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Mini-Workshop: Mathematics of Many-body Fermionic Systems

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ABSTRACT. Fermionic quantum systems are well described by the linear many-body Schrödinger equation. For interacting systems the full Schrödinger theory is extremely complicated and theoretical as well numerical investigations are not feasible. In practice, macroscopic properties of large systems can therefore only be accessed by means of approximate theories. The intention of this workshop was to showcase the most recent advances in the mathematical study of many-body interacting fermionic systems and to stimulate discussions among different research groups.

Mathematics Subject Classification (2020): 35P05, 35Q20, 35Q40, 35Q55, 35Q60, 35Q83, 81Q10, 82B10, 82C10.

Introduction by the Organizers

The mini-workshop *Mathematics of Many-body fermionic systems*, organized by Nikolai Leopold (Basel), Phan Thành Nam (Munich) and Chiara Saffirio (Basel) gathered sixteen participants, including the organizers. The group covered a broad range of expertise and maintained a well-rounded balance in terms of both age and gender. The main goals of the workshop were to showcase the most recent mathematical techniques in many-body interacting fermionic systems and to foster the interaction between different research groups. The newest results in the field were presented in thirteen one-hour lectures. Several free slots as well as an open problem discussion session provided opportunities for in-depth scientific discussions on cutting-edge methodologies and potential future research directions.

The talks were centered on the following core themes: ground state energies of many-body fermionic systems, effective dynamics for quantum systems and quantum systems in interaction with radiation fields.

The majority of the contributions dealt with ground state energies of many-fermion systems. Christian Hainzl opened the workshop with a presentation concerning the correlation energy of the electron gas in the mean-field regime. Related developments were reported by Martin Christiansen about spectral estimates for fermionic n -body operators and reduced density matrices, by Emanuela Giacomelli about the low density Fermi gas in three dimensions towards the Huang-Yang conjecture, and by Blazej Ruba concerning the bosonization for strongly interacting Fermi gases. The topic was in addition addressed by Volker Bach who discussed unitary renormalization group flows for fermion systems, Mathieu Lewin who gave an overview on mathematical results in density functional theory, and Charlotte Dietze who presented semiclassical estimates for Schrödinger operators with Neumann boundary conditions on Hölder domains.

The time evolution of quantum systems was treated by Peter Pickl with his presentation about effective evolution equations for tracer particles in interaction with either bosonic or fermionic gases. François Golse gave insights into the random batch method in the context of large N limit (uniform in \hbar) of the Wigner transform of the single-particle reduced density matrix associated with an N -body quantum system. Jani Lukkarinen's talk was concerned with the propagation of chaos via cumulant hierarchies in two example models: the discrete nonlinear Schrödinger evolution and the stochastic Kac model.

Systems with radiation fields have been considered by Tadahiro Miyao who presented a unified mathematical framework to describe the magnetic properties of ground states in many-electron systems, and Simone Rademacher who discussed the Landau-Pekar conjecture on the effective mass problem for the classical polaron. The workshop ended with the talk of Manfred Salmhofer reviewing results on the Hubbard model and the Fermi liquids, based on renormalization group techniques.

Wednesday morning was devoted to a collaborative discussion session aiming to maximize the interaction between the participants. The attendees were split into four subgroups, each dedicated to exploring a given topic for an hour. Subsequently, the findings were shared in a large plenary session, sparking further discussions. This format, recommended to the organizers by Mathieu Lewin, proved highly successful with many topics continuing to be explored during the traditional afternoon hike. The subjects listed below were the main themes of the discussion.

Correlation estimates: The discussion revolved around the study of the energy in terms of reduced density matrices, and in particular around Coulson's challenge related to the reconstruction of the N -particle states originated from a two-body density matrix. At present it is believed that in practical applications the so-called P-Q-G-T1-T2 conditions on two-body density matrices suffice for the reconstruction of the N -body states up to a very high precision. In 2013, Volker Bach, Hans

Konrad Knörr and Edmund Menge showed that conditions P-Q-G imply the validity of the Hartree-Fock approximation, thus particularly explaining the success of earlier numerical tests by Eric Cancès, Mathieu Lewin and Gabriel Stoltz. On the other hand, the T1 and T2 conditions are obtained by suitable 3-body density inequalities, and they seem to be hidden in recent developments in the correlation energy. Potential links between the P-Q-G-T1-T2 conditions and the random phase approximation were suggested, leading to interesting open problems to be investigated in the upcoming years.

Effective dynamics: The second group focused on the derivation of effective evolution equations for many particle systems. Two key open problems were identified. Firstly, there is an interest in deriving effective equations for longer time scales than those thus far explored. Secondly, a highly desirable goal is to establish the derivation of the Vlasov–Poisson equation from the classical dynamics of many particles with Coulomb interaction. The plenary discussion revolved around the latter challenge, specifically addressing the fact that Sylvia Serfaty and Mitia Duerinckx have successfully derived the Vlasov–Poisson equation with Coulomb potential in the monokinetic case. The discourse then centered on exploring whether the assumptions on the solutions of the pressureless Euler–Poisson equation (linked to monokinetic solutions of the Vlasov–Poisson equation) can be relaxed in the monokinetic derivation. Additionally, it was addressed how a derivation beyond the monokinetic scenario could be accomplished.

Kinetic equations: The group directed its attention towards the derivation of the quantum Boltzmann equation from the many-body Schrödinger equation. The weakly interacting and dilute regime were identified for derivations of the quantum Boltzmann equation with cubic collision operator. Recent findings about the derivation of the quantum Boltzmann equation by Thomas Chen, Michael Hott and Esteban Cárdenas as well as concerning the derivation of the wave kinetic equation by Tristan Buckmaster, Yu Deng, Pierre Germain, Zaher Hani and Jalal Shatah were highlighted. The main focus of the discussion then shifted to the technical aspects of the derivation. On the one hand it was investigated how Gronwall-type estimates could be optimized to be more useful in the kinetic regime. In this context it was discussed if the introduction of randomness could be helpful. On the other hand attention was directed towards finding suitable macroscopic observables for the derivation such as cumulants.

Semiclassical limits (including systems with radiation fields): Natural connections between semiclassical analysis and density functional theory were mentioned, including several problems on semiclassical estimates. In particular, challenging questions on asymptotic behaviors of large Coulomb systems were promoted. Concerning systems with radiation fields it was discussed in which way Maxwell’s equations emerge from the quantized electromagnetic field with large photon number. Existing results were pointed out and a derivation of Maxwell’s equations from non-relativistic quantum electrodynamics in a many-fermion limit as open problem identified. Additionally, the question if it is possible to define and analyze a

microscopic model of a laser was raised. First results in this direction by Jean-Bernard Bru and Walter de Siqueira Pedra were pointed out.

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Abstracts

Correlation energy of the electron gas in the mean-field regime

CHRISTIAN HAINZL

(joint work with M. R. Christiansen and P. T. Nam)

In [5] we prove a rigorous upper bound on the correlation energy of interacting fermions in the mean-field regime for a wide class of interaction potentials. Our result covers the Coulomb potential, and in this case we obtain the analogue of the Gell-Mann–Brueckner formula [6] $c_1\rho \log(\rho) + c_2\rho$ in the high density limit. We do this by refining the analysis of our bosonization method in [3] to deal with singular potentials, and to capture the exchange contribution which is absent in the purely bosonic picture.

In a forthcoming paper we will actually also prove the corresponding lower bound. Before stating the Theorem we give a precise definition of the model.

We consider N (spinless) electrons in the unit torus $\Omega = [0, 2\pi]^3$ (periodic b.c.) where

$$N = |B_F| = |B(0, k_F) \cap \mathbb{Z}^3|, \quad k_F \sim N^{1/3},$$

B_F denoting the Fermi ball and k_{B_F} the Fermi momentum. The N -body Hamiltonian on $L^2_a(\Omega^N)$ has the form

$$H_N = \sum_{i=1}^N (-\Delta_{x_i}) + \frac{1}{k_F} \sum_{1 \leq i < j \leq N} V(x_i - x_j)$$

with mean-field periodic Coulomb potential

$$\frac{1}{k_F} V(x) = \frac{1}{k_F (2\pi)^3} \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \hat{V}_k e^{ik \cdot x}, \quad \hat{V}_k = \frac{4\pi}{|k|^2}.$$

The main theorem about recovering the Gell-Mann-Brueckner formula for the correlation energy reads as follows, where E_{HF} is the Hartree-Fock energy.

Theorem.

$$E_N = E_{\text{HF}} + E_{\text{corr,bo}} + E_{\text{corr,ex}} + o(k_F)_{k_F \rightarrow \infty}$$

with bosonic correlation contribution,

$$E_{\text{corr,bo}} = \frac{1}{\pi} \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \int_0^\infty F \left(\frac{k_F^{-1} \hat{V}_k}{(2\pi)^3} \sum_{p \in L_k} \frac{\lambda_{k,p}}{\lambda_{k,p}^2 + t^2} \right) dt \sim k_F \log(k_F)$$

and exchange correlation contribution

$$E_{\text{corr,ex}} = \frac{1}{4(2\pi)^6} \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \sum_{p, q \in L_k} \frac{k_F^{-2} \hat{V}_k \hat{V}_{p+q-k}}{\lambda_{k,p} + \lambda_{k,q}} \sim k_F$$

$$F(x) = \log(1+x) - x, \quad \lambda_{k,p} = \frac{1}{2}(|p|^2 - |p-k|^2) > 0, \quad p \in L_k = (B_F + k) \setminus B_F.$$

The main idea of the proof can be summarized as follows. Starting from the Hamiltonian in second quantization, one can approximate the main contribution of the Hamiltonian by the following pseudo-quadratic Hamiltonian

$$H_{\text{eff}} \approx \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \sum_{p \in L_k} 2\lambda_{k,p} b_{k,p}^* b_{k,p} + \sum_{k,p,q} \frac{\hat{V}_k k_F^{-1}}{2(2\pi)^3} (2b_{k,p}^* b_{k,q} + b_{k,p} b_{-k,-q} + b_{-k,-q}^* b_{k,p}^*),$$

where the operators $b_{k,p}$ describe a pair of Fermions,

$$b_{k,p} = a_{p-k}^* a_p, \quad p \in L_k = (B_F + k) \setminus B_F,$$

where a_{p-k}^* annihilates a hole in the Fermi sea and a_p annihilates a particle outside the Fermi sea. These $b_{k,p}$'s behave approximately like bosons. Following Sawada [8, 9] we diagonalize the Hamiltonian as if these operators were bosons and obtain the stated result. Since we track the non-bosonicity of the b -operators exactly we also recover the exchange contribution in contrast to Sawada. Using a different approach, more precisely patching the Fermi sea, a similar result for smooth potentials was obtained earlier, see [1, 2]. In a perturbative form a similar result was obtained in [7]. In a similar way one can also track the elementary excitations. Plugging in the Coulomb potential into the final formula, one obtains the so called plasmon spectrum [4].

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Spectral Estimates for Fermionic n -Body Operators

MARTIN RAVN CHRISTIANSEN

Fermionic n -Body Operators. Let \mathfrak{h} be a Hilbert space and let $\Psi \in \bigwedge^N \mathfrak{h}$ be a normalized N -particle state. Then the n -body operator associated to Ψ , $\gamma_n^\Psi : \bigotimes^n \mathfrak{h} \rightarrow \bigotimes^n \mathfrak{h}$, is defined with respect to elementary tensors by

$$\langle (\varphi_1 \otimes \cdots \otimes \varphi_n), \gamma_n^\Psi(\psi_1 \otimes \cdots \otimes \psi_n) \rangle = \langle \Psi, c^*(\psi_1) \cdots c^*(\psi_n) c(\varphi_n) \cdots c(\varphi_1) \Psi \rangle.$$

Here $c^*(\cdot)$ and $c(\cdot)$ denote creation and annihilation operators, which obey the canonical anticommutation relations (CAR)

$$\{c(\varphi), c^*(\psi)\} = \langle \varphi, \psi \rangle, \quad \{c(\varphi), c(\psi)\} = 0 = \{c^*(\varphi), c^*(\psi)\}.$$

γ_n^Ψ is a positive self-adjoint operator on $\bigotimes^n \mathfrak{h}$, and if $(u_k)_k$ is an orthonormal basis for \mathfrak{h} then its action can be recast as

$$\langle \Phi, \gamma_n^\Psi \Phi \rangle = \left\| \sum_{k_1, \dots, k_n} \overline{\Phi_{k_1, \dots, k_n}} c_{k_n} \cdots c_{k_1} \Psi \right\|^2$$

where $\Phi_{k_1, \dots, k_n} = \langle u_{k_1} \otimes \cdots \otimes u_{k_n}, \Phi \rangle$ for $\Phi \in \bigotimes^n \mathfrak{h}$ and $c_k = c(u_k)$ for $k \in \mathbb{N}$.

The n -body operator γ_n^Ψ is trace-class with $\text{tr}(\gamma_n^\Psi) = \frac{N!}{(N-n)!}$. This trivially implies that also $\|\gamma_n^\Psi\|_{\text{op}} \leq \frac{N!}{(N-n)!} \sim N^n$, which is optimal in the bosonic case. For fermions this is untrue however, as e.g.

$$\langle \varphi, \gamma_1^\Psi \varphi \rangle = \langle \Psi, c^*(\varphi) c(\varphi) \Psi \rangle \leq \langle \Psi, \{c^*(\varphi), c(\varphi)\} \Psi \rangle = \|\varphi\|^2$$

by the CAR, which shows that $\|\gamma_1^\Psi\|_{\text{op}} \leq 1$.

In terms of the basis $(u_k)_k$, this can be expressed as $\|\sum_k \alpha_k c_k\|_{\text{op}}^2 \leq \sum_k |\alpha_k|^2$ for any coefficients $(\alpha_k)_k$. This implies an improvement on the bound for $\|\gamma_n^\Psi\|_{\text{op}}$ for any n , since

$$\begin{aligned} \sqrt{\langle \Phi, \gamma_n^\Psi \Phi \rangle} &\leq \sum_{k_1, \dots, k_{n-1}} \left\| \left(\sum_{k_n} \overline{\Phi_{k_1, \dots, k_n}} c_{k_n} \right) c_{k_{n-1}} \cdots c_{k_1} \Psi \right\| \\ &\leq \sqrt{\sum_{k_1, \dots, k_n} |\Phi_{k_1, \dots, k_n}|^2} \sqrt{\sum_{k_1, \dots, k_{n-1}} \|c_{k_{n-1}} \cdots c_{k_1} \Psi\|^2} = \frac{N!}{(N-n+1)!} \|\Phi\| \end{aligned}$$

implies that $\|\gamma_n^\Psi\|_{\text{op}} \leq \frac{N!}{(N-n+1)!} \sim N^{n-1}$.

Yang's Estimates. For $n = 2$ this simply reads $\|\gamma_2^\Psi\|_{\text{op}} \leq N$, which was first proved by Yang in [1], who also showed it to be optimal (for even N). Based on his analysis of the optimizers, he conjectured - and later proved - the following:

Theorem. (Yang, [1, 2]) For any normalized $\Psi \in \bigwedge^N \mathfrak{h}$ it holds that for all $n \in \mathbb{N}$

$$\|\gamma_n^\Psi\|_{\text{op}} \leq C_n N^{\lfloor \frac{n}{2} \rfloor}$$

for constants $C_n > 0$ depending only on n .

This bound follows from two main points. The first is that if we define $\Lambda_n^N = \sup_{\Psi \neq 0} \|\gamma_n^\Psi\|_{\text{op}} \|\Psi\|_{\text{op}}^{-2}$ - i.e. the quantity we wish to control - it is seen that

$$\begin{aligned} \sqrt{\langle \Phi, \gamma_n^\Psi \Phi \rangle} &\leq \sum_{k_1} \left\| \left(\sum_{k_2, \dots, k_n} \overline{\Phi_{k_1, \dots, k_n}} c_{k_n} \cdots c_{k_2} \right) c_{k_1} \Psi \right\| \\ &\leq \sqrt{\Lambda_{n-1}^{N-1}} \sum_{k_1} \sqrt{\sum_{k_2, \dots, k_n} |\Phi_{k_1, \dots, k_n}|^2} \|c_{k_1} \Psi\| \\ &\leq \sqrt{\Lambda_{n-1}^{N-1}} \sqrt{\sum_{k_1, \dots, k_n} |\Phi_{k_1, \dots, k_n}|^2} \sqrt{\sum_{k_1} \|c_{k_1} \Psi\|^2} = \sqrt{N \Lambda_{n-1}^{N-1}} \|\Phi\| \end{aligned}$$

which implies the recursive estimate $\Lambda_n^N \leq N \Lambda_{n-1}^{N-1}$.

The second point is that an argument of Bell [3] implies that $\Lambda_n^N \lesssim C'_n \Lambda_{n-1}^N$ for odd n - combining these two estimates then yields Yang’s estimate $\Lambda_n^N \leq C_n N^{\lfloor \frac{n}{2} \rfloor}$ by induction.

To illustrate Bell’s argument, consider $n = 3$: Then as for $n = 1$

$$\langle \Phi, \gamma_3^\Psi \Phi \rangle \leq \left\langle \Psi, \left\{ \left(\sum_{k,l,m} \overline{\Phi_{k,l,m}} c_m c_l c_k \right)^*, \left(\sum_{k,l,m} \overline{\Phi_{k,l,m}} c_m c_l c_k \right) \right\} \Psi \right\rangle$$

and since 3 is odd, the anticommutator reduces to a sum of terms containing at most 4 creation/annihilation operators, rather than 6. Indeed, assuming without loss of generality that the coefficients $\Phi_{k,l,m}$ are antisymmetric, this anticommutator is

$$9 \sum_k \left| \sum_{l,m} \overline{\Phi_{k,l,m}} c_m c_l \right|^2 - 18 \sum_{k,l} \left| \sum_m \overline{\Phi_{k,l,m}} c_m \right|^2 + 6 \sum_{k,l} |\Phi_{k,l,m}|^2$$

which implies that $\Lambda_3^N \leq 9 \Lambda_2^N + 6$.

Hilbert-Schmidt Estimates for γ_2^Ψ and $\gamma_2^{\Psi,T}$. The argument of Bell was recently used to obtain Hilbert-Schmidt estimates on 2-body operators and their truncated versions $\gamma_2^{\Psi,T} = \gamma_2^\Psi - (1 - \text{Ex})(\gamma_1^\Psi \otimes \gamma_1^\Psi)$.

First let us note that by the identity $\|\gamma_2^\Psi\|_{\text{tr}} = N(N - 1)$ and Yang’s optimal estimate $\|\gamma_2^\Psi\|_{\text{op}} \leq N$, it easily follows that $\|\gamma_2^\Psi\|_{\text{HS}} \leq N^{\frac{3}{2}}$. This can however be improved significantly:

Theorem. ([4]) For any normalized $\Psi \in \wedge^N \mathfrak{h}$ it holds that

$$\|\gamma_2^\Psi\|_{\text{HS}} \leq \sqrt{5}N, \quad \|\gamma_2^{\Psi,T}\|_{\text{HS}} \leq \sqrt{5N \text{tr}(\gamma_1^\Psi - (\gamma_1^\Psi)^2)}.$$

Note that the bound $\|\gamma_2^\Psi\|_{\text{HS}} \leq \sqrt{5}N$ is of the same order with respect to N as Yang’s bound $\|\gamma_2^\Psi\|_{\text{op}} \leq N$ - informally speaking this implies that although γ_2^Ψ can have eigenvalues of order N , it can not have “too many” large eigenvalues. Furthermore, for Slater states Ψ it holds that $\|\gamma_2^\Psi\|_{\text{HS}} = \sqrt{2}N$, so this order is optimal.

The first estimate follows by noting that

$$\mathrm{tr}(A\gamma_2^\Psi) = - \sum_n \left\langle \sum_{k,l,m} \overline{A_{k,l,m,n} c_m^* c_l c_k} \Psi, c_n \Psi \right\rangle$$

for any Hilbert-Schmidt operator A , whence

$$|\mathrm{tr}(A\gamma_2^\Psi)| \leq \sqrt{N \sum_n \langle \Psi, T_n^* T_n \Psi \rangle} \leq \sqrt{N \sum_n \langle \Psi, \{T_n^*, T_n\} \Psi \rangle}$$

for $T_n = \sum_{k,l,m} \overline{A_{k,l,m,n} c_m^* c_l c_k}$. Since this is again a sum of terms with 3 fermionic operators, the anticommutator simplifies significantly, with the consequence that (assuming without loss of generality an antisymmetry condition on $A_{k,l,m,n}$)

$$\sum_n \{T_n^*, T_n\} \leq \sum_{m,n} \left| \sum_{k,l} \overline{A_{k,l,m,n} c_l c_k} \right|^2 + 4 \sum_{k,n} \left| \sum_{l,m} A_{k,l,m,n} c_l^* c_m \right|^2,$$

and since not only $\|\sum_k \alpha_k c_k\|_{\mathrm{op}}^2 \leq \sum_k |\alpha_k|^2$ but also $\|\sum_k \alpha_k c_k^*\|_{\mathrm{op}}^2 \leq \sum_k |\alpha_k|^2$ this can be bounded as

$$\sum_n \{T_n^*, T_n\} \leq 5 \left(\sum_{k,l,m,n} |A_{k,l,m,n}|^2 \right) \left(\sum_k |c_k|^2 \right) = 5N \|A\|_{\mathrm{HS}}^2$$

for the claim. The estimate on $\|\gamma_2^{\Psi,T}\|_{\mathrm{HS}}$ follows by a similar argument after noting the identity

$$\begin{aligned} \left\langle (\varphi_1 \otimes \varphi_2), \gamma_2^{\Psi,T}(\psi_1 \otimes \psi_2) \right\rangle &= \langle \Psi, c(\gamma_1^\Psi \varphi_2) c^*(\psi_1) c^*(\psi_2) c(\varphi_1) \Psi \rangle \\ &\quad - \langle \Psi, c^*(\psi_1) c^*(\psi_2) c(\varphi_1) c((1 - \gamma_1^\Psi) \varphi_2) \Psi \rangle. \end{aligned}$$

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Unitary Flows for Fermion Systems

VOLKER BACH

(joint work with Jakob Geisler, Konstantin Merz)

1. UNITARY FLOWS ON FERMION OPERATORS

1.1. Fermion Systems and Fermi Gases. Here we present a mathematical study of fermion systems. Although we ultimately aim at treating atoms and molecules, we focus on Fermi gases here. For $d, L \in \mathbb{N}$, the configuration space of the system is the d -dimensional torus $\Lambda := \mathbb{R}^d/L\mathbb{Z}^d$ of sidelength $L \gg 1$, the corresponding momentum space is $\Lambda^* = \frac{2\pi}{L}\mathbb{Z}^d$. States of the system are represented by vectors in fermion Fock space $\mathfrak{F} = \mathfrak{F}_f(\mathfrak{h})$, where $\mathfrak{h} = L^2(\Lambda)$ is the Hilbert space of a single fermion. The system's dynamics is generated by the second-quantized Hamiltonian

$$(1) \quad \tilde{\mathbb{H}}_{g,\nu} = \sum_{k \in \Lambda^*} (k^2 - \nu) \hat{a}_k^* \hat{a}_k + \frac{g}{2} \sum_{q, k, k' \in \Lambda^*} \frac{\hat{v}_q}{|\Lambda|} \hat{a}_{k+q}^* \hat{a}_{k'}^* \hat{a}_{k'+q} \hat{a}_k,$$

where $\nu > 0$ is the chemical potential, $g \geq 0$ is the coupling constant, $\hat{v} : \Lambda^* \rightarrow \mathbb{R}_0^+$ is the restriction to $\Lambda \subseteq \mathbb{R}^d$ of the Fourier transform $\mathfrak{F}[V] \in \mathcal{S}(\mathbb{R}^d)$ of a pair potential $V \in \mathcal{S}(\mathbb{R}^d)$, both assumed to be nonnegative, smooth functions of rapid decrease, for simplicity.

The Fermi gas under consideration is characterized by the spectral properties of $\tilde{\mathbb{H}}_{g,\nu}$. These have been an object of research for almost a century, just like quantum mechanics itself. The discovery of High- T_c superconductivity brought these models into the focus of mathematical physics some 35 years ago. Monographs that provide an overview are [10, 7, 9]

1.2. Hartree–Fock Theory and Bogoliubov Transformations. One of the most important approximations to the ground state energy of a many-fermion system is the Hartree–Fock approximation which is defined by restricting the Rayleigh–Ritz variational principle to Slater determinants,

$$(2) \quad E_{\text{HF}}(g, \nu) := \inf \left\{ \langle f_1 \wedge \cdots \wedge f_N | \tilde{\mathbb{H}}_{g,\nu} (f_1 \wedge \cdots \wedge f_N) \rangle \mid N \in \mathbb{N}_0, \langle f_i | f_j \rangle = \delta_{i,j} \right\}.$$

In [6, 2] it was shown that the Hartree–Fock energy $E_{\text{HF}}(g, \nu)$ coincides with the smallest energy expectation value of wave functions, which are Bogoliubov transforms $\mathbb{U}\Omega$ of the vacuum vector Ω ,

$$(3) \quad E_{\text{HF}}(g, \nu) = \inf \left\{ \langle \Omega | \mathbb{U}^* \tilde{\mathbb{H}}_{g,\nu} \mathbb{U} \Omega \rangle \mid \mathbb{U} \in \text{Bog}(\mathfrak{F}) \right\}.$$

Here, $\text{Bog}(\mathfrak{F}) \subseteq \mathcal{U}(\mathfrak{F})$ denote the Bogoliubov transforms on \mathfrak{F} , i.e., all unitary operators that act linearly on creation and annihilation operators. If we impose

translation invariance of $|\mathbb{U}\Omega\rangle\langle\mathbb{U}\Omega|$, then the best choice for \mathbb{U} is

$$(4) \quad h_k^* := \mathbb{U}_\mu \widehat{a}_k^* \mathbb{U}_\mu^* := \widehat{a}_k^*, \quad k^2 \geq \mu,$$

$$(5) \quad \ell_k^* := \mathbb{U}_\mu \widehat{a}_k^* \mathbb{U}_\mu^* := \widehat{a}_k, \quad k^2 < \mu,$$

$$(6) \quad \mathbb{U}_{\mu\Omega} := \left(\prod_{k^2 < \mu} \widehat{a}_k^* \right) \Omega,$$

where $\mu \equiv \mu(g) = \nu + \mathcal{O}(g)$ is chosen as to minimize $\langle \Omega | \mathbb{U}_\mu^* \widetilde{\mathbb{H}}_{g,\nu} \mathbb{U}_\mu \Omega \rangle$. Note that translation invariance of $|\mathbb{U}\Omega\rangle\langle\mathbb{U}\Omega|$ for the minimizing Bogoliubov transformation \mathbb{U} is a plausible assumption and actually violated sometimes; BCS theory builds up on this assumption. For more details see [1] and references therein.

After conjugation with \mathbb{U}_μ , the Hamiltonian reads

$$(7) \quad \mathbb{H}_g := \mathbb{U}_\mu^* \widetilde{\mathbb{H}}_{g,\nu} \mathbb{U}_\mu = E_{\text{tHF}}(g, \nu) + d\Gamma(\omega) + g\mathbb{Q},$$

where $E_{\text{tHF}}(g, \nu)$ is the Hartree–Fock energy restricted to translation-invariant states, $\omega_k = |k^2 - \mu|$, and \mathbb{Q} is purely quartic in h_k^* , ℓ_k^* , h_k , and ℓ_k .

1.3. Flow Equations for Fermion Systems in Standard Representation.

We report on joint work in progress with *J. Geisler* and *K. Merz*. A suggestive formulation of the renormalization group (RG) is given by a family $(\mathbb{W}(t))_{t \geq 0}$ of unitarily equivalent operators determined by the evolution equation

$$(8) \quad \forall t > 0: \quad \dot{\mathbb{W}}(t) = i[\mathbb{G}(t), \mathbb{W}(t)], \quad \mathbb{W}(0) = \mathbb{H}_g,$$

where $\mathbb{G}(t) = \mathbb{G}^*(t)$ is chosen as to eliminate (“diagonalize away”) the undesired terms in \mathbb{H}_g . A concrete implementation of this idea is the Brockett–Wegner flow [5, 11, 3, 4]. A main difficulty for setting up the flow (8) is to find an appropriate Banach space on which it possesses basic properties such as (local and global) existence in the flow parameter $t \geq 0$.

A natural idea is to write $\mathbb{W}(t) = \mathbb{Q}[\underline{w}^{(t)}] \in \mathcal{B}[\mathfrak{F}]$ and $\mathbb{G}(t) = \mathbb{Q}[\underline{g}^{(t)}] \in \mathcal{B}[\mathfrak{F}]$ as images of symbols $\underline{w}^{(t)}, \underline{g}^{(t)} \in \mathcal{W}$ under a linear quantization map $\mathbb{Q}: \mathcal{W} \rightarrow \mathcal{B}[\mathfrak{F}]$, where \mathcal{W} is a suitable Banach space of coefficients. Here and henceforth, we assume, for simplicity, Λ^* to be finite and, hence, the one-fermion space $\mathfrak{h} = \ell^2(\Lambda^*)$ and also the fermion Fock space $\mathfrak{F} = \mathfrak{F}[\mathfrak{h}]$ to be finite-dimensional, so that all operators are bounded. The Banach space $\mathcal{W} = \bigoplus_{m,n \geq 0} \mathcal{W}_{m,n}$ contains collections $\underline{w}^{(t)} = (\underline{w}_{m,n}^{(t)})_{m,n \geq 0}$ and $\underline{g}^{(t)} = (\underline{g}_{m,n}^{(t)})_{m,n \geq 0}$ of antisymmetric functions $\underline{w}_{m,n}^{(t)}, \underline{g}_{m,n}^{(t)}: (\Lambda^*)^m \times (\Lambda^*)^n \rightarrow \mathbb{C}$. Given $\underline{w} = (\underline{w}_{m,n})_{m,n \geq 0} \in \mathcal{W}$, its quantization $\mathbb{Q}[\underline{w}]$ is defined as

$$(9) \quad \mathbb{Q}[\underline{w}] := \sum_{m,n=0}^{\infty} \sum_{x_1^m \in (\Lambda^*)^m} \sum_{y_1^n \in (\Lambda^*)^n} w_{m,n}(x_1^m | y_1^n) a^*(x_1^m) a(y_1^n),$$

where $x_1^m = (x_1, \dots, x_m)$ with $x_1 < \dots < x_m$ and $y_1^n = (y_1, \dots, y_n)$ with $y_1 < \dots < y_n$, for some fixed total order on Λ^* . Moreover, $a^*(x_1^m) = a_{x_1}^* \cdots a_{x_m}^*$ and

$a(y_1^n) = a_{y_n} \cdots a_{y_1}$. Now observe that, for $\underline{v} = (\underline{v}_{m,n})_{m,n \geq 0}$, $\underline{w} = (\underline{w}_{m,n})_{m,n \geq 0} \in \mathcal{W}$, we have

$$(10) \quad \mathbb{Q}[\underline{v}] \mathbb{Q}[\underline{w}] = \mathbb{Q}[\underline{v} * \underline{w}],$$

with the convolution product defined by

$$(11) \quad (\underline{v} * \underline{w})_{M,N}(x_1^M | y_1^N) := \sum_{r=0}^{\infty} \sum_{m=0}^M \sum_{n=0}^N (-1)^{mn+r} r! \binom{m+r}{r} \binom{n+r}{r} \mathcal{A}_{M,N} \left[\sum_{z_1^r \in (\Lambda^*)^r} v_{M-m,n+r}(x_{m+1}^M | z_1^r, y_1^n) w_{m+r,N-n}(z_1^r, x_1^m | y_{n+1}^N) \right],$$

and $\mathcal{A}_{M,N}$ being the antisymmetrization operator. While the parametrization (9) seems natural, the No-Go theorem of Geisler [8] shows that, under some mild assumption on its form, no choice of norm $\|\cdot\|_{\mathcal{W}}$ on \mathcal{W} will

- make the convolution product (11) submultiplicative, i.e.,

$$(12) \quad \forall \underline{v}, \underline{w} \in \mathcal{W} : \quad \|\underline{v} * \underline{w}\|_{\mathcal{W}} \leq \|\underline{v}\|_{\mathcal{W}} \|\underline{w}\|_{\mathcal{W}},$$

- and at the same time control the operator norm, i.e.,

$$(13) \quad \forall \underline{w} \in \mathcal{W} : \quad \|\mathbb{Q}[\underline{w}]\|_{\mathcal{B}[\mathfrak{F}]} \leq \|\underline{w}\|_{\mathcal{W}}.$$

1.4. New Representation of Fermion Operators. We continue to report on joint work in progress with *J. Geisler* and *K. Merz*. Given the negative result of [8] that (12) and (13) plus some further natural assumptions lead to a contradiction, we propose to change the parametrization of operators on fermion Fock space altogether. We replace \mathcal{W} by a different Banach space $\widehat{\mathcal{W}}$ of interaction coupling functions $\underline{\hat{w}} : \mathfrak{P}(\Lambda^*)^3 \rightarrow \mathbb{C}$ of the form $\underline{\hat{w}} = (\hat{w}_{I,J,K})_{I \dot{\cup} J \dot{\cup} K \subseteq \Lambda^*}$, where $\mathfrak{P}(\Lambda^*)$ is the collection of subsets (power set) of Λ^* , and $\dot{\cup}$ denotes disjoint union. The quantization $\widehat{\mathbb{Q}} : \widehat{\mathcal{W}} \rightarrow \mathcal{B}[\mathfrak{F}]$ is defined by

$$(14) \quad \widehat{\mathbb{Q}}[\underline{\hat{w}}] := \sum_{I \dot{\cup} J \dot{\cup} K} \hat{w}_{I,J,K} a_I^* n_K a_J,$$

where the summation is defined as

$$(15) \quad \sum_{I \dot{\cup} J \dot{\cup} K} F(I, J, K) := \sum_{K \subseteq \Lambda^*} \sum_{J \subseteq \Lambda^* \setminus K} \sum_{I \subseteq \Lambda^* \setminus (K \cup J)} F(I, J, K),$$

$a_{\emptyset}^* := a_{\emptyset} := n_{\emptyset} := 1$, and

$$(16) \quad a_A^* := a_{\alpha_1}^* \cdots a_{\alpha_n}^*, \quad a_A := a_{\alpha_n} \cdots a_{\alpha_1}, \quad n_A := a_A^* a_A,$$

for $A = \{\alpha_1, \dots, \alpha_n\} \subseteq \Lambda^*$ with $\alpha_1 < \dots < \alpha_n$. We can show that this quantization possesses the following properties.

- For any $\underline{\hat{v}} = (\hat{v}_{I,J,K})_{I \dot{\cup} J \dot{\cup} K \subseteq \Lambda^*}$, $\underline{\hat{w}} = (\hat{w}_{I,J,K})_{I \dot{\cup} J \dot{\cup} K \subseteq \Lambda^*} \in \widehat{\mathcal{W}}$, the product of their quantizations

$$(17) \quad \widehat{\mathbb{Q}}[\underline{\hat{v}}] \mathbb{Q}[\underline{\hat{w}}] = \widehat{\mathbb{Q}}[\underline{\hat{v}} * \underline{\hat{w}}],$$

induces a convolution product on $\widehat{\mathcal{W}}$ given for disjoint $I, J, K \subseteq \Lambda^*$ by

$$(18) \quad (\hat{v} * \hat{w})_{I,J,K} = \sum_{I' \dot{\cup} J' \dot{\cup} K'} \sum_{I'' \dot{\cup} J'' \dot{\cup} K''} \sum_{G \subseteq J' \dot{\cup} I''} S_{I',J',K'; I'',J'',K''; G}^{I,J,K} \hat{v}_{I',J',K'} \hat{w}_{I'',J'',K''},$$

where $S_{I',J',K'; I'',J'',K''; G}^{I,J,K} \in \{-1, 1\}$ is an explicit function.

- For $\xi, \eta \geq 1$ with $\xi^2 \geq 1 + \eta$ define a norm on $\widehat{\mathcal{W}}$ for $\hat{w} = (\hat{w}_{I,J,K})_{I \dot{\cup} J \dot{\cup} K \subseteq \Lambda^*} \in \widehat{\mathcal{W}}$ by

$$(19) \quad \|\hat{w}\|_{\xi, \eta} := \sum_{I \dot{\cup} J \dot{\cup} K} \xi^{|I|+|J|} \eta^{|K|} |\hat{w}_{I,J,K}|.$$

Then

$$(20) \quad \|\hat{v} * \hat{w}\|_{\xi, \eta} \leq \|\hat{v}\|_{\xi, \eta} \|\hat{w}\|_{\xi, \eta}.$$

- For $\hat{w} \in \widehat{\mathcal{W}}$, the operator norm of $\widehat{\mathcal{Q}}[\hat{w}]$ is bounded by the norm of \hat{w} ,

$$(21) \quad \|\widehat{\mathcal{Q}}[\hat{w}]\|_{\mathcal{B}[\mathfrak{F}]} \leq \|\hat{w}\|_{\xi, \eta}.$$

Our current activity aims at implementing the diagonalizing flow (8) with $\mathbb{W}(t)$ and $\mathbb{G}(t)$ given by $\widehat{\mathcal{Q}}[\hat{w}(t)]$ and $\widehat{\mathcal{Q}}[\hat{g}(t)]$, respectively, for suitable $\hat{w}(t), \hat{g}(t) \in \widehat{\mathcal{W}}$.

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Bosonization for strongly interacting Fermi gases

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(joint work with S. Fournais and J. P. Solovej)

We study a gas consisting of $N \gg 1$ spinless fermions interacting through a two-body potential v modulated by the factor $N^{-\alpha}$, where α is a numerical parameter. The gas is described by the Hamiltonian

$$(1) \quad H_N = \sum_{i=1}^N (-\Delta_i) + N^{-\alpha} \sum_{1 \leq i < j \leq N} v(x_i - x_j)$$

on the Hilbert space of functions in $L^2((\mathbb{R}/\mathbb{Z})^{3N})$ antisymmetric with respect to permutations of the N copies of $(\mathbb{R}/\mathbb{Z})^3$. We are interested mostly in the ground state energy E_N of H_N .

Assuming that the Fourier series of v has non-negative coefficients $\widehat{v}(k)$ satisfying $\sum_k |k| \widehat{v}(k) < \infty$, we have elementary bounds

$$(2) \quad E_N^{(0)} \leq E_N \leq E_N^{(0)} + cN^{\frac{2}{3}-\alpha} \sum_k |k| \widehat{v}(k) + o(N^{\frac{2}{3}-\alpha}),$$

where $c > 0$ is an explicit constant and

$$(3) \quad E_N^{(0)} = \min_{\substack{p_1, \dots, p_N \in 2\pi\mathbb{Z}^3 \\ \text{distinct}}} \sum_{i=1}^N |p_i|^2 + \frac{N^{-\alpha}}{2} \int v - \frac{N^{1-\alpha}}{2} v(0).$$

One may ask whether one of the bounds in (2) is sharp up to $o(N^{\frac{2}{3}-\alpha})$. The answer is, at least for regular enough v : for $\alpha > \frac{1}{3}$ the upper bound is sharp, for $\alpha = \frac{1}{3}$ neither is sharp, and for $\alpha < \frac{1}{3}$ the lower bound is sharp. The last statement is our main new result.

The choice $\alpha = \frac{1}{3}$, often called the mean field scaling, has been studied extensively. In [1] Hamiltonians in the mean field scaling with small and very regular v were studied. It was explained how in such models one can use second order perturbation theory rigorously. If we take $\alpha > \frac{1}{3}$, which corresponds to interactions weaker than in the mean field scaling, the perturbative expansion is an even better approximation. In particular the reasoning in [1] shows that the upper bound in (2) is sharp up to our desired accuracy. The next term in E_N , given by second order of the perturbative expansion, is of order $N^{1-2\alpha} \ll N^{\frac{2}{3}-\alpha}$.

The understanding of the ground state energy in the mean field scaling was further improved in two series of works, [2, 3, 4] and [5, 6], where two approaches to approximate bosonization were developed. In both treatments one introduces operators which, in some sense, satisfy approximate canonical commutation rules and derives an effective Hamiltonian quadratic in the approximate bosons. Then that Hamiltonian is diagonalized using a Bogoliubov transformation. It is unclear whether the last step of this procedure can be justified also for $\alpha < \frac{1}{3}$, because then the generator of the Bogoliubov transformation is so large that it is difficult to control errors of the bosonic approximation.

In order to avoid the difficulties of working with a large Bogoliubov transformation, we do a variational calculation with the class of all vectors which can be obtained from the ground state of a non-interacting gas by acting with a polynomial in approximate bosons. More precisely, we construct a linear map from the Fock space of exact bosons to the fermionic Hilbert space and show that it is approximately isometric and approximately intertwines between H_N and the effective Hamiltonian. The quality of the approximation gets better as N increases, but it deteriorates very rapidly with the number of bosons in the state. Considering general states with $O(1)$ bosons and optimizing over the state after taking the limit $N \rightarrow \infty$ we obtain our result:

$$(4) \quad E_N = E_N^{(0)} + o(N^{\frac{2}{3}-\alpha}).$$

If one performs the Bogoliubov calculation non-rigorously, i.e. without controlling the error terms, one arrives at

$$(5) \quad E_N \approx E_N^{(0)} + \frac{N^{\frac{1-\alpha}{2}}}{\sqrt{2}} \sum_k |k| \sqrt{\widehat{v}(k)}. \quad (\text{conjectural!})$$

It seems that in order to justify this formula using the bosonization method one would have to understand how to control errors in calculations with states involving many bosons.

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Estimation of propagation of chaos via cumulant hierarchies in two example models

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(joint work with Aleksis Vuoksenmaa)

Propagation and generation of “chaos” is an important ingredient in rigorous control of applicability of kinetic theory, in general. Chaos can here be understood as sufficient statistical independence of random variables related to the “kinetic” observables of the system. Cumulant hierarchy of these random variables thus often gives a way of controlling the evolution and the degree of such independence, i.e., the amount of chaos in the system.

Motivated by recent successes of “direct” perturbation expansion results, such as those in [1, 2], we propose a way to combine such techniques into a simpler method to rigorously control the evolution of the cumulant hierarchy in two, qualitatively different, example cases for which kinetic theory is believed to be applicable: the discrete nonlinear Schrödinger evolution (DNLS) with suitable random, spatially homogeneous initial data, and the stochastic Kac model. In both cases, we set up suitable random variables and propose methods to control the evolution of their cumulant hierarchies. In this abstract, we focus only on the latter results.

The stochastic Kac model is a toy model introduced by Mark Kac in 1956 [3] for deriving a Boltzmann equation. It consists of N particles, where only velocities v_i , $i = 1, 2, \dots, N$, of the particles are tracked, and collisions between particles take place stochastically. The collisions are determined by a Poisson clock whose rate is scaled to match the time-scale of the kinetic evolution. Once the clock rings, the labels of the two colliding particles are picked randomly and, for the chosen pair, their velocities are mixed randomly in such a way that the total energy is always preserved in a collision.

Assuming, for simplicity, that the initial distribution has energy density one, it has been proven that the distribution of the system approaches uniform distribution on the corresponding constant energy surface. However, this convergence can be quite slow, taking order N time units for typical initial data. Also, already in his original work, Kac proved a version of propagation of chaos for this system: if the initial data is approximately of a product form, then it will remain approximately in a product form for later times and the single velocity marginal can be well approximated by the solution to a corresponding Boltzmann-type evolution equation. Summary of the related results and literature may be found from [4, 5].

In our work in progress, we have been able to improve these results in two ways: (1) We have fairly accurate estimates for finite cumulants which become very small (consistent with approximate independence) already at times which are order one. (2) Since our initial data is less restricted, we are also able to conclude *generation of chaos* for these cumulants.

A more precise summary, whose proof and detailed assumptions can be found from our upcoming work, is given in the following Theorems. The results concern

cumulants of the energies of the particles, i.e., the random variables $e_i := v_i^2$ and, for simplicity, we only consider the one-dimensional case, $v_i \in \mathbb{R}$.

Theorem 1 (preliminary for non-repeated cumulants). *Assume that the initial distribution is exchangeable, i.e., label permutation invariant. Suppose there is $B \geq 0$ such that the initial non-repeating energy cumulants $M_n^N(0)$ satisfy a bound $|M_n^N(0)| \leq B(n!)^2$. Then there is a constant A which only depends on B , such that the time-evolved non-repeating cumulants $M_n^N(t)$ satisfy the following bound for $n \geq 3$ and $t \geq 0$:*

$$|M_n^N(t)| \leq A^n (n!)^2 \left(\frac{1}{(N-1)^{n-1}} + e^{-\frac{A}{4}t} \right).$$

This indeed proves generation of chaos for all finite order non-repeating cumulants whenever $\ln N \gg \ln n$. The first term in the bound is uniformly $O(N^{-(n-1)})$ hence goes to zero as $N \rightarrow \infty$. This is consistent with the above mentioned convergence to a stationary distribution since the variables e_i are mildly correlated under the uniform distribution on the energy surface.

Theorem 2 (preliminary for general cumulants). *Assume that the initial distribution is exchangeable, i.e., label permutation invariant. Suppose there is $B \geq 0$ such that the initial energy cumulants $\kappa_0^{n,N}(e_s)$ satisfy a bound $|\kappa_0^{n,N}(e_s)| \leq B^{n^2}(n!)^2$. Then there is a constant A , which only depends on B , and $N_0(n) \in \mathbb{N}$, such that for every $N \geq N_0(n)$ the time-evolved cumulants $\kappa_t^{m,N}(e_s)$ satisfy the following bound for any $t \geq 0$ and any sequence s of m labels, $m \in \{3, 4, \dots, n\}$:*

$$|\kappa_t^{m,N}(e_s)| \leq A^{m^2} (m!)^2 \left(\frac{1}{(N-1)^{\text{len}(s)-1}} + e^{-\frac{1}{4}t} \right)$$

In the above, s is a sequence of m labels from $\{1, 2, \dots, N\}$, and $\text{len}(s)$ is the number of different labels in this sequence. The earlier bound for non-repeating cumulants is $e^{-\frac{\text{len}(s)}{4}t}$ while here we are only able to prove $e^{-\frac{1}{4}t}$. The proof is based on using an order on the structure of certain partition classifiers to control the linear part of the evolution and then iteratively propagating the upper bound.

In addition to the above generation of chaos bounds, it would be of interest to also look at relaxation for fixed N : Could we control (exponential) convergence of cumulants to their values in the uniform distribution on the sphere, as $t \rightarrow \infty$ for a fixed N ? Would it be possible to control the accuracy of kinetic theory predictions such as improving the earlier estimates for the accuracy of the solution of the Boltzmann equation?

How much of these techniques can be used for cumulant hierarchies of other models, such as the nonlinear Schrödinger equation, is still under investigation.

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The low density Fermi gas in three dimensions

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(joint work with Marco Falconi, Christian Hainzl, Marcello Porta)

In 1957 Huang-Yang (HY) conjectured a formula for the asymptotic expansion of the ground state energy density of the Fermi gas at low density and in the infinite volume limit (see [1]), the rigorous validation of which is still an open problem. Here we present some recent results aimed at paving the way for rigorously proving the HY formula. We consider N interacting fermions with spin $\sigma = \{\uparrow, \downarrow\}$ in a box $\Lambda_L := [-L/2, L/2]^3$, with periodic boundary conditions. The Hamiltonian of the system is

$$(1) \quad H_N = - \sum_{i=1}^N \Delta_{x_i} + \sum_{i < j=1}^N V(x_i - x_j),$$

and it acts on $L_a^2(\Lambda_L^{N_\uparrow}) \otimes L_a^2(\Lambda_L^{N_\downarrow})$, where $L_a^2(\Lambda_L^{N_\sigma})$ is the antisymmetric tensor product of N_σ copies of $L^2(\Lambda_L)$ with N_σ denoting the number of particles with spin $\sigma = \{\uparrow, \downarrow\}$ ($N = N_\uparrow + N_\downarrow$). Correspondingly, we set $\rho_\sigma := N_\sigma/L^3$ ($\rho = \rho_\uparrow + \rho_\downarrow$). In the following, we will assume that our system is dilute, i.e., $\rho_\sigma \ll 1$. The interaction potential V is such that

$$(2) \quad V(x - y) = \frac{1}{L^3} \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \hat{V}_\infty(p) e^{ip \cdot (x-y)}, \quad \hat{V}_\infty(p) = \int_{\mathbb{R}^3} dx V_\infty(x) e^{-ip \cdot x},$$

where V_∞ is supposed to be non negative, radial, smooth and compactly supported.

We are interested in the thermodynamic limit, meaning that $N_\sigma, L \rightarrow \infty$ keeping ρ_σ fixed. In this setting, it is well known [2] that, in units such that $\hbar = 1$ and putting the masses of the particles equal to $1/2$, the ground state energy per unit volume can be approximated as

$$(3) \quad e(\rho_\uparrow, \rho_\downarrow) = \frac{3}{5} (6\pi^2)^{\frac{2}{3}} (\rho_\uparrow^{\frac{5}{3}} + \rho_\downarrow^{\frac{5}{3}}) + 8\pi a \rho_\uparrow \rho_\downarrow + o(\rho^2) \quad \text{as } \rho \rightarrow 0.$$

The first term in the above expansion is purely kinetic (the kinetic energy of the free Fermi gas), and the fact that this contribution is proportional to $\rho^{5/3}$ is a consequence of the fermionic nature of the wave function. The effect of the interaction appears at the next order, via the parameter a , which is the scattering length of the interaction potential. In particular the contribution $\mathcal{O}(\rho^2)$ in (3) corresponds to the leading order in the asymptotic expansion for the correlation

energy, which is defined as the difference between the ground state energy and that of the free Fermi gas. In [1] Huang-Yang conjectured a refined version of the asymptotics in (3) in the case where $\rho = \rho_\uparrow/2 + \rho_\downarrow/2$:

$$(4) \quad e(\rho) = \frac{3}{5}(3\pi^2)^{\frac{2}{3}}\rho^{\frac{5}{3}} + 2\pi a\rho^2 + \frac{4(11 - 2 \log 2)}{35\pi^2} \left(\frac{3}{4\pi}\right)^{\frac{4}{3}} a^2\rho^{\frac{7}{3}} + o\left(\rho^{\frac{7}{3}}\right).$$

as $\rho \rightarrow 0$. In 2021, the same asymptotics as the one in (3) have been re-derived in [3]. Differently than in [2], in [3] more restrictions are put in the interaction potential, but better error estimates are obtained. However, the main difference between [2] and [3] is the approach taken. In particular, the main novelty in [3] is the use of Bogoliubov theory applied to pairs of fermions (particle-hole pairs) that behave approximately as bosonic particles. Developing further this approach, in [4] refined asymptotics estimates are obtained, as stated below.

Theorem 1. *Let V, V_∞ as in (2) with V_∞ non negative, radial, smooth and compactly supported. There exists $L_0 > 0$ such that for $L \geq L_0$, it holds*

$$(5) \quad e_L(\rho_\uparrow, \rho_\downarrow) = \frac{3}{5}(6\pi^2)^{\frac{2}{3}}(\rho_\uparrow^{\frac{5}{3}} + \rho_\downarrow^{\frac{5}{3}}) + 8\pi a\rho_\uparrow\rho_\downarrow + r_L(\rho_\uparrow, \rho_\downarrow),$$

where a is the scattering length of the interaction potential V_∞ and

$$-C\rho^{2+\frac{1}{5}} \leq r_L(\rho_\uparrow, \rho_\downarrow) \leq C\rho^{\frac{7}{3}}.$$

Note that the upper bound in Theorem 1 is optimal, in the sense that it agrees with the HY formula in (4). We also mention that very recently the ground state energy of the dilute spin-polarized Fermi gas was studied in [6] and with similar techniques an almost optimal upper bound for the ground state energy of a dilute spin 1/2 Fermi gas was derived (via cluster expansion) in [5].

The general strategy of the proof of Theorem 1 is based on the use of almost bosonic operators to describe the low energy excitations around the Fermi ball. These operators are defined as

$$(6) \quad b_{p,\sigma}^* = \sum_{\substack{k \in \mathcal{B}_F^\sigma \\ k+p \notin \mathcal{B}_F^\sigma}} a_{k+p,\sigma}^* a_{k,\sigma}^*, \quad b_{p,\sigma} = \sum_{\substack{k \in \mathcal{B}_F^\sigma \\ k+p \notin \mathcal{B}_F^\sigma}} a_{k,\sigma} a_{k+p,\sigma}$$

where a^*, a are the fermionic creation/annihilation operators. In (6), \mathcal{B}_F^σ denotes the Fermi ball, i.e., $\mathcal{B}_F^\sigma := \{k \in (2\pi/L)\mathbb{Z}^3 \mid |k| \leq k_F^\sigma\}$, and k_F^σ is the Fermi momentum which, for fixed densities and in the limit $L \rightarrow \infty$, can be written as $k_F^\sigma = (6\pi^2)^{1/3} \rho_\sigma^{1/3} + o(1)$. The reason why we refer to the operators in (6) as *almost-bosonic operators* is that, when acting on states with few particles, they approximately behave as bosonic creation/annihilation operators (i.e., they almost satisfy the canonical commutation relations). Once these operators are introduced, the main idea is to express the relevant contributions to the correlation energy in terms of b, b^* and to diagonalise this effective energy via an (almost-bosonic)

Bogoliubov transformation, which is explicitly written as

$$(7) \quad T = \exp \left\{ \frac{1}{L^3} \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \hat{\varphi}(p) \hat{b}_{p,\uparrow} \hat{b}_{-p,\downarrow} - \text{h.c.} \right\}.$$

Note that, the choice of $\hat{\varphi}$ is responsible for getting the right dependence on the scattering length in the constant term we want to extract, i.e., $8\pi a \rho_{\uparrow} \rho_{\downarrow}$. In other words, $\hat{\varphi}$ is related to the scattering equation. Finally, we emphasise that since we are working directly in the thermodynamic limit, both in [3, 4] we need to introduce some localizations in order to obtain decay estimates that are not true in the original setting. More specifically, we need to use a regularised version of the almost bosonic creation/annihilation operators. In [4]¹ this corresponds to discarding some momenta inside the Fermi ball, i.e., all the $k \in (2\pi/L)\mathbb{Z}^3$ in $k_F + \rho^{2/3} < |k| < k_F$ and some others outside², i.e., all the momenta in the annulus $k_F < |k| < 2k_F$ or $|k| > \rho^{-\beta}$. In our approach, however, we not only need to regularise the almost bosonic operators but we also need to localise $\hat{\varphi}$: it turns out that it is convenient to do this localisation in configuration space. The way we do it is different in [3] and [4]. We conclude by comparing these two different approaches. In [3] we take³ $\varphi \equiv \varphi_{\gamma}$, where φ_{γ} is the periodization of the solution of the Neumann problem in a ball $B \equiv B_{\rho^{-\gamma}}(0) \subset \mathbb{R}^3$ centered at zero and with radius $\rho^{-\gamma}$. More precisely, φ_{γ} is the periodization of $\varphi_{\gamma,\infty}$ which is the solution of

$$-2\Delta(1 - \varphi_{\gamma,\infty}) + V_{\infty}(1 - \varphi_{\gamma,\infty}) = \lambda_{\gamma}(1 - \varphi_{\gamma,\infty}), \quad \varphi_{\gamma,\infty} = 2\nabla\varphi_{\gamma,\infty} = 0 \text{ on } \partial B,$$

where $|\lambda_{\gamma}| \leq C\rho^{3\gamma}$. In [4], instead, $\varphi(x)$ is taken to be the periodization of a localized version of the solution of the zero energy scattering equation in \mathbb{R}^3 , which reads as

$$\varphi_{\infty}(x) := \varphi_0(x)\chi(x/\rho^{-1/3}), \quad 2\Delta\varphi_0 V(1 - \varphi_0) = 0, \quad \varphi_0(x) \rightarrow 0 \text{ as } |x| \rightarrow \infty,$$

where χ is a smooth cut-off function in \mathbb{R}^3 , which varies smoothly between 0 and 1 in the annulus $\rho^{-1/3} \leq |x| \leq 2\rho^{-1/3}$. As a consequence of our localization, $\varphi_{\infty} = \varphi_0$ in the support of the interaction potential V_{∞} and it is such that φ_{∞}

$$2\Delta\varphi_{\infty} + V_{\infty}(1 - \varphi_{\infty}) \sim -2a \left[\frac{2\rho^{1/3}}{|x|^2} + \frac{\rho^{2/3}}{|x|} \right] \chi(|x| \sim \rho^{-1/3}),$$

where a is the scattering length of the interaction potential. This different way of doing the localization allows us to better estimate many error terms recovering the optimal estimate in the proof of the upper bound in Theorem 1.

¹In [3] a different choice of the cut-off is used.

²The smoothness of the interaction potential is needed to justify the ultraviolet cut-off.

³In [3], we take $\gamma = 2/9$ for the upper bound and $\gamma = 1/3$ in the lower bound.

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A tracer particle interacting with a cold quantum gas

PETER PICKL

(joint work with Viet Hoang, Maximilian Jeblick, Jonas Lampart,
David Mitroskas, Sören Petrat)

The computation of effective equations in many body systems is an interesting area of research and was the topic of the Oberwolfach Min-Workshop where this presentation was held. In the talk I will present recent findings on the dynamics of a so called tracer particle entering a cold quantum gas. Both cases, gases made of Fermions and of Bosons, will be considered. The question is of physical interest, since the influence of the gas on the dynamics of the tracer can be used to gain information of the underlying interactions of the system. In the Bosonic case it has been shown recently, that – assuming constant density of the gas and a respective scaling of the interaction of the gas particles with the tracer – the system is effectively described by the Bogoliubov-Fröhlich Hamiltonian: the interaction of the tracer will be of leading order influenced by the Bogoliubov excitations in the gas [1] and excite itself further particles of a similar number as the Bogoliubov excitations. In the Fermionic case the rigidity of the Fermi-ball plays an important role for the dynamics of the tracer. It suppresses the effective interaction significantly and leads to free evolution of the tracer for relatively strong couplings [2] respectively an effective interaction between tracers when shooting more than one tracer particle into the gas [3]. At the end of the talk, new, so far unpublished findings for the Fermi gas will be presented. Together with Viet Hoang we could show that, increasing the tracer-gas coupling, the leading order dynamics will be given by a tracer coupled to a phonon field. The phonons describe the pair-excitations in the gas and behave like Bosons.

Possible extensions and open questions are the generalization of these findings to systems of large volumes. Further it should, at least in the case of an absence of interaction within the gas, be possible to extend the time scales for which one can proof validity of the effective descriptions to times polynomial in the density

rather than logarithmic. On large time scales, new physical phenomena should become visible.

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Some mathematical results in Density Functional Theory

MATHIEU LEWIN

(joint work with Elliott H. Lieb and Robert Seiringer)

I review some mathematical results in Density Functional Theory (DFT) following [4]. Consider N electrons in \mathbb{R}^3 and assume that they have the one-particle density ρ (a non-negative function such that $\int_{\mathbb{R}^3} \rho(x) dx = N$). *Lieb’s functional* [5] provides the lowest possible energy of these electrons at the given ρ :

$$(1) \quad F(\rho) := \inf_{\rho_\Gamma = \rho} \text{tr} (H^N(0)\Gamma).$$

The infimum is over all N -particle mixed states Γ on $\bigwedge_1^N L^2(\mathbb{R}^3, \mathbb{C}^2)$ having density $\rho_\Gamma = \rho$. Here

$$H^N(V) := \sum_{j=1}^N (-\Delta_{x_j} + V(x_j)) + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|}$$

is the usual Coulomb N -particle Hamiltonian in an external potential V — in (1) we took $V \equiv 0$. The main interest of $F(\rho)$ is that the ground state energy in any external potential V can be expressed as

$$(2) \quad \min \sigma(H^N(V)) = \inf_{\int_{\mathbb{R}^3} \rho = N} \left\{ F(\rho) + \int_{\mathbb{R}^3} \rho(x)V(x) dx \right\}.$$

This minimization problem is settled in the physical space \mathbb{R}^3 and not in the N -particle space \mathbb{R}^{3N} . If we knew how to compute $F(\rho)$, this would dramatically decrease the computational cost of the ground state energy. Unfortunately, $F(\rho)$ is a highly nonlinear and nonlocal unknown functional which is defined in terms of N -particle states. The cost of computing $F(\rho)$ is probably at least as high as solving Schrödinger’s equation. The purpose of (orbital-free) DFT is to provide simple but efficient approximations of $F(\rho)$.

The most famous is the *Local Density Approximation* (LDA), where it is assumed that ρ is locally flat and the local energy is taken to be that of an infinite gas of constant density, per unit volume:

$$F(\rho) \approx F_{\text{LDA}}(\rho) := \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dx dy + \int_{\mathbb{R}^3} f(\rho(x)) dx,$$

where $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ is the energy per unit volume of the infinite uniform electron gas. The LDA was rigorously justified for the first time in [3], for the grand-canonical version of $F(\rho)$. It is an open problem to justify the LDA for the canonical functional $F(\rho)$.

Another regime is the *large density limit*, where the kinetic energy dominates and the system becomes non-interacting. This limit can be stated as

$$\lim_{\lambda \rightarrow \infty} \frac{F(\rho_\lambda)}{\lambda^2} = T(\rho), \quad \rho_\lambda(x) = \lambda^3 \rho(\lambda x).$$

The kinetic energy can be expressed in terms of the one-particle density matrix γ (a trace-class operator on $L^2(\mathbb{R}^3)$) as

$$(3) \quad T(\rho) = \inf_{\substack{\Gamma \\ \rho_\Gamma = \rho}} \text{tr} \left(\sum_{j=1}^N (-\Delta)_{x_j} \right) \Gamma = \inf_{\substack{0 \leq \gamma = \gamma^* \leq 1 \\ \rho_\gamma = \rho}} \text{tr}(-\Delta)\gamma.$$

Let us now discuss some known bounds on $T(\rho)$ and work in any dimension $d \geq 1$. The Hoffman-Ostenhof inequality state that

$$T(\rho) \geq \int_{\mathbb{R}^d} |\nabla \sqrt{\rho}(x)|^2 dx.$$

This implies that $\sqrt{\rho} \in H^1(\mathbb{R}^d)$ is a necessary condition for $T(\rho)$ to be finite. It was proved in [5] that this is also a sufficient condition. For the proof one takes as trial state the Slater determinant $\Psi = (N!)^{-1/2} \det(\phi_j(x_k))$ with $\phi_j = \sqrt{\rho/N} e^{i\theta_j(x)}$. The phases θ_j are chosen so that the ϕ_j are orthonormal, with $\int_{\mathbb{R}^d} \rho |\nabla \theta_j|^2 < \infty$. It is very hard to construct such phases and get good bounds. In [5] Lieb got

$$T(\rho) \leq \left(\frac{\pi^2}{3} N^2 + CN \right) \int_{\mathbb{R}^d} |\nabla \sqrt{\rho}(x)|^2 dx.$$

This blows up quite fast with N . The growth was later improved to the optimal rate $CN^{2/d}$ in [1]. In fact, an extensive bound cannot only involve gradients. It should at least also include the semi-classical approximation of $T(\rho)$,

$$T(\rho) \approx c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+\frac{2}{d}} dx, \quad c_{\text{TF}} = \frac{\pi^2 d}{(d+2)q^{2/d}} \left(\frac{d}{|\mathbb{S}^{d-1}|} \right)^{\frac{2}{d}}$$

where c_{TF} is the semi-classical (a.k.a. Thomas-Fermi) constant. Here q is the number of spin states, which is $q = 2$ for electrons. Choosing the phases θ_j appropriately, March and Young [6] had already obtained in dimension $d = 1$

$$(4) \quad T(\rho) \leq \frac{\pi^2}{12} \int_{\mathbb{R}} \rho(x)^3 dx + \int_{\mathbb{R}} \left| (\sqrt{\rho})'(x) \right|^2 dx.$$

The first constant is just c_{TF} in $d = 1$, which led them to conjecture the following inequality in any dimension

$$(5) \quad T(\rho) \stackrel{?}{\leq} c_{TF} \int_{\mathbb{R}^d} \rho(x)^{1+\frac{2}{d}} dx + C \int_{\mathbb{R}^d} |\nabla\sqrt{\rho}(x)|^2 dx,$$

This conjecture is still open in dimension $d \geq 2$, but recent works came arbitrarily close to the result in the following sense.

Theorem 1 (Semi-classical estimates on the kinetic energy functional). *Let $d \geq 1$. There exists a constant $C = C(d)$ such that*

$$(6) \quad c_{TF}e^{-\varepsilon} \int_{\mathbb{R}^d} \rho^{1+\frac{2}{d}} - \frac{C}{\varepsilon} \int_{\mathbb{R}^d} |\nabla\sqrt{\rho}|^2 \leq T(\rho) \\ \leq c_{TF}(1 + \varepsilon) \int_{\mathbb{R}^d} \rho^{1+\frac{2}{d}} - \frac{C(1 + \varepsilon)}{\varepsilon} \int_{\mathbb{R}^d} |\nabla\sqrt{\rho}|^2$$

for any $\varepsilon > 0$ and any $\rho \geq 0$ with $\sqrt{\rho} \in H^1(\mathbb{R}^d)$.

The lower bound was first proved in [7] but with the coefficient $C/\varepsilon^{3+4/d}$ in front of the second term. The upper bound was shown in [3], using the simple trial state

$$\gamma = \int_0^\infty \sqrt{\eta\left(\frac{t}{\rho(x)}\right)} \mathbb{1}\left(-\Delta \leq \frac{d+2}{d}c_{TF}t^{\frac{2}{d}}\right) \sqrt{\eta\left(\frac{t}{\rho(x)}\right)} \frac{dt}{t},$$

where $\eta \in C_c^\infty(\mathbb{R}_+, \mathbb{R}_+)$ is so that $\int_0^\infty \eta(t) dt = 1$ and $\int_0^\infty t^{-1}\eta(t) dt \leq 1$. Here the two functions $\sqrt{\eta(t/\rho(x))}$ are interpreted as multiplication operators. The main idea is to locate the places where $\rho(x) \approx t$ using the cut-off function η and to place a free Fermi gas of density t there. Concentrating η about 1 at scale ε one obtains the upper bound in (6). This idea was recently pursued in [8] to also provide the stated lower bound. In fact, taking ε large enough and using the Hofmann-Ostenhof inequality provides a very simple proof of the Lieb-Thirring inequality. If we scale a density ρ as $\rho(\hbar x)$ and take $\varepsilon = \hbar$ in(6), we find

$$T(\rho_\hbar) = c_{TF}\hbar^{-d} \int_{\mathbb{R}^d} \rho^{1+\frac{2}{d}} + O(\hbar^{-d+1}).$$

An interesting open problem is to justify the next order, which is predicted to be

$$\frac{d-2}{3d}\hbar^{-d+2} \int_{\mathbb{R}^d} |\nabla\sqrt{\rho}(x)|^2 dx.$$

The negativity of the coefficient in $d = 1$ is related to the non-optimality of the semi-classical constant for the Lieb-Thirring inequality in dimension $d = 1$ [2].

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Spectral estimates for Schrödinger operators with Neumann boundary conditions on Hölder domains

CHARLOTTE DIETZE

Netrusov and Safarov proved Weyl’s law

$$(1) \quad N(-\Delta_{\Omega}^N - \lambda) = \frac{|B_1^d(0)|}{(2\pi)^d} |\Omega| \lambda^{\frac{d}{2}} + o\left(\lambda^{\frac{d}{2}}\right) \text{ as } \lambda \rightarrow \infty,$$

for γ -Hölder domains Ω with Neumann boundary conditions for all Hölder exponents $\gamma \in (\frac{d-1}{d}, 1)$ [1, Corollary 1.6]. They also showed that Weyl’s law fails for all $\gamma \in (0, \frac{d-1}{d}]$. More precisely, for those γ , there exists a γ -Hölder domain Ω such that (1) is not true [1, Theorem 1.10].

We consider Weyl’s law for Schrödinger operators on Hölder domains Ω

$$(2) \quad N(-\Delta_{\Omega}^N + \lambda V) = (2\pi)^{-d} |B_1^d(0)| \lambda^{\frac{d}{2}} \int_{\Omega} |V|^{\frac{d}{2}} + o\left(\lambda^{\frac{d}{2}}\right) \text{ as } \lambda \rightarrow \infty,$$

where $V : \Omega \rightarrow (-\infty, 0]$. In view of [1], one might expect that (2) holds for all $\gamma \in (\frac{d-1}{d}, 1)$ and $V \in L^{d/2}(\Omega)$. For every $\gamma \in (\frac{d-1}{d}, 1)$ we give an explicit example for a γ -Hölder domain Ω , and $V \in L^{d/2}(\Omega)$, where (2) fails [2, Theorem 1.1]. However, if we assume more integrability on V , namely that it is in some weighted L^p -space for some $p = p(d, \gamma) > d/2$, we prove (2) [2, Theorem 1.3].

The proof of (2) relies on a Cwikel-Lieb-Rozenblum-type bound for the number of negative eigenvalues of the Schrödinger operator $-\Delta_{\Omega}^N + V$ [2, Theorem 1.2]. In the proof of this Cwikel-Lieb-Rozenblum-type bound, we use a new covering theorem, and a new Poincaré-Sobolev inequality for suitably chosen small rectangles intersected with Ω .

Further details and explanations can also be found in [3].

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The Random Batch Method for Quantum Dynamics

FRANÇOIS GOLSE

(joint work with Shi Jin & Thierry Paul)

Consider the quantum Hamiltonian for a system of N identical particles

$$\mathcal{H}_N := \sum_{m=1}^N -\frac{1}{2}\hbar^2 \Delta_{x_m} + \frac{1}{N-1} \sum_{1 \leq l < n \leq N} V(x_l - x_n),$$

where V is an even, real-valued function. The cost of computing the interaction potential is $\frac{1}{2}N(N - 1)$ evaluations of V and additions.

The Random Batch Method (RBM) is, at each time step (1) to replace the total interaction of each particle with the $N - 1$ other particles by the interaction with $p \ll N$ other particles chosen at random multiplied by $(N - 1)/p$ (with a computing cost $Np \ll \frac{1}{2}N(N - 1)$ operations), and (2) to reshuffle the particles at each time step (with a computing cost $O(N)$ by Durstenfeld’s algorithm [3]).

1. FORMULATION OF THE RBM: CASE $p = 2$

Let $N \geq 2$ be an even integer. Let $\sigma_1, \sigma_2, \dots, \sigma_j, \dots$ be a sequence of random mutually independent elements of \mathfrak{S}_N distributed uniformly. Given $\Delta t > 0$, define

$$\mathbf{T}_t(l, n) := \begin{cases} 1 & \text{if } \{l, n\} = \{\sigma_{[t/\Delta t]+1}(2k - 1), \sigma_{[t/\Delta t]+1}(2k)\} \text{ for some } k = 1, \dots, \frac{N}{2}, \\ 0 & \text{otherwise.} \end{cases}$$

and

$$\tilde{\mathcal{H}}_N(t) := \sum_{m=1}^N -\frac{1}{2}\hbar^2 \Delta_{x_m} + \sum_{1 \leq l < n \leq N} \mathbf{T}_t(l, n)V(x_l - x_n).$$

The RBM dynamics is defined by the Cauchy problem

$$i\hbar \partial_t \tilde{R}_N(t) = [\tilde{\mathcal{H}}_N(t), \tilde{R}_N(t)], \quad \tilde{R}_N(0) = R_N^{in}.$$

In the sequel, we seek to compare

$$R_N(t) := e^{-it\mathcal{H}_N/\hbar} R_N^{in} e^{it\mathcal{H}_N/\hbar}, \quad \text{and} \quad \tilde{R}_N(t).$$

2. CONVERGENCE OF THE RBM

The convergence of the RBM is couched in terms of the Wigner function. Any trace-class operator S on $\mathfrak{H} = L^2(\mathbf{R}^d)$ is defined by an integral kernel $s \equiv s(x, y)$ such that (see Lemma 2.1 in [1])

$$z \mapsto [x \mapsto s(x + z, x - z)] \in C_b(\mathbf{R}_z^d; L^1(\mathbf{R}_x^d)) .$$

Its Wigner function is the Fourier transform (in $\mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d)$)

$$W_{\hbar}[S](x, \xi) := \frac{1}{(2\pi)^d} \int_{\mathbf{R}^d} s(x + \frac{1}{2}\hbar y, x - \frac{1}{2}\hbar y) e^{-i\xi \cdot y} dy .$$

We shall also need the dual norm

$$\|f\|_{-m} := \sup \left\{ \left| \int_{\mathbf{R}^{2d}} f(z) \overline{a(z)} dz \right| : a \in C_c^\infty(\mathbf{R}^{2d}) \text{ and } \max_{0 < |\alpha| \leq m} \|\partial^\alpha a\|_{L^\infty} \leq 1 \right\} .$$

Finally, the notion of symmetrized 1-particle marginal $\tilde{R}_{N:1}(t)$ of $\tilde{R}_N(t)$ is defined as follows: for all $A \in \mathcal{L}(\mathfrak{H})$,

$$\text{tr}_{\mathfrak{H}}(\tilde{R}_{N:1}(t)A) := \frac{1}{N} \sum_{k=1}^N \text{tr}_{\mathfrak{H}_N}(\tilde{R}_N(t)J_k A)$$

where $\mathfrak{H}_N = \mathfrak{H}^{\otimes N} = L^2(\mathbf{R}^{dN})$ and

$$J_k A := I_{\mathfrak{H}}^{\otimes(k-1)} \otimes A \otimes I_{\mathfrak{H}}^{\otimes(N-k)} .$$

Theorem. [4] *Assume that V is an even real-valued function on \mathbf{R}^d with Fourier transform $\hat{V} \in L^2(\mathbf{R}^d; (1+|\omega|^2)d\omega)$, while $(R_N^{in})^* = R_N^{in} \geq 0$ satisfies $\text{tr}_{\mathfrak{H}_N} R_N^{in} = 1$. Then, for all $\Delta t, \hbar \in (0, 1)$, all even $N \geq 2$ and all $t \geq 0$,*

$$\begin{aligned} & \| \|W_{\hbar}[\mathbf{E}\tilde{R}_{N:1}(t) - R_{N:1}(t)] \| \|_{-[d/2]-3} \\ & \leq 5\Delta t \cdot \gamma_d L(V) (1 + (1 + 2\sqrt{d})L(V)t) e^{6t \max(1, \sqrt{d}L(V))} , \end{aligned}$$

where $L(V) = (2\pi)^{-d} \|(d + |\omega|^2)\hat{V}\|_{L^1}$.

This result proves the convergence of 1-particle observables for the RBM as the reshuffling time step $\Delta t \rightarrow 0$, uniformly in the particle number N and in the Planck constant \hbar . We have treated only the case $p = 2$; larger values of p can be handled in essentially the same manner — in fact, one expects that the larger p , the better the RB approximation will be.

3. METRIZING THE SET OF DENSITY OPERATORS

Let $\mathcal{D}(\mathfrak{H}) = \{R = R^* \in \mathcal{L}(\mathfrak{H}) : R \geq 0 \text{ and } \text{tr}_{\mathfrak{H}}(R) = 1\}$ the set of density operators on \mathfrak{H} . For $R, S \in \mathcal{D}(\mathfrak{H})$, set

$$d_{\hbar}(R, S) := \sup_{A \in \mathcal{L}(\mathfrak{H})} \{ |\text{tr}_{\mathfrak{H}}((R - S)A)| : \sup_{1 \leq j, k \leq d} SC_{j,k}(A) \leq 5\hbar^2 \} ,$$

where

$$\begin{aligned} SC_{j,k}(A) := & \hbar \| [x^j, A] \| + \hbar \| [-i\partial_{x^j}, A] \| + \| [x^k, [x^j, A]] \| \\ & + \| [-i\hbar\partial_{x^k}, [x^j, A]] \| + \| [-i\hbar\partial_{x^k}, [-i\hbar\partial_{x^j}, A]] \| . \end{aligned}$$

Proposition. [4]

- (1) The functional $d_{\hbar} : \mathcal{D}(\mathfrak{H}) \times \mathcal{D}(\mathfrak{H}) \rightarrow [0, +\infty]$ is an extended metric.
- (2) There exists $\gamma_d > 0$ depending only in the space dimension d such that

$$\| \|W_{\hbar}[R - S]\| \|_{-[d/2]-3} \leq \gamma_d d_{\hbar}(R, S), \quad R, S \in \mathcal{D}(\mathfrak{H}) .$$

The proof of this proposition is based on the duality formula

$$\int_{\mathbf{R}^{2d}} W_{\hbar}[T](x, \xi) \overline{a(x, \xi)} dx d\xi = \text{tr}_{\mathfrak{H}}(TA^*)$$

where A is the Weyl operator with symbol a , and on the Calderón-Vaillancourt theorem [2].

The definition of d_{\hbar} is reminiscent of the Kantorovich-Rubinstein duality formula (Theorem 1.14 in [6]) for the Monge-Kantorovich distance \mathcal{MK} between Borel probability measures on \mathbf{R}^n with finite first order moment

$$\mathcal{MK}(\mu, \nu) := \sup_{\text{Lip}(\phi) \leq 1} \left| \int_{\mathbf{R}^n} \phi(z) \mu(dz) - \int_{\mathbf{R}^n} \phi(z) \nu(dz) \right|$$

The quantum analogue of this metric for $R, S \in \mathcal{D}(\mathfrak{H})$ is

$$MK_{\hbar}(R, S) := \sup_{A \in \mathcal{L}(\mathfrak{H})} \{ |\text{tr}_{\mathfrak{H}}((R - S)A)| : \sup_{1 \leq j \leq d} \widetilde{SC}_j(A) \leq \hbar \},$$

where

$$\widetilde{SC}_j(A) = \max(\| [x^j, A] \|, \| [-i\hbar \partial_{x^j}, A] \|).$$

The analogy comes from the correspondence principle, which says that

$$\frac{i}{\hbar} [x^j, \cdot] \rightarrow \{x^j, \cdot\} = -\partial_{\xi^j}, \quad \frac{i}{\hbar} [-i\hbar \partial_{x^j}, \cdot] \rightarrow \{\xi^j, \cdot\} = \partial_{x^j},$$

where $\{\cdot, \cdot\}$ is the Poisson bracket defined on pairs of C^1 functions on phase space, while ξ^j is the j -th component of the classical momentum variable ξ , which is conjugate to the j th position coordinate x^j .

The proof of the theorem of convergence of the RBM is based on proving that

$$d_{\hbar}(\mathbf{E}\tilde{R}_{N:1}(t), R_{N:1}(t)) \leq 5\Delta t L(V)(1 + (1 + 2\sqrt{d})L(V)t)e^{6t \max(1, \sqrt{d}L(V))}$$

by a duality argument. In the course of the proof, one needs to control commutators with the interaction potential V in terms of d_{\hbar} . This is done with the following lemma.

Lemma. Let $f \equiv f(x)$ such that \hat{f} and $\widehat{\partial_x f}$ belong to $L^1(\mathbf{R}^d)$. Then

$$\| [f, T] \| \leq \max_{1 \leq j \leq d} \| [x^j, T] \| \cdot \frac{1}{(2\pi)^d} \sum_{j=1}^d \| \widehat{\partial_{x^j} f} \|_{L^1} .$$

For a quick proof of this inequality, see formula (55) in [5].

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Magnetic properties of ground states in many-electron systems

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(joint work with K. Nishimata, H. Tominaga)

In crystals, electrons exhibit the following fundamental properties: (i) Fermi statistics, (ii) spin, (iii) Coulomb repulsion, and (iv) itinerancy. Explaining ferromagnetism in metals solely based on these properties remains a significant goal in condensed matter physics.

In 1963, Gutzwiller, Kanamori, and Hubbard proposed a simple model to describe electrons on a crystal lattice and analyzed the magnetic properties of the ground state [1, 2, 3]. This model, known today as the Hubbard model, is one of the simplest models that captures the four fundamental properties mentioned earlier.

Subsequently, various studies, including numerical calculations, have been conducted on this model in theoretical physics. However, a precise explanation of the quantum origin of metallic ferromagnetism remains incomplete.

In this talk, I will first explain fundamental issues in the rigorous analysis of metallic ferromagnetism. Next, I will elaborate on the basic theorems in this field, namely the Marshall–Lieb–Mattis theorem [5, 6], Lieb’s theorem [4], and their stability [9, 10]. After revealing the similar structures inherent in these three theorems, I will consider the following problem: constructing a unified mathematical theory that can describe them all. In this talk, I will formulate this theory using the standard form of von Neumann algebras. As a result, I will establish the existence of a set of Hamiltonians \mathcal{C}_{MLM} possessing the following properties [11, 13]:

- (1) All ground states of Hamiltonians in \mathcal{C}_{MLM} exhibit properties akin to those stated in the Marshall–Lieb–Mattis theorem for the ground states of Heisenberg models.
- (2) \mathcal{C}_{MLM} contains a countably infinite number of elements.

We refer to \mathcal{C}_{MLM} as the Marshall–Lieb–Mattis (MLM) stability class. The MLM stability class enables the explanation of the magnetic properties of ground states in half-filling many-electron systems on bipartite lattices. For instance, it is demonstrated that Hamiltonians describing systems where many electrons interact

with phonons or photons belong to \mathcal{C}_{MLM} . Consequently, the magnetic properties of the ground states of these Hamiltonians satisfy the aforementioned property (1), see [9, 10, 11]. This implies the stability of magnetic properties in the ground states under electron-lattice interactions.

In addition to the MLM stability class, several stability classes can be constructed, such as the Nagaoka–Thouless stability class [11, 13, 14]. These stability classes are determined by factors such as the filling factor, crystal structure, and Coulomb interaction, each corresponding to different scenarios in many-electron systems. Each stability class describes the stability of magnetic states in many-electron systems in different situations.

A modified version of the MLM stability class, known as the deformed MLM stability class, encompasses models such as the Kondo lattice model and the periodic Anderson model. Moreover, it includes Hamiltonians derived by introducing electron-phonon interactions to these models [12, 15]. Consequently, the stability of magnetic properties in the ground states of the Kondo lattice model and periodic Anderson model, influenced by these interactions, can be expounded through the attributes of this deformed MLM stability class.

In this talk, due to time constraints, I will elucidate findings pertaining to finite lattice systems. For discussions on the infinite volume limit using conditional expectations between von Neumann algebras, please refer to [13].

In addition to the rigorous results mentioned here, the flat-band ferromagnetism theory proposed by Mielke and Tasaki is considered to describe more realistic many-electron systems [7]. A methodology for constructing stability classes describing flat band ferromagnetism is becoming evident, and I am presently engaged in the detailed investigation of this phenomenon.

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The effective mass problem for the classical polaron

SIMONE RADEMACHER

(joint work with Dario Feliciangeli and Robert Seiringer)

The polaron is a quasi-particle that models an electron in a charged crystal. While moving through the crystal, the electron interacts with its self-induced polarization field that is mathematically either described by a quantum field (Fröhlich model) or by a classical field (Landau-Pekar equations). Here we consider the classical field description: For that we consider a pair $(\psi, \varphi) \in H^1(\mathbb{R}^3) \times L^2_\varepsilon(\mathbb{R}^3)$ where ψ denotes the L^2 -normalized wave function of the electron and φ the polarization field that is an element of the weighted L^2 -space

$$(1) \quad L^2_\varepsilon(\mathbb{R}^3) := \{f : \mathbb{R}^3 \rightarrow \mathbb{C} \mid \int \varepsilon(k) |f(k)|^2 dk < \infty\}$$

for a positive function $\varepsilon : \mathbb{R}^3 \rightarrow \mathbb{R}_+$. The dynamics of the classical polaron is given by the solution (ψ_t, φ_t) to the Landau-Pekar (LP) equations

$$(2) \quad i\partial_t \psi_t = h_{\sqrt{\alpha}\varphi_t} \psi_t, \quad i\varepsilon^{-1}(k) \partial_t \varphi_t(k) = \varphi_t(k) + \sqrt{\alpha} \sigma_{\psi_t}(k)$$

where $\alpha > 0$ denotes the coupling constant and

$$(3) \quad h_\varphi := -\frac{\Delta}{2m} + 2\operatorname{Re} \int v(k) \varphi(k) e^{ik \cdot x} dk, \quad \sigma_\psi(k) = (2\pi)^{3/2} \frac{v(k)}{\varepsilon(k)} |\widehat{\psi}|^2(k)$$

for some $v : \mathbb{R}^3 \rightarrow \mathbb{R}$. Landau and Pekar [5, 6, 9] first described the classical polaron in the strong coupling regime, $\alpha \rightarrow \infty$, by (2) with the choice

$$(4) \quad v(k) = |k|^{-1}, \quad \varepsilon = 1$$

for the form factor resp. the dispersion of the underlying medium.

The dynamics of the polaron is closely related to the polaron’s effective mass: While interacting with the self-induced polarization field, the electron slows down; and thus the polaron’s effective mass increases. Landau and Pekar [6] formulated a quantitative conjecture on the effective mass of the polaron in the strong coupling regime, whose mathematical verification is an outstanding open problem. For the effective mass problem of the quantum (Fröhlich) polaron there is recent progress for lower [1, 2, 10] and upper bounds [3] improving earlier results [11].

Here we address the effective mass problem for the classical polaron given by (2) as originally studied by Landau and Pekar. The heuristic arguments of Landau and Pekar are based on traveling wave solutions to (2) that are given for $v \in \mathbb{R}^3$ by initial states (ψ_v, φ_v) such that

$$(5) \quad (\psi_t(x), \varphi_t(k)) = (e^{i\omega_v t} \psi_v(x - vt), e^{ik \cdot v} \varphi_v(k))$$

solves the Landau-Pekar equations (2) for some phase factor $\omega_v \in \mathbb{R}$. Due to a vanishing speed of sound for the choice (4) we, however, conjecture that there are no traveling wave solutions for the classical polaron with the choice (4).

Considering a regularized polaron model with non-vanishing speed of sound, i.e. considering the dispersion ε of the underlying medium such that

$$(6) \quad v_c := \inf_k \varepsilon(k)/|k| > 0$$

for $v \leq v_c$, I prove [8] that there exist traveling wave solutions of the form (5):

Theorem 1. [8] *Let ε satisfy (6) and $v/\varepsilon^{1/2} \in L^2_{(|k|+1)^4}(\mathbb{R}^3)$, $v/\varepsilon^{1/2}(k) \geq |k|^{-1/4}$. For $|v| \leq v_c$ there exist traveling wave solutions of the form (5).*

In this case, the heuristic arguments of Landau and Pekar can be made rigorous and the effective mass of the classical regularized polaron can be defined through an energy-velocity expansion of sub-sonic traveling waves, i.e.

$$(7) \quad (\psi_v, \varphi_v) \text{ satisfying (4) with } |v| \leq v_c, \omega_v \geq -e_\alpha + v^2/4$$

that have low energy, i.e. such that

$$(8) \quad \mathcal{G}(\psi_v, \varphi_v) = \langle \psi_v, h_{\varphi_v} \psi_v \rangle + \|\varphi\|_{L^2_\varepsilon}^2 < e_\alpha + \kappa$$

for sufficiently small $\kappa > 0$ and where $e_\alpha = \inf_{\psi, \varphi} \mathcal{G}(\psi, \varphi)$. I prove the following expansion for states of the set

$$(9) \quad \mathcal{I}_v := \{(\psi_v, \varphi_v) \in H^1(\mathbb{R}^3) \times L^2_\varepsilon(\mathbb{R}^3) \mid (7), (8) \text{ hold} \}.$$

Theorem 2. [8] *Let ε satisfy (6) and $v/\varepsilon^{1/2} \in L^2_{(|k|+1)^4}(\mathbb{R}^3)$, $v/\varepsilon^{1/2} \geq |k|^{-1/4}$. Then for all $\alpha \geq \alpha_0$, and $\alpha \ll 1$, it is*

$$(10) \quad E_v := \inf_{\mathcal{I}_v} \mathcal{G}(\psi, \varphi) = e_\alpha + \frac{m_{\text{eff}} v^2}{2} + O(\alpha v^3).$$

The constant m_{eff} is explicitly given and, in particular, satisfies in the strong coupling limit

$$(11) \quad \lim_{\alpha \rightarrow \infty} \alpha^{-1} m_{\text{eff}} = \lim_{\alpha \rightarrow \infty} \alpha^{-1} \lim_{v \rightarrow 0} \frac{E_v - e_\alpha}{v^2/2} = \frac{2(2\pi)^3}{3} \|k v \varepsilon^{-3/2}\|_2^2$$

that agrees with findings for the effective mass the regularized (quantum) Fröhlich model [7]. Moreover, I prove in [8] that alternatively the effective mass can be defined based on an energy-momentum expansion of low-energy states with fixed total momentum.

However, for the Landau-Pekar equations with the choice (4) for the dispersion relation resp. the form factor, as originally considered by Landau and Pekar, non of these two approaches work (the reason is related to the vanishing speed of

sound in this case). In [4] we therefore provide a novel approach for the definition of the effective mass based on an energy-velocity expansion for solutions to the LP equations with that gives a first verification the conjecture of Landau and Pekar for the classical polaron.

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Hubbard Models, Fermi Liquids, and Renormalization

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I review some ideas and results in mathematical condensed-matter physics, specifically about many-electron models for metals, magnets, and superconductors, along the lines of [1].

A prototypical such model is the *Hubbard model*, a quantum many-body system on a square or cubic lattice, introduced independently by Gutzwiller, Hubbard, and Kanamori [4] in the late 1950s. The particles obey Fermi statistics, their kinetic term is the discrete Laplacian, and their interaction is an on-site repulsion. More general Hubbard-type models involve different lattices, general short-range hopping amplitudes in the kinetic term, and also more general short-range interactions that may also be attractive. Since the late 1980s these models have received enormous attention as microscopic models for high-temperature superconductors [2, 3]. Because the high- T_c materials have a layered structure, where hopping amplitudes between layers are at least one order of magnitude smaller than those within a layer, the Hubbard model on a two-dimensional lattice is of particular interest.

For fermions on a finite lattice, the Fock space is finite-dimensional. Thus the Hamiltonian H is bounded below, the ground state is well-defined, and so is the thermal state of quantum statistical mechanics in finite volume, as a positive linear functional on the fermionic C^* algebra, given by the appropriately normalized trace with $e^{-\beta(H-\mu N)}$, where $\beta > 0$ is the inverse temperature (the grand canonical ensemble, with the number operator N and the chemical potential μ fixing the average density). The interest lies in finding and proving statements that hold in the thermodynamic limit where the volume becomes infinite, or that are uniform in volume at large volumes.

In spite of the simplicity of the Hamiltonian, many of the properties of the ground state and the thermal state remain controversial. Some remarkable rigorous results, in particular about magnetism in these models, are reviewed in [4, 5].

In the physical application, the interaction is very often strong, i.e. the typical two-body interaction energy is much larger than the band width defined by the kinetic term. But it is already very nontrivial to treat the weakly coupled case, which arises from noninteracting Fermi gases at positive particle density when a weak, short-range interaction is included. The positive density implies that the Fermi gas has an extended Fermi surface, in particular the spectrum of the kinetic energy operator is gapless in the infinite-volume limit.

This property is essential for much of the phenomenological importance of these models – the presence of a Fermi surface is the basis for metallic behaviour – but it also presents an essential mathematical difficulty, in that naive perturbation theory diverges at zero temperature and gives a wrong temperature dependence at small positive temperatures. This necessitates renormalization to give a rigorous treatment of interaction effects.

It is a fundamental question whether the low-lying excitations of the weakly interacting system, i.e. the states energetically just above the ground state, have the character of fermionic quasiparticles, which very loosely speaking means that the states in Hilbert space correspond to wave packets with a small damping, which satisfy Fermi statistics. Landau's *Fermi liquid (FL) theory* asserts that a rather general class of fermion systems (which also includes ones with strong interactions) has this property [6, 7]. From the mathematical point of view, FL theory remained largely conjectural for some time, partly because a precise definition of a Fermi liquid is not straightforward, partly because of the difficulty of the problem. In one dimension, the exact solution of the Luttinger model shows that FL theory is not valid. This was proven to extend to Hubbard-type models in one dimension in [8, 9]. FL theory was very successful in many three-dimensional fermion systems, but its limitations became obvious in the high- T_c materials, which exhibit striking deviations from the predictions of FL theory, such as a linear rise of electrical resistivity as a function of temperature above the critical temperature for superconductivity.

A mathematically precise condition for a weakly interacting Fermi system to be a Fermi liquid at positive temperature was formulated in [10], as follows. The quantum-field theoretical fermionic two-point function of a Fermi gas has Fourier

transform $\hat{C}(\omega, k) = (i\omega - e(k))^{-1}$, where ω is an odd multiple of $\frac{\pi}{\beta}$, $e(k) = \varepsilon(k) - \mu$, and $k \mapsto \varepsilon(k)$ is the Fourier transform of the hopping amplitude. The level set $S = \{k : e(k) = 0\}$, where \hat{C} becomes large, and singular in the zero-temperature limit $\beta \rightarrow \infty$, is called Fermi surface in three dimensions, and Fermi curve in two dimensions (for brevity, always referred to as the Fermi surface in the following). The system with an interaction with coupling strength λ is a Fermi liquid at sufficiently low temperatures (say, $\beta > 1$) if there is $C > 0$, independent of the volume, such that (a) renormalized perturbation theory converges on the set \mathcal{R} of all pairs (λ, β) satisfying $|\lambda| \log \beta < C$ and (b) on \mathcal{R} , the fermionic two-point function has Fourier transform $\hat{G}(\omega, k) = (i\omega - e(k) - \Sigma(\lambda, \omega, k))^{-1}$ and the *fermionic self-energy* Σ is a C^2 function of (ω, k) , with sup norms of the second derivatives bounded uniformly on \mathcal{R} .

This condition is fine enough to separate FL from the one-dimensional Luttinger liquids: in one dimension, (a) holds but (b) fails, since already the first derivative of Σ diverges on the zero set of e (which in one dimension is a set of two points). This second-order divergence is the first indication for the anomalous decay exponents of the full solution in one dimension. In two spatial dimensions, the detailed calculation of the order- λ^2 contribution to the self-energy [14] shows that (b) is the best one can hope to get, and in the limit $\beta \rightarrow \infty$, the second derivative blows up.

The deeper motivation for condition (a) is that, because of the Kohn-Luttinger effect [11], one should not expect a Fermi system that satisfies $e(-k) = e(k)$ to be a FL at zero temperature. Specifically, for $\varepsilon(k) = k^2$ the ground state will be superconducting for any $\mu > 0$, i.e. it has off-diagonal long range order that spontaneously breaks the $U(1)$ particle number symmetry of the action. In other words, the restriction to the set \mathcal{R} places the temperature β^{-1} above the critical temperature for the superconducting transition.

When analyzing the Fermi system, it becomes clear that the validity or failure of FL theory in this sense is intimately tied to the geometry of the Fermi surface S : if the Fermi surface is regular, i.e. $\nabla e(k) \neq 0$ for all $k \in S$, and if it obeys a relatively weak non-nesting condition, then the first derivatives with respect to momentum and frequency are bounded [12, 13]. (The singularity in one dimension arises because there is no curvature.) If the interior of S is strictly convex and if S is regular and positively curved, (b) holds. These properties were proven to all orders in λ in all dimensions $d \geq 2$ in [13, 14, 15]. In subsequent work, the above FL condition was proven to hold for models with positively curved Fermi surfaces in two dimensions in [17, 18, 19, 20, 21]. Conversely, it was proven not to hold in the half-filled case, where the Fermi surface is perfectly nested [22]. It was also shown that even in the absence of nesting, the presence of Van Hove singularities, i.e. points $k \in S$ where $\nabla e(k) = 0$, leads to singularities in the fermionic self-energy Σ that violate (b) [23, 24]. The regularity of Σ as a function of ω and of k is different, unlike in the one-dimensional Luttinger model [24].

Fermi systems with $e(-k) \neq e(k)$ (defined by precise conditions) were shown to be Fermi liquids in a more general sense by Feldman, Knörrer, and Trubowitz [25].

Remarkably, their proof holds in the limit of zero temperature, $\beta \rightarrow \infty$, i.e. in [25] the region \mathcal{R} plays no role, and the only condition on the coupling is $|\lambda| < \text{const.}$ The intuitive reason is that the asymmetry of the band function in k removes the Cooper pairing instability, but the full proof requires more, namely rather subtle bounds on particle-hole contributions to the effective interaction. The result of [25] includes the proof that the fermionic occupation density has a discontinuity at the Fermi surface (which is never true at any positive temperature).

In all the above proofs, mathematical renormalization group methods [26, 27, 28] were used; the same methods also serve to prove an inversion theorem [16] that justifies renormalization. A variant of these methods have also been successful in theoretical physics studies. Their application to the Hubbard model in the parameter range interesting for the high- T_c materials explains the phase diagram of these systems and sheds light on the interplay of antiferromagnetic and superconducting correlations in the Hubbard model [24, 29, 30, 31, 1].

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