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Many-Body Quantum Systems and Effective Theories

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Abstract. In the last years, substantial progress has been made in many areas of mathematical physics. The goal of this workshop was to bring together researchers working on analytic and probabilistic aspects of many-body quantum systems and quantum statistical mechanics, to discuss recent developments, exchange ideas and propose new challenges and research directions. Among the questions addressed during the workshop were the derivation of effective equations, the analysis of physically interesting nonlinear partial differential equations emerging from microscopic theories, the study of open quantum systems in and out of equilibrium, and the investigation of the ground state properties and of the dynamics of quantum spin systems.

Mathematics Subject Classification (2010): 82B10, 82C10, 81Q05, 81Q10, 35Q40, 35Q20, 35Q41, 35Q55, 35Q56.

Introduction by the Organisers

During the workshop there were 21 lectures, ranging in topic from the mathematical description of many-particle systems of fermions, bosons and anyons, quantum spin systems, topological phases of matter and the non-equilibrium statistical mechanics of open quantum systems. In addition, there were evening sessions on open problems in the field, which resulted in lively discussions. The first was given on Monday evening by Bruno Nachtergaele, covering quantum spin systems, in particular the existence of spectral gaps, in general for dimensions greater than two and in certain one-dimensional models, e.g. the Haldane spin chain. The second was given by Jan Philip Solovej on Thursday, and concerned open problems in atomic physics, in particular the ionization conjecture and other conjectures concerning

the size of atoms with large nuclear charge and the connection to Thomas-Fermi theory.

The workshop covered the following subjects, all of which have received a lot of attention in the mathematical physics community in the last years.

1. Derivation of effective theories

One of the most important questions of statistical mechanics is the justification of effective theories, like Thomas-Fermi, Vlasov and BCS theories, starting from a microscopic description of many-body systems. In this line of research, Mathieu Lewin presented a new general approach to understand the ground state energy of fermionic systems in the mean-field limit, generalizing previous results restricted to very special cases, like systems with Coulomb interaction. Michael Sigal discussed the existence of vortices and vortex lattices in superconductors described by the Bogoliubov-de-Gennes equations. Nicolas Rougerie presented a derivation of effective many-body anyonic systems starting from a model of fermions, where the anyonic degrees of freedom effectively arise in a suitable parameter regime. Alissa Geisinger discussed the question of translational symmetry breaking in the BCS model.

2. Analysis of quantum many-body systems

The focus here is on the analysis of physically interesting properties of many-body systems, described either on the microscopic level, or through approximate theories. For example, Heinz Siedentop presented a derivation of the Scott correction for large atoms for a pseudo-relativistic model of atoms. Ian Jauslin explained a renormalization-group construction of bilayer graphene. Jakob Yngvason discussed his recent work on the incompressibility of Laughlin-type wave functions. Anyons were also the topic of Douglas Lundholm's lecture, in particular Lieb-Thirring inequalities and their dependence on the statistics parameter. Phan Thanh Nam discussed results on the ionization conjecture for various effective theories of atoms, including the Thomas-Fermi-Dirac-von-Weizsäcker theory and the Müller density matrix functional. Stefan Teufel presented an alternative view on particular annihilation, described via boundary conditions on Fock space.

3. Mathematical analysis of nonlinear partial differential equations

Nonlinear partial differential equations arising in the description of many-body quantum systems are the source of several challenging mathematical problems. In the workshop, we had three talks addressing such questions. Enno Lenzmann discussed the existence of solutions of the half-wave-map, an analogue of the wave map with the Laplacian replaced by its square root. Julien Sabin explained the extension of Strichartz inequalities to systems of orthonormal functions. Rupert Frank analyzed the phase transition occurring in a certain model of flocking.

4. Open quantum systems

New phenomena emerge when quantum systems are coupled to large reservoirs, allowing energy and particles to flow. In this setting, Gian Michele Graf discussed the adiabatic crossing of infinitely degenerate energy levels and applications to open quantum systems. Marco Merkli presented applications of the spin-boson model in quantum biology. Wojtech De Roeck explained the effects of periodic driving on quantum systems, and Annalisa Panati discussed energy fluctuations and the full counting statistics.

5. Quantum spin systems

Quantum Spins systems provide toy models in statistical mechanics, which are analytically easier to handle than full many-body theories but, at the same time, capture many of the essential features, like phase transitions, long-range order, correlations and entanglement. They were the subject of two talks in the workshop. Daniel Ueltschi presented new correlations inequalities for the quantum XY model. Yoshiko Ogata explained her work on the classification of frustration free one-dimensional Hamiltonian and corresponding quantum phases.

6. Other

Finally, two talks addressed topics which do not fit precisely in the previous sections but, nevertheless, were related to many-body quantum systems. Felix Finster gave an overview of his work on the causal action principle, in an attempt to try to connect his theory to more traditional approaches. Jonas Lampart discussed the applicability of density functional theory in the time-dependent setting.

Acknowledgement: The MFO and the workshop organizers would like to thank the National Science Foundation for supporting the participation of junior researchers in the workshop by the grant DMS-1049268, "US Junior Oberwolfach Fellows".

Workshop: Many-Body Quantum Systems and Effective Theories

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Abstracts

The semi-classical limit of large fermionic systems

Mathieu Lewin
(joint work with Søren Fournais & Jan Philip Solovej)

For many-particle systems, the *mean-field* regime is a limit of high-density and low interactions, in which the system is appropriately described by a simplified effective equation involving a mean-field (self-consistent) potential. A high density is needed to ensure that each particle meets many others, and low interactions are necessary for a law of large number to hold.

In mathematical terms the Hamiltonian describing N quantum particles takes the form

$$H_{\hbar,N} = \sum_{j=1}^{N} \big(-i\hbar\nabla_j + A(x_j)\big)^2 + V(x_j) + \frac{1}{N} \sum_{1\le k<\ell\le N} w(x_k - x_\ell). \tag{1}$$

The small coupling constant $1/N$ makes the two-body interaction (which contains $N(N-1)/2$ terms) of the same order as the one-body part (which has N terms).

For bosons this operator must be restricted to the subspace of $L^2(\mathbb{R}^{dN})$ containing all the functions that are symmetric under exchange of variables. In the limit $N \to \infty$ with $\hbar$ fixed, one then obtains the Gross-Pitaevskii theory, based on the nonlinear functional

$$\mathcal{E}^{V,A}_{\rm GP}(u) = \int_{\mathbb{R}^d} \big(| -i\hbar\nabla u(x) + A(x)u(x)|^2 + V(x)|u(x)|^2 \big)\, dx + \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} w(x-y)|u(x)|^2|u(y)|^2\, dx\, dy.$$

This convergence has been proved both for stationary states and for the time-dependent equation. We refer to [5] for a list of references and an optimal result for ground states.

For fermions, $H_{\hbar,N}$ must be restricted to the subspace of $L^2(\mathbb{R}^{dN})$ containing *anti*symmetric functions. Those functions have a kinetic energy that will typically grow much faster than N. Indeed, the Lieb-Thirring inequality [6] states that

$$\sum_{j=1}^{N} \int_{\mathbb{R}^{dN}} |(-i\hbar\nabla_j + A(x_j))\Psi|^2 \ge C\hbar^2 \int_{\mathbb{R}^d} \rho_\Psi^{1+\frac{2}{d}} \ge C|\Omega|^{-\frac{2}{d}}\hbar^2 \left(\int_\Omega \rho_\Psi\right)^{1+\frac{2}{d}} \tag{2}$$

for any bounded set Ω and with the one-particle density

$$\rho_\Psi(x) := N \int_{\mathbb{R}^{d(N-1)}} |\Psi(x, x_2, ..., x_N)|^2\, dx_2 \cdots dx_N.$$

As we expect that there will be of the order of N particles in a suitable domain Ω, the right side of (2) will behave as $\hbar^2 N^{1+2/d}$ and this suggests to take $\hbar \sim N^{-1/d}$ in order to compensate this growth. For this reason the mean-field limit for fermions is naturally coupled to a semi-classical limit.

The limiting effective theory obtained in this limit is based on the Vlasov energy

$$\mathcal{E}^{V,A}_{\rm Vla}(m) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} |p+A(x)|^2 m(x,p)\,dx\,dp + \int_{\mathbb{R}^d} V(x)\rho_m(x)\,dx + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-y)\rho_m(x)\,\rho_m(y)\,dx\,dy. \tag{3}$$

Here $\rho_m(x) = (2\pi)^{-d}\int_{\mathbb{R}^d} m(x,p)\,dp$ and $m(x,p)$ is a probability measure on the phase space $\mathbb{R}^d\times\mathbb{R}^d$ that must satisfy the additional constraint $0\le m\le 1$. This condition says that one cannot put more than one particle at x with a momentum p, as is appropriate for fermions. With this constraint, the Vlasov energy is minimized for measures of the form

$$m_\rho(x,p) = \mathbb{1}\left(|p+A(x)|^2 \le c_{\rm TF}\,\rho(x)^{2/d}\right) \tag{4}$$

where $c_{\rm TF} = 4\pi^2\left(d/|S^{d-1}|\right)^{2/d}$ and ρ now minimizes the *Thomas-Fermi energy*

$$\mathcal{E}^V_{\rm TF}(\rho) := \mathcal{E}^{V,A}_{\rm Vla}(m_\rho) = \frac{d}{d+2}c_{\rm TF}\int_{\mathbb{R}^d}\rho(x)^{1+\frac{2}{d}}\,dx + \int_{\mathbb{R}^d} V(x)\rho(x)\,dx + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-y)\rho(x)\,\rho(y)\,dx\,dy. \tag{5}$$

In the following we denote by

$$e^V_{\rm TF} = \inf_{\substack{\rho\ge 0\\ \int_{\mathbb{R}^d}\rho=1}} \mathcal{E}^V_{\rm TF}(\rho) = \inf_{\substack{0\le m\le 1\\ \int_{\mathbb{R}^{2d}} m=(2\pi)^d}} \mathcal{E}^{V,A}_{\rm Vla}(m)$$

the Thomas-Fermi ground state energy and by $\mathcal{M}$ the set of all the weak limits of minimizing sequences (ρ_n) for $e^V_{\rm TF}$. In the 'good' cases where no particle is lost, this is just the set of all the minimizers of the Thomas-Fermi problem.

Theorem 1 (Convergence to Thomas-Fermi [2])**.** *Assume that V, w and $|A|^2$ are in $L^{1+d/2}(\mathbb{R}^d)+L^\infty_\varepsilon(\mathbb{R}^d)$. Then we have for the first (fermionic) eigenvalue*

$$\lim_{\substack{N\to\infty\\ \hbar N^{1/d}\to 1}} \frac{\lambda_1(H_{\hbar,N})}{N} = e^V_{\rm TF}.$$

Let Ψ_N be any sequence of fermionic states such that $\langle\Psi_N, H_{\hbar,N}\Psi_N\rangle/N \to e^V_{\rm TF}$. Then there exists a subsequence and a probability measure μ on the set $\mathcal{M}$ such that for every fixed $k\ge 1$, the k-particle Wigner function

$$\mathcal{W}^{(k)}_{\Psi_N}(x_1,p_1,...,x_k,p_k) := \frac{N!}{(N-k)!}\int_{\mathbb{R}^{dN}} \Psi(x_1+y_1/2,...,y_{k+1},...,y_N)\times \overline{\Psi(x_1-y_1/2,...,y_{k+1},...,y_N)} e^{-i\hbar^{-1}\sum_{\ell=1}^k p_\ell\cdot y_\ell}\,dy_1\cdots dy_N$$

converges in the sense of distributions to

$$\mathcal{W}^{(k)}_{\Psi_{N'}}(x_1,p_1,...,x_k,p_k) \rightharpoonup \int_{\mathcal{M}}\prod_{j=1}^k m_\rho(x_j,p_j)\,d\mu(\rho).$$

The statement gives the convergence of the many-particle ground state(s) to that of Thomas-Fermi theory. Results of this form have been known for a long time in particular cases. Lieb and Simon proved it for atoms in [7, 8] in the limit $N \sim Z \to \infty$ which can be recast in the above form after changing the units of length by a factor $N^{1/3}$. Lieb, Thirring and Yau have considered in [9, 10] the case of stars where $V \equiv 0$ and $w(x) = -1/|x|$.

The proof uses ideas from [5] and in particular the classical de Finetti-Hewitt-Savage theorem [1, 3] which says that the law of an infinite family of exchangeable random variables must be the convex combination of iid ones. For fermions, this means that if we have a family $m^{(k)}$ of symmetric positive measures on $(\mathbb{R}^{2d})^k$ such that

$$0 \leq m^{(k)} \leq 1 \qquad \text{and} \qquad (2\pi)^{-d} \int_{\mathbb{R}^{2d}} m^{(k)}(\cdot, x_k, p_k)\, dx_k\, dp_k = m^{(k-1)},$$

then there exists a probability measure μ such that

$$m^{(k)} = \int_{\substack{0 \leq m \leq 1 \\ \int_{\mathbb{R}^{2d}} m = (2\pi)^d}} m^{\otimes k}\, d\mu(m).$$

In other words, these must necessarily be combinations of factorized states.

The proof uses this theory for the *Husimi measures* of Ψ_N in a coherent state basis, which have better positivity properties than Wigner measures. The link with the Wigner measures is made through the use of the Calderon-Vaillancourt theorem. The main difficulty in carrying the whole argument is to deal with the possible lack of compactness due to the escape of some particles at infinity. This is quantified using a technique developed in [4, 5].

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No translational symmetry breaking in the BCS model with radial pair interactions

Alissa Geisinger
(joint work with Andreas Deuchert, Christian Hainzl, Michael Loss)

We consider a sample of fermionic atoms in a cold gas in the framework of BCS theory. It is convenient to think of the sample as infinite and periodic, since this setting avoids having to deal with boundary conditions. The BCS functional for the free energy at temperature $T \geq 0$, with chemical potential $\mu \in \mathbb{R}$, interaction potential $V \in L^2(\mathbb{R}^d)$ and entropy

$$S(\Gamma) = -\frac{1}{2}\mathrm{Tr}_\Omega[\Gamma \log \Gamma + (1-\Gamma)\log(1-\Gamma)],$$

is then given by

$$\mathcal{F}(\Gamma) = \mathrm{Tr}_\Omega[(-\Delta - \mu)\gamma] + \int_{\Omega\times\mathbb{R}^d} V(x-y)|\alpha(x,y)|^2 \,\mathrm{d}(x,y) - TS(\Gamma),$$

where for $\Omega = [0,1]^d$ and Tr_Ω denotes the trace per unit volume. We describe periodic BCS states by operators Γ on $L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$ which satisfy $0 \leq \Gamma \leq 1$ and can be represented by 2×2 operator-valued matrices of the form

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1-\overline{\gamma} \end{pmatrix}, \tag{1}$$

where γ and α are periodic operators with period one. In (1), $\overline{\alpha} = C\alpha C$, where C denotes complex conjugation. We call Γ of the form (1) an *admissible* BCS state if $\mathrm{Tr}_\Omega(-\nabla^2+1)\gamma < \infty$ and denote the set of admissible BCS states by $\mathcal{D}$.

In this talk, we treat the question of whether there is translational symmetry breaking in the BCS model. More precisely, we study the minimization problem

$$\inf\{\mathcal{F}(\Gamma) \,|\, \Gamma \in \mathcal{D}\}$$

and, in particular, whether the infimum of $\mathcal{F}$ is attained by the minimizers of the translation-invariant BCS functional. In three dimensions, this is already known to be the case if $\hat{V} \leq 0$ (see [FHSS12, HS16]).

The translation-invariant BCS functional $\mathcal{F}^{\mathrm{ti}}$ is obtained from $\mathcal{F}$ by restricting the domain $\mathcal{D}$ of $\mathcal{F}$ to the set translation-invariant states. We denote the set of admissible translation-invariant BCS states by $\mathcal{D}^{\mathrm{ti}}$. The translation-invariant BCS functional then takes the form

$$\mathcal{F}^{\mathrm{ti}}(\Gamma) = \int_{\mathbb{R}^d} (p^2-\mu)\gamma(p)\,\mathrm{d}p + \int_{\mathbb{R}^2} V(x)|\alpha(x)|^2\,\mathrm{d}x - TS(\Gamma),$$

where the entropy S can in this case be written as

$$S(\Gamma) = -\frac{1}{2}\int_{\mathbb{R}^2} \mathrm{tr}_{\mathbb{C}^2}[\Gamma(p)\log\Gamma(p) + (1-\Gamma(p))\log(1-\Gamma(p))]\,\mathrm{d}p.$$

It was shown in [HHSS08, Theorem 1] that a certain linear operator determines the critical temperature. In order to define this linear operator, we introduce the function

$$K_T(p) = \frac{p^2 - \mu}{\tanh((p^2 - \mu)/(2T))}.$$

Then, $K_T(-i\nabla)$ defines an operator on $L^2(\mathbb{R}^d)$ given by multiplication by $K_T(p)$ in Fourier space. It is easy to see that the essential spectrum of $K_T + V$ is given by $\sigma_{\mathrm{ess}}(K_T + V) = [2T, \infty)$. The monotonicity of K_T in T allows us to define the critical temperature for the BCS functional as the value of T for which zero is the lowest eigenvalue of $K_T + V$, that is,

$$T_c = \inf\{T \geq 0 \,|\, K_T + V \geq 0\}.$$

Note that in two dimensions and for radial potential V the linear operator $K_T + V$ is rotation invariant and consequently all its eigenstates are of the form

$$\hat{\alpha}_\ell(p) = e^{i\ell\varphi}\sigma_\ell(p), \tag{2}$$

for some even $\ell \in 2\mathbb{Z}$, where $|p|$ and φ denote the polar coordinates of $p \in \mathbb{R}^2$ and σ_ℓ is a radial function. We use this fact to define critical temperatures on the sectors of angular momentum ℓ, $\mathcal{H}_\ell = \big\{f \in H^1(\mathbb{R}^2) | f \text{ is of the form (2)}\big\}$, by

$$T_c(\ell) = \inf\left\{T \geq 0 \,\middle|\, (K_T + V)\big|_{\mathcal{H}_\ell} \geq 0\right\}.$$

One easily sees that $T_c(\ell) = T_c(-\ell)$ and that

$$T_c = \max\left\{T_c(\ell) | \ell \in 2\mathbb{N}\right\}.$$

The following theorem shows that the translational symmetry in the BCS model is not broken for temperatures $T \in (T_c(\ell_1), T_c)$, if $T_c = T_c(\ell_0) > T_c(\ell_1) \geq T_c(\ell)$ for all $\ell \in 2\mathbb{N} \setminus \{\ell_0\}$. More precisely, if $\ell_0 = 0$, the periodic BCS functional has a unique (up to a phase) radial minimizer (γ_0, α_0) for $T \in (T_c(\ell_1), T_c)$. If $\ell_0 \neq 0$, the periodic BCS functional has two minimizers, namely $(\gamma_{\ell_0}, \alpha_{\ell_0})$ and $(\gamma_{\ell_0}, \alpha_{-\ell_0})$, with γ_{ℓ_0} radial and $\alpha_{\pm\ell_0}$ of the form (2).

Theorem 1. *Let $V \in L^2(\mathbb{R}^2)$ with $\hat{V} \in L^r(\mathbb{R}^2)$, where $r \in [1, 2)$, be radial and such that $T_c > 0$. Suppose that there exist $\ell_0, \ell_1 \in 2\mathbb{N}$ satisfying*

$$T_c(\ell_0) > T_c(\ell_1) \geq T_c(\ell)$$

for all $\ell \in \mathbb{N} \setminus \{\ell_0\}$. If

$$(\gamma_{\ell_0}, \sigma_{\ell_0}) \in \mathcal{D}_{\ell_0}$$

minimizes $\mathcal{F}_{\ell_0}$, then

$$(\gamma_{\ell_0}, \alpha_{\ell_0}) \text{ and } (\gamma_{\ell_0}, \alpha_{-\ell_0}) \in \mathcal{D}^{\mathrm{ti}},$$

where $\hat{\alpha}_{\pm\ell_0}(p) = e^{\pm i\ell\varphi}\sigma_{\ell_0}(p)$ are the only minimizers (up to a phase) of $\mathcal{F}$ for $T \in (T_c(\ell_1), T_c)$.

Remark 1. *It is shown in* [FL16]*, amongst other things, that for every* $\ell \in 2\mathbb{N}$ *one can find a radial potential such that the ground state of* $K_{T_c} + V$ *is of angular momentum* ℓ*. For small interaction potentials, the methods of* [FHNS07, HS08] *can be applied to determine the angular momentum* ℓ_0 *of the ground state of* $K_{T_c} + V$*. Furthermore, in the case of weak coupling, these methods allow one to verify that* $T_c(\ell_0) \neq T_c(\ell_1)$ *or rather characterize interaction potentials for which* $T_c(\ell_0) = T_c(\ell_1)$*.*

In the special case $\ell_0 = 0$, Theorem 1 also holds in three dimensions. We let $\mathcal{H}_3 = \{f \in H^1(\mathbb{R}^3, \mathrm{d}p) |\, f \text{ radial }\}$ and

$$T' = \inf \left\{ T \geq 0 \,\middle|\, (K_T + V)\big|_{(\mathcal{H}_3)^\perp} \geq 0 \right\},$$

which corresponds to $T_c(\ell_1)$ in the two dimensional case. We then have the following theorem.

Theorem 2. *Let* $V \in L^2(\mathbb{R}^3)$ *with* $\hat{V} \in L^r(\mathbb{R}^3)$ *for some* $r \in [1, 12/7)$ *be radial and such that* $T_c > 0$*. Assume that zero is a non-degenerate eigenvalue of* $K_{T_c} + V$*. Then, for* $T \in (T', T_c)$*, the only minimizer (up to a phase) of* $\mathcal{F}$ *is given by* (γ_0, α_0)*, where* γ_0 *and* α_0 *are radial functions.*

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Ground state construction of bilayer graphene

Ian Jauslin

(joint work with Alessandro Giuliani)

Graphene is a two-dimensional crystal of carbon atoms in a honeycomb lattice structure (see figure 1). It occurs naturally as the elementary building block of a common crystal, called graphite, which consists in many layers of stacked graphene, and was first isolated in 2004, by the group of A. Geim and K.Novoselov [NGe04].

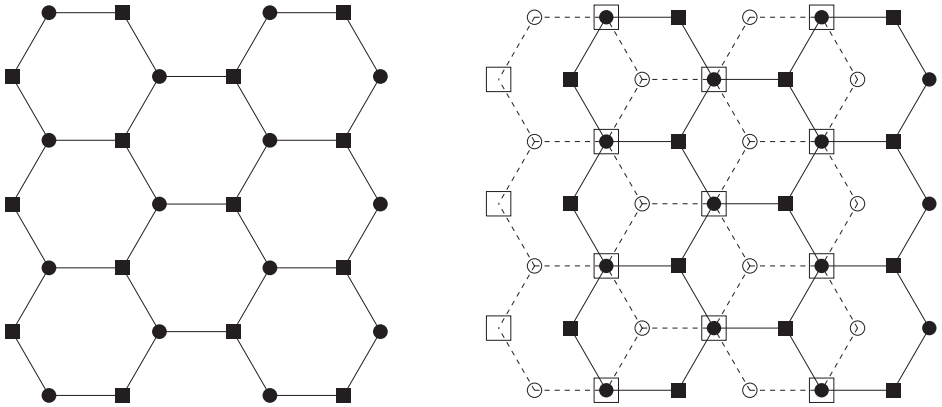

FIGURE 1. The lattice structure of monolayer graphene (left) and bilayer graphene (right). Full and empty circles and squares represent carbon atoms, and solid and dashed lines represent valence bonds. Dashed lines and empty circles and squares represent another graphene layer, which lies below the layer represented using solid lines and filled circles and squares. Even though the atoms are all carbon, they are rendered as circles or squares, depending on where they are located in the lattice, to emphasize the fact that there are 2 inequivalent atoms in graphene and 4 in bilayer graphene, which cannot be obtained from one another by translations.

It has, since, received a lot of attention for its uncommon electronic properties, namely the fact that electrons in graphene behave like *massless* Dirac Fermions, which ensures robust and efficient charge transport.

Here, we study bilayer graphene, which is obtained by stacking two graphene layers, as shown in figure 1. The model we consider, is one for the electrons in bilayer graphene, in which the atoms are fixed at the vertices of the lattice. The Hamiltonian is of the form

$$\mathcal{H} = \mathcal{H}_0 + V \tag{1}$$

where $\mathcal{H}_0$ is the kinetic term of the electrons, and V is their interaction.

The kinetic term is postulated to be that obtained by a *tight-binding* approximation, in which every electron is bound to an atom of the lattice, and may tunnel from one atom to another. Formally,

$$\mathcal{H}_0 = \sum_{x,y} \alpha_{x,y} c_y^\dagger c_x \tag{2}$$

where the sum runs over all pairs of atoms, c_x is the *annihilation operator* at x and $c_x^\dagger$ is the *creation operator* at y, and $\alpha_{x,y}$ is the so-called *hopping strength* of the tunneling process from the atom at x to the atom at y. The hoppings that we consider here are (see figure 2)

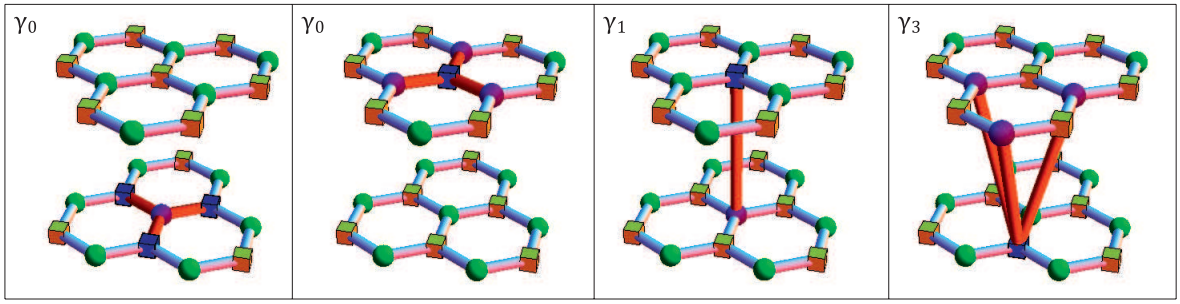

FIGURE 2. The different type of hoppings.

- $\alpha_{x,y} = \gamma_0 > 0$ if x and y belong to the same layer and are nearest neighbors among the atoms in that layer (which represents a hopping between a full circle and a full square, or an empty circle and an empty square, see figures 1 and 2)
- $\alpha_{x,y} = \gamma_1 > 0$ if x and y belong to different layers and are vertically aligned (which represents a hopping between a full circle and an empty square, see figures 1 and 2)
- $\alpha_{x,y} = \gamma_3 > 0$ if x and y belong to different layers, are not vertically aligned, and are nearest neighbors among the atoms that belong to different layers (which represents a hopping between an empty circle and a full square, see figures 1 and 2)
- $\alpha_{x,y} = 0$ otherwise.

Experimental values give [MNe07], in units in which $\gamma_0 = 1$, $\gamma_1 \approx 0.10$ and $\gamma_3 \approx 0.034$. Here, we will take $\gamma_1 \equiv \epsilon \ll 1$ and $\gamma_3 \sim \epsilon$.

The interaction term is a short-range force, which is thought of as a screened Coulomb interaction. Formally,

$$V = U \sum_{x,y} v(x-y) \left(c_x^\dagger c_x - \frac{1}{2} \right) \left(c_y^\dagger c_y - \frac{1}{2} \right) \tag{3}$$

in which U is the *interaction strength* and is small, and v is smooth and satisfies $|v(x-y)| \leqslant e^{-(\text{const.})\ |x-y|}$.

The non-interacting model, that is, the model with $U = 0$, is integrable, in that the Hamiltonian $\mathcal{H}_0$ can be explicitly diagonalized. As a consequence, one can compute a number of thermodynamic observables, like the specific free energy

$$f_0 := -\frac{1}{\beta|\Lambda|} \mathrm{Tr}(e^{-\beta \mathcal{H}_0}) \tag{4}$$

in which β is the inverse temperature and $|\Lambda|$ is the number of atoms in the crystal, and the two-point correlation function

$$\langle c_x^\dagger c_y \rangle_0 := \frac{\mathrm{Tr}(e^{-\beta \mathcal{H}_0} c_x^\dagger c_y)}{\mathrm{Tr}(e^{-\beta \mathcal{H}_0})} \tag{5}$$

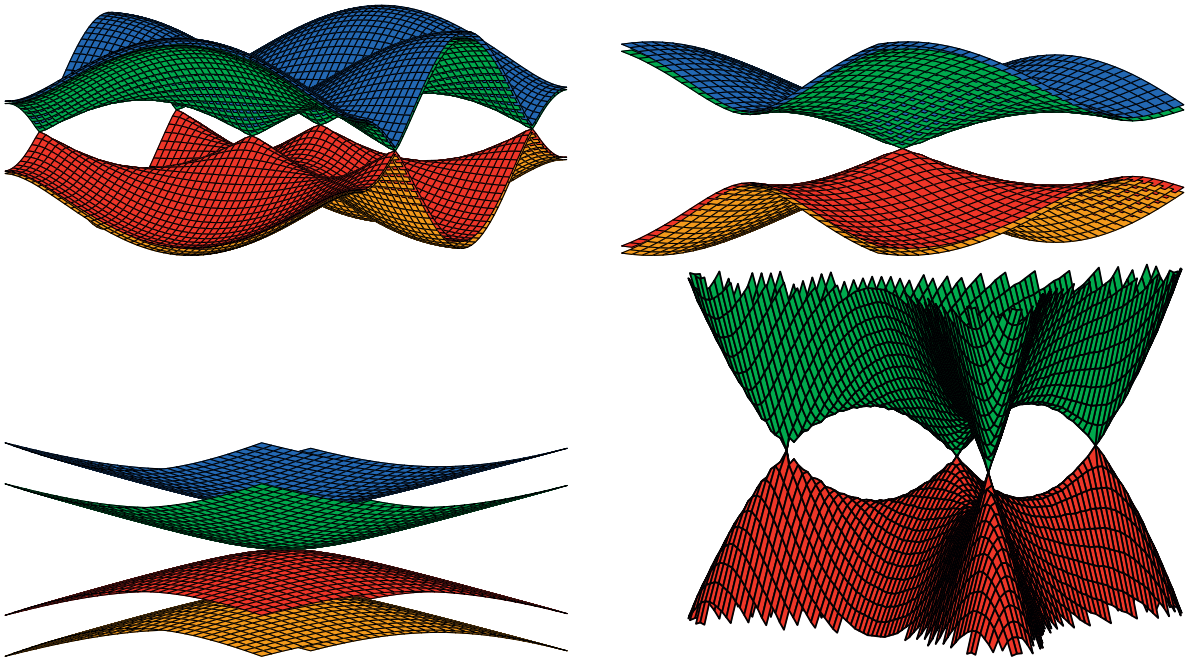

FIGURE 3. The band structure of bilayer graphene. Top-left: full bands, there are four bands because there are four inequivalent atoms in the lattice. Top-right: zoom around one of the singularities, which looks, at this scale, conical. Bottom-left: further zoom around a singularity, which turns out to be parabolic. Bottom-right: further zoom, which reveals three additional singularities, which are conical.

which, in this case, is the Green's function of the Hamiltonian $\mathcal{H}_0$.

Our main result [GJ16] is that, provided ϵ is sufficiently small and β and $|\Lambda|$ are sufficiently large (independently of the size of ϵ), then the free energy and two-point correlation functions of the interacting model are analytic functions of U, whose radius of convergence is positive, yet small, though independently so of ϵ, β and $|\Lambda|$. This has rather profound implications: first of all, this means that one can compute these important thermodynamic observables as convergent power series in U, and, in addition, that there are no singularities as a function of U, which means that there cannot be any phase transitions when introducing weak interactions.

The proof is based on the rigorous renormalization group methods introduced in [BG90], which have been used to compute the free energy and correlation functions of electrons in single layer graphene in [GM10]. The extension to bilayer graphene is non-trivial, since the qualitative properties of the non-interacting system are somewhat more involved. Specifically, the band structure of the non-interacting Hamiltonian has singularities at two quasi-momenta, and their behaviour around these singularities exhibits qualitative changes as one zooms in closer and closer, see figure 3.

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Dynamical crossing of an infinitely degenerate critical point

Gian Michele Graf

(joint work with Sven Bachmann, Martin Fraas)

A quantum evolution can be qualified as adiabatic or sudden in relation to the time dependence of the Hamiltonian. The canonical crossover behavior between these two cases is expressed for two-level systems by a formula about nearly avoided crossings found independently by Landau, Majorana, and Zener. I discussed the dynamical behavior in two variations of that situation: (a) in presence of decoherence (dephasing) and, more extensively, (b) for a model of a dynamical phase transition. The signature of the latter is that the discrete energy spectrum of the system becomes ever denser as the critical point is approached, where it turns to a continuum (or nearly so), just to return being discrete past that point. The model is solvable and exhibits the Kibble-Zurek mechanism, according to which excitations are generated by the transition out of the vacuum. Concretely, the model is a time-dependent harmonic oscillator and the solution is expressed in terms of squeezed states.

Emergent anyons in quantum Hall physics

Nicolas Rougerie

Anyons are by definition particles with quantum statistics different from those of bosons and fermions. They can occur only in low dimensions, 2D being the most relevant case for this proposal. They have hitherto remained hypothetical, but there is good theoretical evidence that certain quasi-particles occuring in quantum Hall physics should behave as anyons.

A possible description for anyons (so-called magnetic gauge picture) is to treat them as ordinary bosons or fermions coupled to magnetic flux tubes whose vector

potential is felt by all other particles in the system. This leads to a model in terms of a strongly interacting bosonic or fermonic Hamiltonian, which contains long-range (and rather peculiar) two- and three-body interactions. An important question is whether this effective Hamiltonian can emerge in some physically relevant scenario.

Recently, we have considered the case of tracer particles immersed in a so-called Laughlin liquid. We argued that, under certain circumstances, these become anyons, as made manifest by the emergence of the aforementioned Hamiltonian in an effective description of their motion.

The anyon Hamiltonian is notoriously hard to solve even in simple cases, and well-controled simplifications are highly desirable. In another paper we have discussed a possible mean-field approximation, leading to a one-particle energy functional with self-consistent magnetic field. The derivation can be made mathematically rigorous in some well-defined asymptotic limit.

The proposed talk will be based on recent joint works with Douglas Lundholm [1, 2]. I would also possibly mention works in progress with Michele Correggi and numerical simulations done by Romain Duboscq, dealing with the analysis of the mean-field functional derived in [1].

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Some Open Problems in Quantum Spin Systems

Bruno Nachtergaele

An after-dinner discussion on open problems in quantum spin systems was started by introducing two issues that are as stimulating as they are challenging.

The first problem concerns proving a positive, system size independent, lower bound for the spectral gap above the ground state of one of the two-dimensional models with $SU(2)$-invariant short-range interactions that are expected to have a unique ground state. The AKLT models on the hexagonal and square lattices are good candidates for this. On the hexagonal lattice this is a spin 3/2 model with a nearest neighbor interaction given by $P^{(3)}$, the orthogonal projection onto the spin 3 subspace of a pair of spin 3/2's. On the square lattice one has a spin 2 at each site and the nearest interaction is $P^{(4)}$, the orthogonal projection onto the spin 4 subspace of a pair of spin 3/2's. Both models were introduced by Affleck, Kennedy, Lieb, and Tasaki in [3]. For the model on the hexagonal lattice it was shown that the ground states for a broad class of boundary conditions the thermodynamic limit yields a unique state with exponential decay of correlations [10], which provides strong evidence for the uniqueness of the ground state and the existing of a spectral gap. For the model on the square lattice exponential

decay is proved only for periodic boundary conditions but there is also numerical evidence for a non-vanishing gap. A proof of the gap for either model has eluded all attempts so far. This is in stark contrast to the situation in one dimension, where one can prove the uniqueness of the ground state, exponential decay of correlations, and estimate the spectral gap for a large class of generalizations of the AKLT model [6, 11].

Homework #1: Prove that the two-dimensional AKLT models on the hexagonal and square lattices have a unique ground state in the thermodynamic limit and prove (or disprove) the existence of a spectral gap above the ground state. Note that it is known in general that a positive spectral gap implies exponential decay of correlations [12, 8].

The second problem poses the question of the existence of a universal many-body localized phase for strongly disordered quantum spin systems. As a prototypical model one may consider the Heisenberg model or one of its relatives with a translation-invariant nearest neighbor interaction $h = h^*$ and a random field of the form $\vec{B}_x(\omega) \cdot \vec{S}_x$ at each site x, with i.i.d. random variables B_x with values in $\mathbb{R}^3$. For the XY model in a random external field, Hamza, Sims, and Stolz showed dynamical localization expressed as a zero-velocity Lieb-Robinson bound [7]. The open problem is to generalize the zero-velocity Lieb-Robinson bounds to general disordered finite-range spin models on $\mathbb{Z}^d$. For $d \geq 2$, many-body-localization may be seen only at low energies, although in what sense is still a matter of debate (see, e.g., [4, 5]). Here is a conjecture.

Homework # 2: Let P_E denote the spectral projection onto the energy interval $[E_0, E_0 + E]$, with E_0 the ground state energy. Show that there exist constants $C, c, \mu > 0$, and $q \geq 0$, a function $g_E(t)$ such that for any pair of finite disjoint subsets $X, Y \subset \mathbb{Z}^d$, and observables A and B supported on X and Y, respectively, one has for $0 \leq E \leq c\mathrm{dist}(X, Y)^q$, the bound

$$\mathbb{E}(\|[\tau_t^\omega(P_E A P_E), B]\|) \leq C\|A\|\|B\||X|g_E(t)e^{-\mu d(X,Y)}, t \in \mathbb{R}. \tag{1}$$

Here, $\mathbb{E}$ denotes the expectation with respect to the disorder, τ_t^ω is the Heisenberg dynamics generated by the random Hamiltonian, and one is interested in showing the inequality with a function $g_E(t)$ of moderate growth. E.g., a good example would be $g_E(t) \sim |t|^\alpha$, for some $\alpha \geq 0$. The standard Lieb-Robinson bound for systems with a bounded finite-range interaction holds with $g_E(t) = C\exp(v|t|)$, where $v > 0$ is a bound for the Lieb-Robinson velocity. For translation invariant systems ballistic propagation, i.e., with a positive velocity, is in general expected to occur. Therefore, a bound of Lieb-Robinson type with $v = 0$ can be an indicator of dynamical localization. In particular, an estimate of the form (1) with any function g_E which grows strictly slower than exponential would provide non-trivial new information.

It is worth noting that, as was the case with the first problem, the situation in one dimension is better understood in several respects than the problem in two and higher dimensions. First, in partial similarity to the case of one-body Anderson localization, many-body localization is expected to occur at all energies when the

disorder strength exceeds a critical value, i.e., one can set $P_E = \mathbb{1}$. Second, we can learn much from special results for exactly solvable one-dimensional models such as the XY chain [2], the quantum Ising chain [9], and Tonks-Girardeau gas [13]. See [1] for a survey of these results.

Both 'homework' problems are of direct relevance for current research in condensed matter physics. Numerous questions from the audience led to a lively discussion on these two problems and related topics.

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The causal action principle and quantum field theory

Felix Finster

The theory of causal fermion systems is an approach to describe fundamental physics. It gives quantum mechanics, general relativity and quantum field theory as limiting cases and is therefore a candidate for a unified physical theory (see [3] or the survey articles [6, 1]). From the mathematical perspective, causal fermion systems provide a general framework for desribing and analyzing non-smooth geometries (see [4, 5] or the introduction in [3, Section 1.1.]). The dynamics is described by the so-called causal action principle (see [3, §1.1.1 and Section 1.4]).

In the talk, I focus on how the dynamics of causal fermion systems can be described effectively with Fock spaces. To this end, after introducing the causal action principle in the simplest possible setting for a system of spinorial wave functions in Minkowski space, I explain the concept of microscopic mixing as introduced in [2] (see also [3, §1.5.3]). A few constructions are mentioned which will be used in [7]. A few open problems are discussed.

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Correlation inequalities for the quantum XY model

Daniel Ueltschi

(joint work with Costanza Benassi, Benjamin Lees)

Correlation inequalities were initially proposed by Griffiths [4] and they have been an invaluable tool in the study of classical spin systems. We discuss generalisations that apply to quantum XY models [1]. They extend an earlier result of Gallavotti [2]. In fact, we discovered recently that our inequalities had already been proposed 40 years ago by Suzuki [6]. His complicated proof was later simplified by Pearce [5]; our independent proof is essentially a clean version of Pearce's, and is also based on Ginibre's method [3].

These correlation inequalities are elegant and potentially useful. It is a pity that the subject has been dormant for so long, and that important results have been largely forgotten. It therefore seemed useful to discuss them in Oberwolfach and to devote a short report on them.

Let Λ denote the (finite) set of sites that host the spins. The Hilbert space of the model is $\mathcal{H}_\Lambda = \otimes_{x\in\Lambda}\mathbb{C}^2$. Let S^i, $i = 1, 2, 3$ denote usual spin operators (Pauli matrices) on $\mathbb{C}^2$, and let $S^i_x = S^i \otimes \mathbb{1}_{\Lambda\setminus\{x\}}$ be the spin operator at site x. We consider the hamiltonian

$$H_\Lambda = -\sum_{A\subset\Lambda} \Big(J^1_A \prod_{x\in A} S^1_x + J^2_A \prod_{x\in A} S^2_x \Big). \tag{1}$$

Here, J^i_A is a nonnegative coupling constant for each subset of $A \subset \Lambda$ and each spin direction $i \in \{1, 2\}$. The expected value of an observable a (that is, an operator

on $\mathcal{H}_\Lambda$) in the Gibbs state with hamiltonian H_Λ is

$$\langle a \rangle = \frac{1}{Z(\Lambda)} \mathrm{Tr}\, a\, \mathrm{e}^{-H_\Lambda}\,, \tag{2}$$

where the normalisation $Z(\Lambda)$ is the partition function $Z(\Lambda) = \mathrm{Tr}\ \mathrm{e}^{-H_\Lambda}$. Traces are taken in $\mathcal{H}_\Lambda$. We also consider Schwinger functions that are defined for $s \in [0,1]$ by

$$\langle a; b \rangle_s = \frac{1}{Z(\Lambda)} \mathrm{Tr}\, a\, \mathrm{e}^{-sH_\Lambda}\, b\, \mathrm{e}^{-(1-s)H_\Lambda}\,. \tag{3}$$

Theorem 1. *Assume that $J_A^i \geq 0$ for all $A \subset \Lambda$ and all $i \in \{1,2\}$. Then for all $A, B \subset \Lambda$, and all $s \in [0,1]$, we have*

$$\Big\langle \prod_{x\in A} S_x^1; \prod_{x\in B} S_x^1 \Big\rangle_s - \Big\langle \prod_{x\in A} S_x^1 \Big\rangle \Big\langle \prod_{x\in B} S_x^1 \Big\rangle \geq 0;$$
$$\Big\langle \prod_{x\in A} S_x^1; \prod_{x\in B} S_x^2 \Big\rangle_s - \Big\langle \prod_{x\in A} S_x^1 \Big\rangle \Big\langle \prod_{x\in B} S_x^2 \Big\rangle \leq 0.$$

A consequence of Theorem 1 is the monotonicity of certain spin correlations with respect to the coupling constants:

Corollary 2. *Under the same assumptions as in the above theorem, we have for all $A, B \subset \Lambda$ that*

$$\frac{\partial}{\partial J_A^1} \Big\langle \prod_{x\in B} S_x^1 \Big\rangle \geq 0;$$
$$\frac{\partial}{\partial J_A^1} \Big\langle \prod_{x\in B} S_x^2 \Big\rangle \leq 0.$$

The first inequality states that correlations increase when the coupling constants increase (in the same spin direction). The second inequality is perhaps best understood classically; if the first component of the spins increases, the other components must decrease because the total spin is conserved. Corollary 2 follows immediately from Theorem 1 since

$$\frac{1}{\beta} \frac{\partial}{\partial J_A^i} \Big\langle \prod_{x\in B} S_x^j \Big\rangle = \int_0^1 \Big[\Big\langle \prod_{x\in B} S_x^j; \prod_{x\in A} S_x^i \Big\rangle_s - \Big\langle \prod_{x\in B} S_x^j \Big\rangle \Big\langle \prod_{x\in A} S_x^i \Big\rangle \Big] \mathrm{d}s. \tag{4}$$

These correlation inequalities allow to compare the critical temperatures of the quantum XY model with that of Ising. Indeed, let us define the magnetisation m_Λ by

$$m_\Lambda(\beta)^2 = \Big\langle \frac{1}{|\Lambda|^2} \sum_{x,y\in\Lambda} S_x^1 S_y^1 \Big\rangle, \tag{5}$$

where the expectation is taken with respect to the Gibbs state with hamiltonian βH_Λ. Let $m(\beta)$ denote the infinite-volume limit, and let

$$T_\mathrm{c} = \sup\{\tfrac{1}{\beta} : m(\beta) > 0\}. \tag{6}$$

It follows from Corollary 2 that $m(\beta)$ is decreasing with respect to J_A^2, so that

$$T_{\mathrm{c}}^{\mathrm{XY}} \leq T_{\mathrm{c}}^{\mathrm{Ising}}. \tag{7}$$

The latter refers to an Ising model with coupling constants $2^{-|A|}J_A^1$, because of factors $1/2$ present in Pauli matrices. In the case of the three-dimensional cubic lattice with nearest-neighbour interactions, numerical calculations have revealed that $T_{\mathrm{c}}^{\mathrm{XY}} = 1.01$ and $T_{\mathrm{c}}^{\mathrm{Ising}} = 1.13$. These values are quite close.

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Spectral cluster bounds for orthonormal functions

Julien Sabin

(joint work with Rupert L. Frank)

Let (M, g) a smooth, compact, boundaryless Riemannian manifold of dimension $N \geqslant 2$, and denote by Δ_g the (non-negative) Laplace-Beltrami operator on M. A general question in semi-classical analysis is to describe the behaviour of eigenfunctions of Δ_g corresponding to large eigenvalues. More precisely, one is interested in the concentration properties of these eigenfunctions: do they concentrate around some points or submanifolds of M, or do they rather spread evenly on M? One extreme example is given by the sphere, where there are spherical harmonics which concentrate on poles or on an equator. Such concentration can be measured by looking at the growth of the L^p norms of these functions, for $p > 2$ (assuming that they are L^2-normalized). Indeed, such spherical harmonics have growing L^p norms as the eigenvalue gets bigger. A radically different phenomenon happens on the torus $\mathbb{T}^2$, where eigenfunctions are uniformly bounded in L^4 regardles s of the eigenvalue. One thus sees that the growth of L^p norms of eigenfunctions is very dependent of the underlying geometry.

If one looks at functions in *spectral clusters* rather than eigenfunctions, that is functions in the space

$$E_\lambda := \Pi_\lambda L^2(M), \quad \Pi_\lambda = \mathbb{1}(\lambda^2 \leqslant \Delta_g < (\lambda+1)^2),$$

it is a striking result of Sogge [5] that we have a uniform behaviour regardless of the geometry: he proved that for $2 \leqslant p \leqslant \infty$, there exists $C > 0$ such that for all

$\lambda > 0$ and for all $f \in E_\lambda$ one has

$$\|f\|_{L^p(M)} \leqslant C\lambda^{s(p)} \|f\|_{L^2(M)},$$

with

$$s(p) = \begin{cases} N\left(\frac{1}{2} - \frac{1}{p}\right) - \frac{1}{2} & \text{if } \frac{2(N+1)}{N-1} \leqslant p \leqslant \infty \\ \frac{N-1}{2}\left(\frac{1}{2} - \frac{1}{p}\right) & \text{if } 2 \leqslant p \leqslant \frac{2(N+1)}{N-1}. \end{cases}$$

Furthermore, he showed that on *any* M, these bounds (that is, the powers of λ) are optimal: there are functions that saturate the growth in λ given by these bounds. What makes spectral clusters more 'universal' than eigenspaces is explained by the Weyl law with a sharp remainder term, due to Avakumović [1], Levitan [4] and vastly generalized by Hörmander [3, Thm. 1.1], which implies that

$$\dim E_\lambda \sim \lambda^{N-1},$$

also regardless of the geometry, while for instance on the sphere or on the torus, the degeneracies of eigenvalues are of completely different order.

We are interested in the following question: can we say something about the concentration of orthonormal functions on M? More precisely, given a subspace $Q \subset E_\lambda$, and (f_j) an orthonormal basis of Q, define its density as

$$\rho^Q := \sum |f_j|^2.$$

We discuss the concentration properties of the density ρ^Q, depending on the dimension of Q. When $\dim Q = 1$, we are in the context of the result of Sogge since we are dealing with a single function. In the other extreme case where $Q = E_\lambda$, it is also a consequence of the pointwise Weyl law that

$$\left\|\rho^{E_\lambda}\right\|_{L^\infty(M)} \lesssim \lambda^{N-1}.$$

Hence, for any $p \geqslant 1$ one has

$$\lambda^{N-1} \sim \dim E_\lambda = \left\|\rho^{E_\lambda}\right\|_{L^1} \leqslant \left\|\rho^{E_\lambda}\right\|_{L^p} \leqslant \left\|\rho^{E_\lambda}\right\|_{L^\infty} \lesssim \lambda^{N-1},$$

meaning that all L^p-norms of ρ^{E_λ} are of the same order, a symptom of *non-concentration* (or spreading) of ρ^{E_λ}.

We thus see that for $\dim Q = 1$, one has concentration of ρ^Q while for $Q = E_\lambda$, one has no concentration. In [2], we show how the transition between concentration and non-concentration occurs: for any $2 \leqslant p \leqslant \infty$ there exists $C > 0$ such that for any $\lambda > 0$ and any $Q \subset E_\lambda$ we have

$$\left\|\rho^Q\right\|_{L^{p/2}(M)} \leqslant C\lambda^{2s(p)}(\dim Q)^{1/\alpha(p)},$$

with $\alpha(p)$ satisfying

$$2s(p) + \frac{N-1}{\alpha(p)} = N - 1.$$

When $\dim Q = 1$, we recover the result of Sogge while for $Q = E_\lambda$, the estimate is sharp by Weyl's law and the relation defining $\alpha(p)$.

We also discuss a stronger notion of optimality for our result. Namely, pick any sequence (r_λ) such that $1 \ll r_\lambda \ll \dim E_\lambda$. Does there exists subspaces $Q_\lambda \subset E_\lambda$ with $\dim Q_\lambda \sim r_\lambda$, such that

$$\left\|\rho^{Q_\lambda}\right\|_{L^{p/2}(M)} \geqslant c\lambda^{2s(p)} r_\lambda^{1/\alpha(p)},$$

for some $c > 0$ independent of λ? We prove such a result for $M = \mathbb{S}^2$, but a construction in the general case remains open.

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A class of asymmetric gapped Hamiltonians on quantum spin chains and its characterization

Yoshiko Ogata

In this talk, I discussed about the possibility to have a simple representation of ground state structures, in gapped systems. For bulk ground state, Matsui showed the following: if 1. Hamiltonian is gapped, 2. the bulk ground state is unique, 3. Hamiltonian is frustration free, and 4. the ground state degeneracy is uniformly bounded from above, then the unique bulk ground state is a matrix product state, given by a primitive n-tuple of matrices. In this talk, we considered the "edge-version" of this. We consider the following system. 1. Hamiltonian is gapped, 2. the bulk ground state is unique, 3. Hamiltonian is frustration free, 4. the ground state degeneracy is uniformly bounded from above, 5. the boundary effect decays exponentially fast, and 6. the distance from any edge ground state and its space translation gets smaller than 2 for some translation. We showed that for such a system, there exists an n-tuple of matrices, with which the ground state on finite/infinite intervals can be represented. This n-tuple has a special form which I call Class A.

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On the Bogolubov-de Gennes (and Hartree-Fock-Bogolubov) Equations

Israel Michael Sigal

The Bogolubov-de Gennes and Hartree-Fock-Bogolubov equations describe quantum phenomena on macroscopic and mesoscopic scales, namely, the superconductivity and superfluidity. They are among the latest additions to the family of important effective equations of mathematical physics. Together with the Hartree-Fock and Ginzburg-Landau equations, they are the quantum members of this illustrious family consisting of such luminaries as the heat, Poisson, Euler, Navier-Stokes and Boltzmann equations.

There are still many fundamental questions about these equations which are completely open. Generally, there are three types of questions one would like to ask about an evolution equation:

- Derivation;
- Well-posedness;
- Special solutions (say, stationary solutions or traveling waves) and their stability.

Some rigorous results on the derivation of the Hartree-Fock-Bogolubov (HFB) equations can be found in [7, 10, 11]. The well-posedness (or existence) for the time-dependent HFB equations for confined systems (see below) was proven in [1]. The well-posedness theory for the time-dependent Bogolubov-de Gennes (BdG) equations is largely open and is addressed in [3]. Some important stationary solutions of the BdG and HFB equations were found in [8] and [12, 13, 1], respectively.

In this talk I discussed recent work on the BdG and HFB equations, jointly with Li Chen ([4, 5]) and Volker Bach, Sébastien Breteaux, Thomas Chen and Jürg Fröhlich ([1]), respectively. For the time sake, I talked mainly about the BdG equations, which present an equivalent formulation of the BCS theory.

The three works dominate the subject, [2, 8, 6] (see for an excellent, recent review [9]). The results I discussed are complementary to this work. The hart of the talk dealt with special solutions of Bogoliubov-de Gennes equations: normal, superconducting and mixed or intermediate states. For type II superconductors, the latter consist of vortices and vortex lattices. An important role here are played by the magnetic flux quantization and the critical magnetic fields. Below, I list the topics I prepared for the talk.

- Quasifree reduction
- For time reasons, we concentrate on Bogolubov-de Gennes (BdG) equations.
- Bogoliubov-de Gennes equations
- Symmetries of the Bogoliubov-de Gennes equations
- Hamiltonian structure and conservation laws
- Stationary Bogoliubov-de Gennes equations
- Free energy
- Special solutions of Bogoliubov-de Gennes equations

- Hamiltonian structure and conservation laws.
- Critical temperature T_c.
- Critical magnetic fields.
- Type I and II superconductors.

In the actual talk, I covered, to a large extend, topics 1–4 and 6–8, but I did not manage to get to the remaining topics, most importantly, the critical temperature and the critical magnetic fields, which play a central role in the subject. An expanded version of the talk can be found on arXiv.

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The Energy of Heavy Atoms

Heinz Siedentop
(joint work with Michael Handrek)

We consider heavy atoms in a physically realistic model, namely we use the no-pair Hamiltonian in the Furry picture. We prove that the ground-state energy $E(Z)$ of heavy atoms, i.e., large atomic number Z and the quotient $\gamma := Z/c$ fixed (c speed of light), has the asymptotic expansion

$$E(Z) = e_{\mathrm{TF}} Z^{7/3} + (\frac{1}{2} + s(\gamma))Z^2 + o(Z^2).$$

Here e_{TF} is the Thomas-Fermi energy of the non-relativistic hydrogen atom. The correction term to the non-relativistic Scott correction $Z^2/2$ is given by the sum of the differences of the Dirac and Schrödinger eigenvalues of the hydrogenic atom with coupling constant γ all divided by γ^2. The error term is uniform on any compact subinterval of $[0, 1)$. (See [1] for details.)

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Recent studies of anyons

Douglas Lundholm

(joint work with Simon Larson, Nicolas Rougerie, Jan Philip Solovej)

Quantum systems confined to planar geometries may exhibit effective particles with unusual statistics, called anyons. These can be modeled as identical particles (bosons or fermions) in 2D with magnetic flux attached to them. In my talk I reviewed recent progress on the understanding of the anyon gas, focusing on universal lower bounds for the ground-state energy for the ideal and the extended gas by means of magnetic Hardy inequalities and local exclusion principles.

Ideal anyons may be characterized by a single statistics parameter $\alpha \in [0, 2)$ defining the phase factor $e^{i\alpha\pi}$ for the many-body wave function under two-particle exchange, with $\alpha = 0$ or 1 corresponding to bosons or fermions, respectively. In work with Solovej [8] it was found that the ideal anyon gas obeys a non-trivial lower bound for its ground-state energy depending on α via the quantity

$$\alpha_* := \inf_{p,q\in\mathbb{Z}} |(2p+1)\alpha - 2q| = \begin{cases} 1/\nu, & \text{if } \alpha = \mu/\nu \in \mathbb{Q} \text{ reduced, } \mu \textbf{ odd}, \nu \geq 1, \\ 0, & \text{otherwise.} \end{cases}$$

This bound has subsequently been supplemented and improved in further work with Solovej [9, 10] and recent work with Larson [1] to the bounds

$$2C_1\alpha_* \leq C_1(j'_{\alpha_*})^2 \leq e(\alpha, 0) \leq C_2,$$

for some universal constants $C_1, C_2 > 0$, where $e(\alpha, 0)$ denotes the ground-state energy per particle and unit density of the homogeneous ideal anyon gas. Comparing with bosons and fermions, one has $e(0, 0) = 0$ and $e(1, 0) = 2\pi$. The expressions α_* and j'_{α_*} respect the periodicity of α and are plotted in Figure 1. Also possible matching upper bounds using trial states have been discussed in [9, 2, 3], although not yet with rigorous implications.

Extended anyons are more realistic [6, 7] magnetically interacting particles with smeared out magnetic flux. These have an additional dimensionless density parameter $\gamma \geq 0$ defined as the ratio of the size of the particles to the average interparticle distance. In the work [1] with Larson we have proved lower bounds to the ground-state energy $e(\alpha, \gamma)$ per particle and unit density of such an extended homogeneous anyon gas (see Figure 2).

One of the mathematical tools that is useful for the study of such interacting many-body systems is a new family of Lieb–Thirring inequalities, which is based on a general local formulation of the exclusion principle and has been developed together with Nam, Portmann and Solovej [8, 10, 5, 4].

See also the talk of Rougerie concerning the emergence of anyons and of an effective self-interacting one-body model for almost-bosonic anyons, i.e. for $\alpha \to 0$ under certain conditions on γ.

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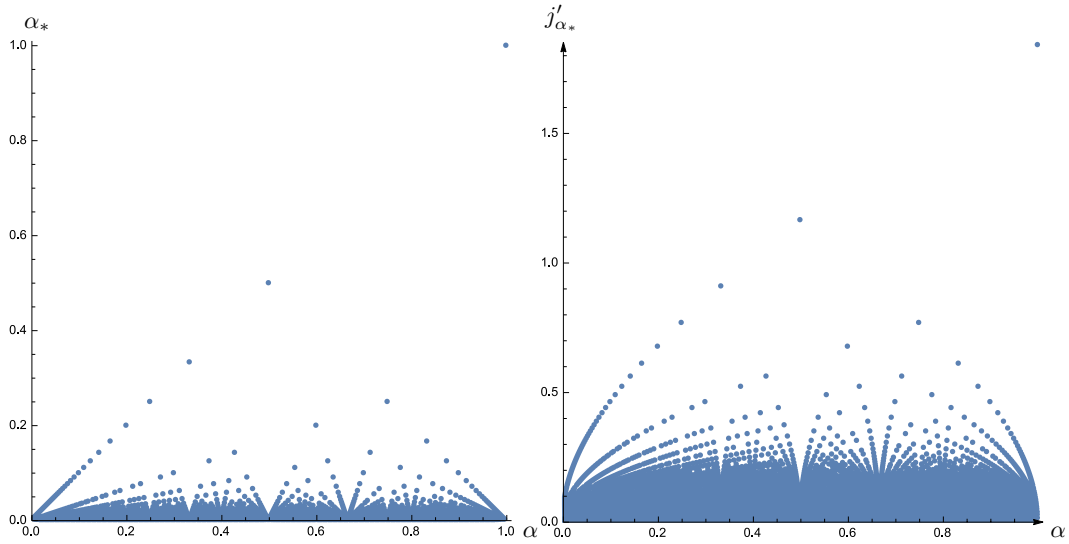

FIGURE 1. Plots of α_* respectively j'_{α_*} for $0 \leq \alpha \leq 1$. These can be continued to all $\alpha \in \mathbb{R}$ using periodicity and reflection (complex conjugation) symmetry.

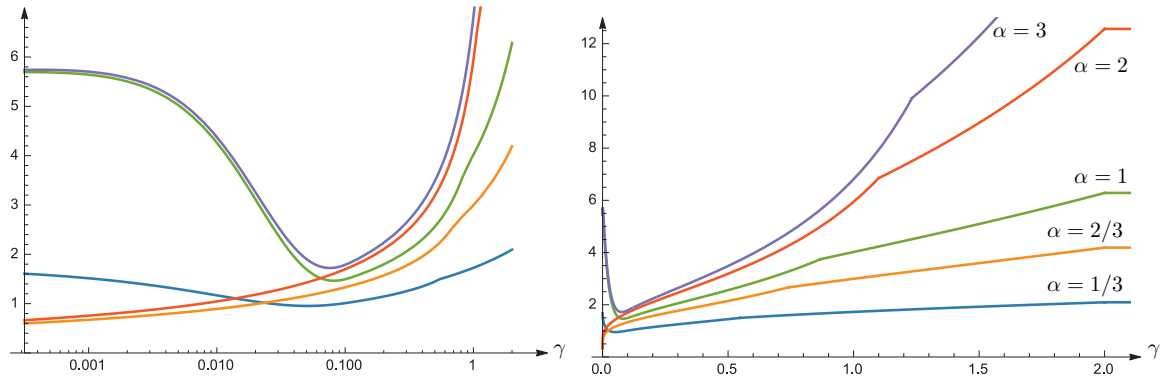

FIGURE 2. Current universal lower bounds for the g.s. energy $e(\alpha, \gamma)$ (from [1] with scales chosen for purposes of illustration) of the extended anyon gas as a function of the statistics parameter α and the dimensionless density parameter $\gamma \geq 0$. Left: logarithmic scale, displaying an α_*-dependent behavior in the dilute limit $\gamma \to 0$. Right: general behavior over the full range, with a linear dependence in the dense regime $\gamma \gtrsim 1$.

Two-dimensional electrostatics and the density of quantum fluids

JAKOB YNGVASON
(joint work with Elliott H. Lieb, Nicolas Rougerie)

The Nobel prize winning Laughlin state of electrons in the lowest Landau level [2] is one of the basic constructs in our physical understanding of the Fractional Quantum Hall Effect. It has long been plausibly assumed that it is not possible to increase the density of electrons in this level while simultaneously retaining the correlations built in the Laughlin state. In the talk a mathematically rigorous proof [3, 4] of this physically important rigidity of the Laughlin state was outlined.

A Laughlin wave function has the form

$$\Psi^{(\ell)}_{\text{Laugh}}(z_1, \dots, z_N) = C_{N,\ell} \prod_{i<j} (z_i - z_j)^\ell e^{-\sum_{i=1}^N |z_i|^2/2} \tag{1}$$

with ℓ a positive integer, $z_i \in \mathbb{C} \simeq \mathbb{R}^2$, and $C_{N,\ell}$ is a normalization constant. For fermions, ℓ is odd and ≥ 3, while for bosons $\ell \geq 2$ is even. Bosonic functions of this type are potentially relevant for cold atomic gases in artificial magnetic fields.

In order to allow for a response of the Laughlin state to perturbations generated by impurities or external potentials we consider normalized wave functions of the form

$$\Psi_F(z_1, \dots, z_N) = F(z_1, \dots, z_N) \Psi^{(\ell)}_{\text{Laugh}}(z_1, \dots, z_N) \tag{2}$$

with F analytic and symmetric under exchange of the z_i. This is the most general type of a wave function that minimizes the magnetic kinetic energy by staying in the lowest Landau level and at the same time avoids repulsive interactions between the particles by vanishing as $(z_i - z_j)^\ell$ as z_i and z_j come together.

The 1-particle density of the wave function Ψ_F is, by definition,

$$\rho^{(1)}(z) = N \int |\Psi_F(z, Z')|^2 dZ' \tag{3}$$

with $Z' = (z_2, \ldots, z_N)$. For $F = 1$, i.e., the wave function (1), Laughlin argued in [2] that the density distribution has, for large N, the form of a circular droplet of radius $\sqrt{\ell N}$ where the density takes the constant value $(\pi\ell)^{-1}$. Rigorous mean-field analysis [7, 8, 5, 6] has confirmed this result and extended the density bound to functions Ψ_F with special pre-factors F. The density bound is a fundamental property expressing the rigidity of the Laughlin quantum liquid and it is important to prove it for *general* pre-factors F.

Numerical studies [1] indicate that a pointwise density bound cannot be expected for finite N but we prove that it holds in a suitable weak sense for large N. In order to study the $N \to \infty$ limit it is convenient to change variables and consider the scaled N-particle probability density

$$\mu^{(N)}(z_1, \ldots, z_N) := N^N \left| \Psi_F \left(\sqrt{N} z_1, \ldots, \sqrt{N} z_N \right) \right|^2 \tag{4}$$

corresponding to the wave-function (2). Integrating over the $N - 1$ variables $Z' = (z_2, \ldots, z_N)$ we obtain the scaled 1-particle probability density

$$\mu^{(1)}(z) = \int \mu^{(N)}(z, Z') dZ'. \tag{5}$$

The 1-particle density (3) is then $\rho^{(1)}(z) = \mu_F^{(1)}(N^{-1/2}\, z)$.

For an external potential V we define

$$E_\ell(V, N) = \inf \left\{ \int V(z) \mu^{(1)}(z)\, dz \ : \Psi_F \text{ of the form (2)} \right\}. \tag{6}$$

We also define the 'bathtub energy' corresponding to the density bound $(\pi\ell)^{-1}$ as

$$E_V^{\mathrm{bt}}(\ell) := \inf \left\{ \int V(z) \rho(z)\, dz \,\middle|\, 0 \le \rho \le \frac{1}{\pi\ell},\ \int \rho = 1 \right\}. \tag{7}$$

Our main result can be stated as follows.

Theorem. *For $V \in C^2(\mathbb{R}^2)$, increasing at infinity,*

$$\liminf_{N \to \infty} E_\ell(V, N) \ge E_\ell^{\mathrm{bt}}(V). \tag{8}$$

A bound of the type (8) for general F was first proved in [6] but with ℓ replaced by $\ell/4$. The proof [3, 4] of the optimal bound is based on a generalization of the potential theoretic arguments used in [6]

As in the previous work [7, 8, 5, 6], the first step in the proof is to write the N-particle probability density as a Boltzmann-Gibbs factor

$$\mu^{(N)}(z_1, \ldots, z_N) = \mathcal{Z}_N^{-1} \exp\left(-\tfrac{1}{T} H(z_1, \ldots, z_N) \right), \tag{9}$$

with temperature $T = N^{-1}$ and the Hamiltonian

$$H(z_1, \ldots, z_N) = \sum_{j=1}^{N} |z_j|^2 - \frac{2\ell}{N} \sum_{i<j} \log |z_i - z_j| + W(z_1, \ldots, z_N) \tag{10}$$

where

$$W(z_1, \ldots, z_N) = -\frac{2}{N} \log \left| F\left(\sqrt{N} z_1, \ldots, \sqrt{N} z_N\right) \right|. \tag{11}$$

The density $\mu^{(N)}$ minimizes the free energy functional corresponding to this Hamiltonian and the temperature $T = N^{-1}$.

The main step towards the density bound for $\mu^{(1)}$ is the establishment of an upper bound on the local density of points in a minimizing configuration of the Hamiltonian H:

Proposition. *If $(z_1^0, \ldots, z_N^0)$ is a minimizing configuration for H then the local density of the points z_i^0 is everywhere bounded above by $N(\pi\ell)^{-1}(1+o(1))$ for large N.*

This bound is obtained by studying an auxiliary Thomas-Fermi energy functional of a special kind. This functional depends on the density distribution of a fictitious "electron" cloud that interacts with itself and with "nuclei" at fixed positions through a two-dimensional Coulomb potential. The density of the "electrons" is required to lie between 0 and 1. The functional captures the neutralizing effect of the quadratic first term of H which can be interpreted as the electrostatic potential of a uniform background charge competing with the logarithmic Coulomb repulsion of the second term. The last term of H, $W(z_1, \ldots, z_N)$, is plurisuperharmonic because F is analytic. Potential theoretic arguments imply that a minimizing configuration $(z_1^0, \ldots, z_N^0)$ for H has a certain *exclusion property*: No z_i^0 can lie in a set $\Sigma^{\mathrm{TF}}(z_1^0, \ldots, z_{i-1}^0, z_{i+1}^0, \ldots, z_N^0)$ that is defined as the support of the electron cloud neutralizing the "nuclei" at the positions z_j^0, $j \neq i$ in the Thomas-Fermi model. Once this has been established the proof of the Proposition is completed by showing that every configuration having this exclusion property satisfies the required density bounds.

The study of the Thomas-Fermi model requires some effort because it is not of standard type. The details are given in [3, 4].

Besides the Proposition the effect of the entropic part of the free energy has to be taken into account. Here it is crucial that the temperature scales as N^{-1} which implies that the main contribution to the Gibbs state (9) comes from minimum configurations of the Hamiltonian H. As in [6] the bound (8) is proved by perturbing H with εU where U is a suitable modification of V and using a Feynman-Hellmann type argument.

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Can quantum dynamics be described by the density alone?

Jonas Lampart

(joint work with Søren Fournais, Mathieu Lewin, Thomas Østergaard Sørensen)

Density Functional Theory proposes methods to calculate, or approximate, the one-particle density of an N-particle quantum system directly – without first calculating the full N-body wave-function. Such methods are popular computational tools, due to their moderate cost. This leads to the question how much information about the full system is contained in the one-body density. More specifically, one may ask which quantities in the full system may be reconstructed from the density, given some a priori information, such as what kind of particles constitute the system. We will address this question here for a time-dependent problem. We assume that the quantum system in question consists of N fermions or bosons, and that its time-dependent Hamiltonian, defined on $L^2_{\mathrm{a}}(\mathbb{R}^{dN})$ or $L^2_{\mathrm{s}}(\mathbb{R}^{dN})$, is of the form

$$H_V(t) := H_0 + \sum_{i=1}^{N} V(x_i, t)\,,$$

with

$$H_0 = \sum_{i=1}^{N} -\Delta_{x_i} + V_0(x_i) + \sum_{1\leq i<j\leq N} W(x_i - x_j)\,.$$

The conditions on the potentials V, V_0, W on $\mathbb{R}^d$ will be discussed in detail later. We consider V_0 and W as quantities which are a priori known. If, for example, the particles in our system are electrons they will interact via Coulomb forces $W(x) = 1/|x|$. In the time-independent case of ground-states, it is known that for $V, V_0, W \in L^{d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ (for $d \geq 3$) the potential V is uniquely determined

by the ground state density

$$\rho(x) = N \int |\psi(x, y_1, \ldots, y_{N-1})|^2 \, dy_1 \cdots dy_{N-1} \,.$$

That is, if $V_1, V_2 \in L^{d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ differ by more than a constant and have ground states ψ_1, ψ_2, then the corresponding one-particle densities ρ_1 and ρ_2 are different. Equivalently, if $\rho_1 = \rho_2$, then $V_1 = V_2 + \text{const.}$. This statement is known as the Hohenberg-Kohn Theorem [HK64], see Lieb [Li83] for a proof.

Runge and Gross [RG84] have argued that a similar property should hold for time dependent systems. That is, the time-dependent density $\rho(x,t)$ should determine the external potential $V(x,t)$ up to a constant $C(t)$ if the system starts with a given initial wave-function ψ_0. The argument is based on an order-by order analysis of the Taylor series in time of the density $\rho(x,t)$ obtained from the solution $\psi(t)$ of the Schrödinger equation with initial condition ψ_0 and time-dependent Hamiltonian H_V. Such an expansion clearly relies on smoothness of ρ and V w.r.t. the time-variable, which cannot always be guaranteed. This has recently led to a discussion in the physical-chemistry literature regarding the validity of the argument, see e.g. [YB13].

The first mathematical work concerning this question is our article [FLLS16], where we discuss the possibility of choosing a set $\mathcal{I}$ of admissible initial conditions and $\mathcal{V}$ of external potentials for which the statement above can be proven rigorously, using an argument similar to that of Runge and Gross. In order to avoid pathologies, these sets should satisfy the following conditions:

- The set $\mathcal{I}$ is invariant under the dynamics generated by H_V for any $V \in \mathcal{V}$.
- $0 \in \mathcal{V}$ and if $V(x,t)$, $t \in [0,T)$ is an admissible potential, then so is the time-independent potential $V(x,t_0)$ for any $t_0 \in [0,T)$.
- If the time-independent potential $V(x) \in \mathcal{V}$, then any eigenvectors of H_V are admissible initial conditions.

In order to have smooth solutions, we also need to restrict the set of initial conditions

$$\mathcal{I} \subset \bigcap_{V(x) \in \mathcal{V}} C^\infty(H_V) \,,$$

where the intersection is over all time-independent potentials and $C^\infty(H_V) := \bigcap_{k \in \mathbb{N}} D(H_V^k)$ denotes the set of H_V-smooth vectors. Now, depending on the set $\mathcal{V}$, the intersection above may be very small – and will in general not be invariant under the dynamics of the operators H_V. In order to avoid this we have to restrict $\mathcal{V}$ so that

$$C^\infty(H_V) = C^\infty(H_0) \tag{1}$$

for every $V \in \mathcal{V}$. This condition clearly shows that the possible choice of $\mathcal{V}$ depends strongly on H_0 – and thus on V_0 and W.

1. Smooth potentials

If the potentials V_0 and W are smooth, we have natural choices for $\mathcal{I}$ and $\mathcal{V}$ and the Runge-Gross argument becomes a rigorous theorem. To be more precise, let $V_0, W \in C_b^\infty(\mathbb{R}^d, \mathbb{R})$, W even, and set

$$\mathcal{I} = \bigcap_{k\in\mathbb{N}} H^{2k}(\mathbb{R}^{dN}) \cap L^2_{\mathrm{a/s}}(\mathbb{R}^{dN})$$
$$\mathcal{V} = C_b^\infty([0,T)\times\mathbb{R}^d, \mathbb{R})$$

for some $T > 0$. We then have:

Theorem 1. *Let $V_1, V_2 \in \mathcal{V}$ and $\psi_0 \in \mathcal{I}$ with one-particle density ρ_0. Denote by $\psi_k(t)$, $k \in 1, 2$ the solution at time $t \in [0, T)$ of the Schrödinger equation with Hamiltonian H_{V_k} and initial condition $\psi_k(0) = \psi_0$. Denote by ρ_k the corresponding one-particle density. If $\rho_1 = \rho_2$, then for all $\ell \in \mathbb{N}$*

$$\int_{\mathbb{R}^d} \rho_0(x)|\nabla\partial_t^\ell(V_1 - V_2)|^2(x, 0)dx = 0\,. \tag{2}$$

If additionally the set $\rho_0^{-1}(0)$ has zero Lebesgue measure, then $\partial_t^\ell V_1(x) = \partial_t^\ell V_2(x) + c_\ell$ for some constant c_ℓ. If furthermore $(V_1 - V_2)(x, t)$ is real-analytic in t for every x we also have $V_1(x, t) = V_2(x, t) + C(t)$, with $C(t) = \sum_{\ell\in\mathbb{N}} \frac{c_\ell}{\ell!} t^\ell$.

For the proof of this theorem, one first applies a result of Kato [Ka53] to show that $\psi_k(t) \in \mathcal{I}$ depends smoothly on time. Then Equation (2) is obtained recursively by calculating weak time-derivatives of $\rho_1 - \rho_2$ at $t = 0$, which must equal zero since $\rho_1 = \rho_2$. For instance, the weak second derivative yields

$$0 = \frac{d^2}{dt^2}\bigg|_{t=0} \int_{\mathbb{R}^d} \varphi(x)(\rho_1 - \rho_2)(x, t)dx = 2N \int (\nabla\varphi)(x)\nabla(V_2 - V_1)(x, 0)dx\,,$$

so choosing the test-function $\varphi = V_2 - V_1$ gives (2) for $\ell = 0$. The additional statements follow easily from (2).

2. Singular potentials

If V_0 or W are not smooth, the condition (1) will lead to strong restrictions on the set $\mathcal{V}$. For example, it is easy to see that if H_0 is the one-dimensional Schrödinger operator with a delta-potential at $x = 0$, any potential satisfying (1) must be smooth on $\mathbb{R}$ and vanish to infinite order at $x = 0$. We expect this statement to hold generically for non-smooth potentials V_0. The restrictions on $\mathcal{V}$ are far more severe for singular interactions. We have the following:

Proposition 1. *Let $d = 3$, $N = 2$, $V_0 = 0$, $W(x) = \frac{1}{|x|}$ be the Coulomb-interaction and H_0 the operator acting on symmetric functions given by these choices. If $V \in C_b^6(\mathbb{R}^3)$ satisfies $D(H_V^4) = D(H_0^4)$ then V is constant.*

To prove this, one separates the relative and centre-of-mass coordinates and then applies similar arguments as in the case of a singular one-body potential V_0. This yields $\Delta V = 0$ and thus proves that V is constant.

We thus see that for the Coulomb-interaction Equation (1) already implies that V is constant, and there is nothing of interest to prove afterwards. Equation (2) can still be shown to hold for $\ell \leq 3$ ($\ell \leq 4$ for fermions), under reasonable assumptions. In order to obtain more information, a new approach that avoids Taylor expansions of high order is clearly necessary.

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Effective evolution of open dimers

Marco Merkli

(joint work with G.P. Berman, R.T. Sayre, S. Gnanakaran, M. Könenberg, A.I. Nesterov and H. Song)

We consider a quantum process where electric charge, or excitation energy, is exchanged between two agents, and in the presence of a thermal environment. In some chemical processes in biology (photosynthesis), the agent-reservoir interaction energy is large, at least of the same size as the agents' energy difference. We present a rigorous analysis of the effective dynamics of the agents in this coupling regime, valid for all times. In particular, we derive a generalization of the Marcus formula from quantum chemistry, predicting the reaction rate. Our generalization shows that by coupling one agent more strongly to the environment than the other one, a significant speedup of the process can be achieved. Our analytic method is based on a resonance expansion of the reduced agent dynamics, cast in the framework of the strongly coupled spin-boson system.

This talk is based on three recent papers. In [3] we establish a Mourre theory for the strongly coupled spin-boson system and we show ergodicity ('return to equilibrium'). The technically simpler spectral deformation techniques are *not* applicable to the system at hand (in the strong coupling regime, the 'perturbation' operator behaves badly under deformation). In [2] we build a method to extract decay rates and decay directions in Hilbert space from Mourre theory. In spirit, this work is similar to [1], but the latter applies only to zero-temperature systems and the weak coupling regime. Finally, in [5] we apply the resonance expansion for the dynamics established in [2] to a dimer (two-level system) strongly coupled

to a thermal bath. This is a basic relevant model to describe excitation transfer as it is observed, for instance, in chlorophyll molecules during photosynthesis [4].

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Periodic driving and breakdown of linear response

Wojciech De Roeck

We consider many-body quantum systems with a time-periodic Hamiltonian. We prove that, for a time $t(\nu)$, exponentially long in the frequency ν, the system is well-described by an effective time-independent Hamiltonian. This implies absence of heating and pre-thermalization for such systems.

Maximum ionization in Thomas-Fermi-Dirac-Weizsäcker theory

Phan Thành Nam

(joint work with Rupert L. Frank and Hanne Van Den Bosch)

While experiments tell us that a neutral atom can bind at most one or two extra electrons, justifying this fact from the first principles of quantum mechanics is a long standing open problem, often referred to as the *ionization conjecture* (see [10, Chapter 12]). In the full many-body Schrödinger theory, it is known that a nucleus of charge Z can bind at most $\min\{2Z+1, 1.22\,Z+3Z^{1/3}, Z+CZ^{5/7}+C\}$ where C is a universal constant (see [9], [14] and [3, 16] respectively). The uniform bound $Z+C$ is established only in some much simpler theories, such as Thomas-Fermi [11], Thomas-Fermi-von Weizsäcker [2] and Hartree-Fock [17].

In my talk, I have proved the uniform bound $Z+C$ in the Thomas-Fermi-Dirac-von Weizsäcker theory. More precisely, we minimize the TFDW energy functional

$$\int_{\mathbb{R}^3}\Big(c^{\mathrm{TF}}\rho(x)^{5/3}-c^{\mathrm{D}}\rho(x)^{4/3}+c^{\mathrm{W}}|\nabla\sqrt{\rho(x)}|^2-\frac{Z\rho(x)}{|x|}\Big)\mathrm{d}x+\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho(x)\rho(y)}{|x-y|}\mathrm{d}x\mathrm{d}y$$

under the constraint

$$0\leq\rho\in L^1(\mathbb{R}^3)\cap L^{5/3}(\mathbb{R}^3),\quad \int\rho=N.$$

Our main result in [5] is that for all given positive constants c^{TF}, c^{W} and c^{D}, if the TFDW functional has a minimizer, then

$$N \leq Z + C$$

for a constant C independent of Z.

One of the key feature of the Thomas-Fermi-Dirac-von Weizsäcker theory is that some electrons at infinity may form a nontrivial bound state (see [12, 15]). This makes the ionization problem difficult because we cannot apply the standard strategy of 'multiplying the Euler-Lagrange equation by $|x|$' by Benguria and Lieb (see [1, 8, 9]). The ionization problem for 'the infinity model' (the case $Z = 0$) has been solved recently by Lu and Otto [13] by a completely different strategy. Unfortunately, the method in [13] relies on the translation-invariance of the model and fails to apply when $Z > 0$.

In our work [5], we introduce a novel method to replace the 'multiplying by $|x|$' strategy. This method is inspired by ideas in a recent proof of the nonexistence in the liquid drop model by R. Killip and two of us [4]. Roughly speaking, the argument is to exploit the binding inequality by localizing the minimizing by half-planes and taking the average. This allows us to prove $N \leq (2 + o(1))Z$ easily.

To achieve the much improved bound $N \leq Z + C$, we apply our new technique to control only the particles far from the nucleus. We may still lose a factor 2 but this is not a serious problem because the number of the exterior particles is much smaller than Z. The interior particles are controlled by comparing with the Thomas-Fermi theory, following Solovej's proof of the ionization conjecture in the Hartree-Fock theory [17].

The main technical tool in the whole approach is to show that the screened nuclear potential (i.e. the attraction of the nucleus screened by the electrons in the interior region) is approximated well by the Thomas-Fermi screened potential up to the distance o(1) from the nucleus. In the semi-classical distance $O(Z^{-1/3})$, it is well-known that the Thomas-Fermi theory is valid and the approximation of the screened potentials follows easily. However, to extend this approximation to the much larger distance o(1), we need to combine the new bound on exterior particles with Solovej's delicate bootstrap argument [17].

As a by-product of our approach, we can deduce that the atomic radius in TFDW theory is close to that in Thomas-Fermi theory.

Our approach has been adapted to solve the ionization problem in Müller density-matrix-functional theory [6] and a related theory [7].

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Interior boundary conditions on Fock space

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(joint work with Jonas Lampart, Julian Schmidt, Roderich Tumulka)

It is well known that the operator

$$H_\delta = \mathrm{d}\Gamma(-\Delta + E_0) + a(\delta) + a^*(\delta)$$

on symmetric Fock space $\mathcal{F}_s(L^2(\mathbb{R}^3))$ can neither be defined as an operator nor as a form perturbation of the free operator $\mathrm{d}\Gamma(-\Delta)$. However, for $E_0 > 0$ a very simple "energy renormalization" procedure (cf. [1]) allows to define it as the limit of a sequence of UV-cutoff Hamiltonians,

$$H_\delta^{\mathrm{ren}} := \lim_{n\to\infty} (H_{\delta_n} + E_{\delta_n})\,. \tag{1}$$

Here $\delta_n \to \delta$ is a suitable sequence of L^2-functions approximating the δ-distribution and E_{δ_n} is a sequence of real numbers with $\lim_{n\to\infty} E_{\delta_n} = \infty$. The convergence in (1) is in the strong-resolvent sense and while each H_{δ_n} is self-adjoint on the domain of the free operator $\mathrm{d}\Gamma(-\Delta)$, the domain of the limit H_δ^{ren} turns out to be different.

Our aim in [4] is to rigorously pursue in this simple example a recent proposal for defining Hamiltonians without UV-regularization directly [6], i.e. without the need

for a renormalization, in terms of so called interior-boundary conditions (IBC). The basic idea is to think of those configurations

$$\mathcal{C}^n := \Big\{ x = (x_1, \dots, x_n) \in \mathbb{R}^{3n} \,\Big|\, \prod_{i=1}^{n} \|x_i\| = 0 \Big\} \subset \mathbb{R}^{3n} \,,$$

where at least one particle hits the "source" at the origin, as the "boundary" ($\mathcal{C}^n$ has codimension 3) of the n-particle sector of configuration space $\mathbb{R}^{3n} \setminus \mathcal{C}^n$ and to allow for a non-vanishing probability current through this "boundary" into or out of the $n-1$-particle sector. Then the IBC domain D_{IBC} for H_δ contains functions that may be singular at $\mathcal{C}^n$ (only for singular functions a non-vanishing probability current into or out of the set $\mathcal{C}^n$ is possible) and whose boundary value at $\mathcal{C}^n$ is connected to the value of the wave function one sector below,

$$\lim_{r\to 0} r\, \psi^{(n+1)}(r\omega, x_1, \dots, x_n) \sim \psi^{(n)}(x_1, \dots, x_n) \,.$$

We specify D_{IBC} explicitly and show that H_δ^{IBC} defines for $E_0 > 0$ a self-adjoint operator on D_{IBC}, which agrees, up to a finite additive constant, with the operator H_δ^{ren} obtained from the renormalization procedure described above. For $E_0 \geq 0$ the operator H_{IBC} is bounded below and for all $E_0 \in \mathbb{R}$ it is essentially self-adjoint. Moreover, the intersection of $D_{\mathrm{IBC}} = D_{\mathrm{ren}}$ with the domain of the free Hamiltonian $\mathrm{d}\Gamma(-\Delta)$ contains only the zero-vector, $D_{\mathrm{IBC}} \cap D(\mathrm{d}\Gamma(-\Delta)) = \{0\}$. We prove similar results for models with any finite number of point sources and for a (probably exhaustive) family of different interior boundary conditions.

In summary, we provide an explicit and physically transparent characterization of the natural domain of a simple model Hamiltonian for creation and annihilation of particles at point sources.

Similar ideas appeared as early as 1930 in the physics literature [5]. The natural restriction of the operator H_{IBC} to the one and zero-particle sectors of Fock space was discussed in [8] and a closely related model in [7]. Interior boundary conditions in one spatial dimension were studied recently in [3]. A somewhat related study of the domain of the Fröhlich Hamiltonian can be found in [2].

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Energy conservation and fluctuation relations for open quantum systems

Annalisa Panati
(joint work with Tristan Benoist, Vojkan Jakšić, Yan Pautrat and Claude-Alain Pillet)

The fluctuations of thermodynamic quantities in classical systems have been successfully studied through symmetries of associated (moment) generating functions. They have led to a better understanding of classical non-equilibrium systems beyond linear response (see e.g. [4] for a historical account), and various efforts have been made to extend this analysis to the quantum setting.

We consider the generating functions associated with the statistics of a two-time measurement (also known as full counting statistics) of the energy variation for each reservoir of an open quantum system, under an assumption of regularity of the coupling term with respect to the free evolution.
The notion of full counting statistics introduced by Lesovik and Levitov in the study of charge transport (see [3]). It therefore has a simple operational meaning, and in addition it has been shown to satisfy the celebrated Evans-Searles symmetry ([2, 5]), which is associate to a refinement of second law or thermodynamics.

We show in addition that it satisfies an additional symmetry, more precisely a translation-invariance property, as suggested in [1].
We explore its consequences on energy conservation, leading to a strengthening of the first law of thermodynamics for open quantum system. More explicitly in the case of two reservoirs we show that the fluctuations of the heat flows in the first and second reservoir have identical distributions, and that one is almost-surely the opposite of the other.

Moreover, as it was shown in [1], the combination of the two symmetries allow to recover the linear response theory (Green-Kubo formula and Onsager reciprocity relations).

Finally, the general theory can be illustrated on a number of concrete fermonic models, such as the spin-Fermion model, the Electronic Black box and the Spin XY chain.

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A phase transition in a model for swarming

Rupert L. Frank
(joint work with Elliott H. Lieb)

For a parameter $\alpha > 0$ we consider the functional

$$\mathcal{E}_\alpha[\rho] := \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \rho(x) \left(\frac{1}{|x-y|} + |x-y|^\alpha \right) \rho(y)\, dx\, dy$$

and the corresponding minimization problem

$$E_\alpha(m) := \inf \left\{ \mathcal{E}_\alpha[\rho] :\ 0 \leq \rho \leq 1\,,\ \int_{\mathbb{R}^3} \rho(x)\, dx = m \right\}.$$

This is a very simple model of swarming of birds or some other condensation phenomenona. The function ρ describes the spatial density of birds (or 'particles') and m their total number. The two terms in the energy functional $\mathcal{E}_\alpha$ correspond to a two-body repulsive interaction between pairs of birds (or 'particles') and to a two-body attractive interaction that engenders swarming (or 'condensation'), respectively. The condition that $\rho \leq 1$ is a many-body hard-core repulsion at short range. It imposes a maximum density, beyond which the birds would be crushed. Its analogy in statistical physics is a bound on the allowed density of atoms in a liquid, namely the density of the solid state. The above model was introduced in [1] and we refer to this paper, to [2] and to the references therein for background on mathematical models for biological aggregations.

It is easy to see that for any $m > 0$ the minimization problem $E_\alpha(m)$ has a minimizer. Our main result in [2] is that there is a qualitative change in the shape of minimizers as m is increased, which is analogous to a 'liquid-solid' phase transition. More precisely, we prove

Theorem. *Let $\alpha > 0$. Then there are $0 < m_{c_1}(\alpha) \leq m_{c_2}(\alpha) < \infty$ such that for $m < m_{c_1}(\alpha)$ any minimizer ρ for $E_\alpha(m)$ satisfies $|\{\rho = 1\}| = 0$ and for $m > m_{c_2}(\alpha)$ any minimizer ρ for $E_\alpha(m)$ satisfies $|\{0 < \rho < 1\}| = 0$.*

The case $\alpha = 2$ is explicitly solvable [1] and in this case one has $m_{c_1}(2) = m_{c_2}(2)$. In general, however, there might be an intermediate region between $m_{c_1}(\alpha)$ and $m_{c_2}(\alpha)$ where a liquid part $\{0 < \rho < 1\}$ coexists with a solid part $\{\rho = 1\}$.

We expect that the results in the theorem remain valid for a much larger class of interaction kernels $k(|x|)$, typically satisfying $k(r) \to \infty$ as $r \to 0$ and $r \to \infty$ and having a unique local minimum inbetween. Our proof of the theorem, however, uses specific properties of the Coulomb-like behavior $k(r) \sim r^{-1}$ as $r \to 0$.

Technically, we make use of the Coulomb-like behavior by taking the Laplacian of the Euler equation, which holds on the set $\{0 < \rho < 1\}$. Since the regularity of the latter set is not clear, we need the following general result about Sobolev functions.

Lemma. *Let $\Omega \subset \mathbb{R}^d$ be open, $k \in \mathbb{N}$ and $u \in W^{k,1}_{\mathrm{loc}}(\Omega)$. Then $\partial^\alpha u = 0$ almost everywhere on $\{u = 0\}$ for all $\alpha \in \mathbb{N}_0^d$ with $|\alpha|_\infty \leq k$.*

When taking the Laplacian of the Euler equation, we also encounter a term $\Delta k * \rho$ and we note that the monotonicity properties of Δk with respect to the radius are different according to whether α is smaller or larger than 2. In the favorable case we can bound $\Delta k * \rho$ simply by rearrangement inequalities using the L^1 and L^∞ constraints on ρ.

In the unfavorable case, we need additional information about minimizers ρ, namely, that their support is not too large. We prove

Proposition. *Let $\alpha > 0$. Then there is a $C_\alpha > 0$ such that for all $m > 0$ and all minimizers ρ of $E_\alpha(m)$ one has*

$$\operatorname{diam} \operatorname{supp} \rho \leq C_\alpha \max\left\{1, m^{1/3}\right\}.$$

We emphasize that, while we state this proposition only for the specific interaction kernels $k(r) = r^{-1} + r^\alpha$, here the Coulomb-like behavior for small distances does not play an important role and a similar result should hold for a much larger class of interaction kernels.

Finally, we note that

$$E_\alpha(m) \sim m^{2+\alpha/3} \frac{1}{2} \iint_{\mathcal{B}\times\mathcal{B}} |x-y|^\alpha \, dx\, dy \qquad \text{as } m \to \infty,$$

where $\mathcal{B}$ is a ball in $\mathbb{R}^3$ of volume 1. This raises the interesting open question whether there is an $m'_{c_2}(\alpha) < \infty$ such that for $m > m'_{c_2}(\alpha)$ any minimizer of $E_\alpha(m)$ is a characteristic function of a ball of volume m. This would, of course, be consistent with the diameter bound from the proposition.

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