of systems in contact with an environment. The group has also worked out a platform of very robust and flexible homemade numerical tools developed over the years. These unique codes thus allow the Agrégats group to explore non-linear scenarios in clusters and molecules under extreme conditions, processes that are not accessible by other techniques. Few groups in the world can actually compete with such a microscopic description of non-linear processes.

The Agrégats group has also longstanding contacts with experimental groups working in related fields, which provide promising opportunities for the applications of the developed formalisms. Furthermore, one should stress that the problems considered by the Agrégats group call for deep formal developments at the side of Time-Dependent Density Functional Theory (TDDFT). This latter aspect also constitutes a major axis of investigation in the Agrégats group. The close connexion with elaborate numerical modeling provides, in this context, a unique opportunity to test in truly realistic situations the formal developments. Following these general considerations, the Agrégats group identifies three major complementary axes of work:

- Formal developments and implementation of simplified Self-Interaction Correction (SIC) approximations for a correct treatment of ionization and electronic transport.
- Non-adiabatic dynamics of irradiated organic molecules embedded in rare gas droplets, in relation with an experimental group in Lyon (via the follow-up of the joined ANR project MIRRAMO).
- Microscopic description of the interaction of clusters with extreme light (attosecond pulses, X-ray free electron lasers), in connection with the forthcoming data from experiments using these new laser technologies.

Simplified SIC approximations

Relying on the previously TDSIC scheme established in the past three years, there is an urgent need to develop further simplified SIC formulations. Indeed, although formal problems have been clarified, the techniques developed up to now are very costly numerically and almost prevent any practical use of such a correction in realistic cases. Thus, starting from full TDSIC calculations on a broad selection of different and typical reference systems, we will develop approximate treatments of the TDSIC along the line of approximate Optimized Effective Potential (OEP) schemes previously developed. The strategy will thus be twofold here. In parallel to the development of simplified TDSIC approximations, we shall constitute a set of benchmark calculations for validating the implementation of approximations in realistic test cases. A preferred class of test cases will concern organic systems, in relation to some of our other projects. Such systems are furthermore more demanding than the simpler metal clusters used in some of our other projects. They thus constitute a sound basis for testing the elaborate formal developments we shall work on.

Organic molecules in helium droplets

The ANR project MIRRAMO, joined with an experimental group in Lyon, aims at elucidating at the microscopic level the damage on water-coated biomolecules when interacting with a high-energy projectile. The use of rare gas droplets as a next step of these experiments allows to control the external conditions (temperature, orientation) under which irradiation takes place. From the theoretical point of view, the simplest assumption is that the rare gas mostly provides a low temperature heat (cold) bath. But a high precision description has to account also for the side-effects due to the embedment. This task implies the extension of our hierarchical model to the case of organic molecules in/on rare gas droplets. It will benefit from the solid experience acquired in the case of metals in/on rare gases. The basis of modeling will remain the same, namely the description of rare gases by classical atoms dressed with (classical) dynamical polarizabilities. The core of the work here will consist in defining model potentials for the various combinations of C, N, O, H and rare gases, relying on benchmark computations from the literature, especially from ab initio quantum chemistry, when available. We also have the capability to perform our own ab-initio calculations and will do that if necessary.

Irradiation of clusters by extreme laser light

High-intensity X-ray/XUV Free Electron Lasers (FEL) are now available and will allow new, possibly time-resolved (TR), spectroscopies for imaging the electronic motion on its natural time-scale and at the length-scale of a molecule. The availability of attosecond pulses will furthermore even reduce the time scale at which dynamics will be resolved. While there was for years no urgent need to perform such studies, the recent new experiments in these fields open exciting areas in cluster and molecular physics. However, accurate theoretical descriptions are still missing. Our previously developed theoretical and numerical methods are ideally suited to tackle these opening domains in the case of clusters and molecules in extreme light. Indeed, intense fields as provided by these lasers inevitably excite complex dynamics. The success of imaging techniques depends on our understanding of these largely unknown dynamics, creating demand for the theory of complex polyatomic systems in non-perturbative and ultrashort external fields. One of our goal here will to establish time-resolved photoelectron spectra and angular distributions of electrons emitted after the interaction of a cluster/molecule with an extremely short-pulse and/or high-frequency laser. This will allow us to explore the mechanism of light absorption and electronic emission in such new processes.

Evolution of the Agrégats *group*

The Agrégats group is strongly linked to Prof. P.-G. Reinhard at the University of Erlangen in Germany, with which it has a long tradition of collaboration on the dynamics of finite fermions systems (nuclei in the early 1990's, clusters since the mid 1990's). The whole set of computational platforms has been developed together. This closely-knit team allows an active and fruitful partnership. Prof. Reinhard usually supervises 1 PhD student and 1-2 diploma students per year, to be added to the 2.5 PhD students and 0.5 post-doctorant fellow per year in average in the Agrégats group. Recently the visit in 2007/08 of a PhD student from Prof. F. S. Zhang's theory group at the Normal University of Beijing has furthermore initiated a close partnership with China for the future, in addition to the continuing collaborations with experimental groups in France (Lyon) and Germany (Rostock), and the theoretical partnership with Russia (Dubna) and Spain (Valencia). There is also a growing community of interest with the biophysics subgroup of the PhyStat group at LPT, in which the water interface is also a question of great importance. Complementing viewpoints on these questions might in the future constitute an interesting basis for closer contacts.

Nevertheless, the low workforce of the Agrégats group, constituted of only 2 permanent positions (and moreover 2 teaching positions), strongly levels off its scientific production. There is an urgent need for a third permanent position, ideally a CNRS "CR2" researcher (Section 04 or 05). Such a support would be especially welcome either in the projects on irradiation theory or in the ones on extreme light, which are both highly competitive worldwide and where the group has still succeeded to remain at the top front of theoretical and computational developments.

The multidisciplinary nature of the physics studied in the group nevertheless makes such a recruitment delicate. Our activities lie at the border of strong-field physics, laser physics, physics of collisions, quantum chemistry, many-body theory, ultra-fast molecular dynamics and software development. This means connections with sections 02, 04, and 05 of CNRS... The Agrégats group is thus in contact with many communities but fully included in none. This may be welcome from a purely scientific point of view but not simple from the institutional point of view.

Laboratoire de Physique Théorique
UMR5152 CNRS/Université Paul Sabatier
IRSAMC
118, route de Narbonne
31062 TOULOUSE
+33 (0)5 61 55 75 72 (tél.)
+33 (0)5 61 55 60 65 (fax)
www.lpt.ups-tlse.fr