

Research Overview

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My research is centered on effective theories arising in interacting many-body quantum systems. The fundamental problem is always the same: the number of degrees of freedom in many-body systems is enormous - starting from tens of thousands of particles in Bose-Einstein condensates up to 10^{58} particles in stars. While the fundamental equations (at least for not too high energies) are known and mathematically well-defined, they cannot be solved analytically and are also beyond the scope of numerical methods. The challenge was summarized by Robert B. Laughlin and David Pines [14] as

“[The Schrödinger equation] cannot be solved accurately when the number of particles exceeds about 10. No computer existing, or that will ever exist, can break this barrier because it is a catastrophe of dimension. [...] The central task [...] is no longer to write down the ultimate equations but rather to catalogue and understand emergent behavior in its many guises”.

Effective theories are the key in this endeavor: they reduce many-body systems to simpler systems described by a small number of emergent degrees of freedom.

In my research, I attack this challenge from the mathematically rigorous point of view: many effective theories have been proposed and are widely used – but often it remains unclear in which domain of validity these theories emerge, and a quantitative control of the approximation errors is missing. I apply methods of functional analysis and quantum field theory to develop a better understanding of effective theories in bosonic, fermionic and spin systems. My research spans over dynamics, spectral theory, and statistical mechanics.

Dynamics of Many-Boson Systems. A gas of N bosonic particles can be described by the Hamiltonian

$$H_N = \sum_{j=1}^N (-\Delta_{x_j} + V_{\text{ext}}(x_j)) + \sum_{1 \leq i < j \leq N} N^2 V(N(x_i - x_j)), \quad (1)$$

acting as a densely defined, self-adjoint operator on the Hilbert space $L^2_{\text{symm}}((\mathbb{R}^3)^N)$ consisting of functions that are invariant under permutation of the N particles. The potential $V_{\text{ext}} : \mathbb{R}^3 \rightarrow \mathbb{R}$ models the confinement in a trap, and $V : \mathbb{R}^3 \rightarrow \mathbb{R}$ is a repulsive interaction potential. The N -dependence of the interaction models the dilute physical regime (called the Gross-Pitaevskii scaling regime), where the length scale of the potential is much shorter than the average distance between particles. Typically $N \geq 50.000$, so we think of the asymptotics as $N \rightarrow \infty$. The ground state $\psi_{\text{gs}} \in L^2_{\text{symm}}((\mathbb{R}^3)^N)$ of this system shows the phenomenon of Bose-Einstein condensation [15], meaning that its one-particle reduced density matrix $\gamma_{\psi_{\text{gs}}}^{(1)} := \text{tr}_{2,\dots,N} |\psi_{\text{gs}}\rangle\langle\psi_{\text{gs}}|$ (where $|\psi_{\text{gs}}\rangle\langle\psi_{\text{gs}}|$ denotes the projection onto $\text{span}\{\psi_{\text{gs}}\}$, and $\text{tr}_{2,\dots,N}$ denotes a partial trace) converges in trace norm to a rank-one projection operator,

$$\|\gamma_{\psi_{\text{gs}}}^{(1)} - |\varphi_{\text{GP}}\rangle\langle\varphi_{\text{GP}}|\|_{\mathfrak{S}^1} \rightarrow 0 \quad (N \rightarrow \infty),$$

where $\varphi_{\text{GP}} \in L^2(\mathbb{R}^3)$ is the normalized minimizer of the Gross-Pitaevskii energy functional

$$\mathcal{E}_{\text{GP}}(\varphi) = \int dx (|\nabla\varphi|^2 + V_{\text{ext}}|\varphi|^2 + 4\pi a_0|\varphi|^4), \quad a_0 = \text{scattering length of } V. \quad (2)$$

In typical experiments one observes the time evolution after switching off the confining trap (i. e., setting $V_{\text{ext}} = 0$). This evolution is described by the Cauchy problem of the Schrödinger equation,

$$i\partial_t\psi_t = H_N\psi_t, \quad \psi_0 = \psi_{\text{gs}}. \quad (3)$$

This is a partial differential equation of $3N$ variables. To be able to make predictions about typical observables, one would like to approximate (3) by an effective evolution equation with a small number of variables. In [2] we introduced a new technique, based on approximating the initial data by a squeezed coherent state (a state that can be described in Fock space by applying a Weyl operator and a Bogoliubov transformation to the vacuum vector), and thus proved that for all times $t \in \mathbb{R}$ there is a $C(t) \in \mathbb{R}$ such that

$$\|\gamma_{\psi_t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|\|_{\mathfrak{S}^1} \leq \frac{C(t)}{\sqrt{N}} \quad (N \rightarrow \infty),$$

where φ_t is the solution of the time-dependent Gross-Pitaevskii equation (or cubic non-linear Schrödinger equation)

$$i\partial_t\varphi_t = -\Delta\varphi_t + 8\pi a_0|\varphi_t|^2\varphi_t, \quad \varphi_0 = \varphi_{\text{GP}}.$$

Dynamics of Many-Fermion Systems. For fermionic systems one is interested in describing similar experimental situations: a system of many interacting fermions is prepared in its ground state in an external trapping potential; then the trap is switched off and the time evolution observed. The Hartree–Fock approximation consists in looking for the best approximation within the set of Slater determinants; the corresponding effective evolution equation is called the time-dependent Hartree–Fock equation.

A rigorous derivation of the time-dependent Hartree–Fock equation is more difficult than for bosons because for fermions already the simplest physical situation, the mean-field scaling regime, is inevitably linked to the semiclassical regime. This means that the relevant Schrödinger equation is

$$i\varepsilon\partial_t\psi_t = \left[\sum_{j=1}^N -\varepsilon^2\Delta_{x_j} + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j) \right] \psi_t \quad (4)$$

with a semiclassical parameter $\varepsilon := N^{-1/3} \rightarrow 0$. Here $\psi_t \in L^2_{\text{antisymm}}((\mathbb{R}^3)^N)$, meaning that transposition of two particles changes the sign of the wave function ψ_t .

In [6], we proved that the time-dependent Hartree–Fock equation indeed approximates the many-body Schrödinger evolution, again in the sense that the difference of one-particle reduced density matrices converges to zero, with rate N^{-1} . A key idea in our work is to propagate commutator bounds which quantify the semiclassicality of the state along the solution of the time-dependent Hartree–Fock equation.

We also extended this result to fermions with relativistic dispersion relation [5] and initial data prepared at positive temperature as a mixed state[3]. The proof of the latter result uses purification of quantum states combined with the Araki-Wyss representation.

Hartree–Fock–Bogoliubov Equations and the Dirac–Frenkel principle. Where in the systems described above it is easy to see which effective evolution equation constitutes the optimal approximation, this is more difficult for example in fermionic systems with non-vanishing pairing

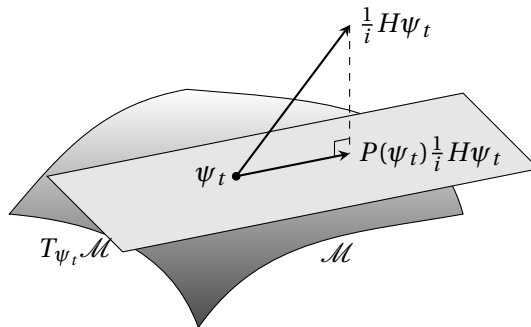


Figure 1: Consider the Schrödinger equation $i\partial_t\psi_t = H\psi_t$ in a Hilbert space \mathcal{H} , and a submanifold $\mathcal{M} \subset \mathcal{H}$. The Dirac–Frenkel principle constructs the optimal approximation $t \mapsto \psi_t \in \mathcal{M}$ to the solution of the Schrödinger equation: at every “time step”, the derivative $\frac{1}{i}H\psi_t$ of the exact evolution is orthogonally projected into the tangent space $T_{\psi_t}\mathcal{M}$. Figure from [7].

density. Physically, models with non-vanishing pairing density describe superconductors. A systematic way of deriving effective equations (although without providing strong error bounds) is the Dirac–Frenkel principle illustrated in Figure 1. However, the Dirac–Frenkel principle was originally formulated in the Hilbert space of many-body wave functions even though the reduced density matrix is more relevant for the approximation of typical observables. For this reason, in [7] we formulated a Dirac–Frenkel principle in terms of the reduced density matrix, and proved its equivalence to the formal quasifree reduction procedure. We thus established that the optimal approximation for reduced density matrices in systems with pairing is given by the Hartree–Fock–Bogoliubov equations (also called the Bogoliubov–de-Gennes equations or BCS equations). We also extended the result to the analogous bosonic setting.

A complete proof of well-posedness for the Hartree–Fock–Bogoliubov equations in the physically most important case of Coulomb interactions was absent from the literature at that point. In [7] we showed that the Banach fixed point theorem cannot be applied in kinetic energy space. Instead we gave a fixed point argument in a larger Banach space. We then constructed a regularization compatible with the conservation laws, and thus proved global well-posedness also in kinetic energy space.

Spin-Wave Theory. The ferromagnetic quantum Heisenberg model is a model proposed to describe the origin of magnetism. In its simplest version, it describes spins placed on the simple cubic lattice, interacting only with their nearest neighbours. Let Λ be a finite subset of \mathbb{Z}^3 , for simplicity a box. The Hilbert space of the model is given by

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathbb{C}^{2S+1}, \quad S \in \frac{1}{2}\mathbb{N},$$

and each copy of \mathbb{C}^{2S+1} carries a spin- S representation of $SU(2)$. The corresponding angular momentum operator at site $x \in \Lambda$ is denoted by $\mathbf{S}_x = (S_x^1, S_x^2, S_x^3)$ with the S_x^i constituting a basis for the representation of the Lie algebra $\mathfrak{su}(2)$. The Hamiltonian is

$$H_\Lambda = \sum_{\substack{(x,y) \in \Lambda \times \Lambda: \\ |x-y|=1}} (S^2 - \mathbf{S}_x \cdot \mathbf{S}_y).$$

The size of the box Λ is to be sent to infinity to describe the thermodynamic limit.

In two groundbreaking papers [10, 11], Dyson argued that the Heisenberg model at low temperatures can be understood in terms of spin waves, delocalized collective excitations of the

ground state that behave as bosonic particles. This was made rigorous by [9], who used the Holstein-Primakov transformation to prove that the free energy, asymptotically for temperature $T \rightarrow 0$, is to leading order given by non-interacting bosons. However, Dyson made a second remarkable claim: the corrections due to interaction between spin waves should be extremely small, namely of order T^4 (whereas the leading term is $T^{3/2}$). In [1] I confirmed this claim to first order in S^{-1} and as an upper bound.

Optimal Upper Bound on the Correlation Energy of the Fermi Gas. Recently I have started to study the spectral theory of the mean-field Fermi gas, as introduced in (4). According to [13] the ground state energy (when constraining to a box)

$$E_N := \inf_{\substack{\psi \in L^2_{\text{antisymm}}((\mathbb{R}^3)^N) \\ \|\psi\|=1}} \langle \psi, H_N \psi \rangle, \quad H_N = \sum_{j=1}^N -\varepsilon^2 \Delta_{x_j} + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j),$$

is well approximated by the infimum of the Hartree-Fock energy functional

$$\mathcal{E}_{\text{HF}}(\omega) = \text{tr}(-\varepsilon^2 \Delta \omega) + \frac{1}{2N} \int V(x-y) \omega(x,x) \omega(y,y) \, dx \, dy - \frac{1}{2N} \int V(x-y) |\omega(x,y)|^2 \, dx \, dy.$$

The minimization of $\mathcal{E}_{\text{HF}}(\omega)$ is over all rank- N orthogonal projection operators ω on $L^2(\mathbb{R}^3)$, corresponding to reduced density matrices of N -particle Slater determinants. The diagonals $\omega(x,x)$ are defined using the spectral decomposition.

A long-standing open problem is to obtain the next order of the ground state energy beyond Hartree-Fock theory, called the correlation energy. For the jellium model (a gas of charged particles with Coulomb repulsion in a uniform background of the opposite charge), a formula for the two leading contributions to the correlation energy, called the Gell-Mann–Brueckner formula, has been conjectured based on extrapolation from the highly divergent perturbation theory [12]. Bohm and Pines [8] and Sawada et al. [16] already suggested that the correlation energy is related to emergent bosonic modes in the Fermi gas, most prominently the plasmon mode, which have the effect of screening the long-range tail of the Coulomb potential.

In [4] we established a rigorous procedure to describe the dominant excitations of the mean-field Fermi gas as emergent, approximately bosonic particles. We embed $L^2_{\text{antisymm}}((\mathbb{R}^3)^N)$ in fermionic Fock space and use the formalism of creation and annihilation operators. We then introduce collective creation operators for delocalized particle-hole pairs as

$$b_{\alpha,k}^* := \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in B_F^c \cap B_\alpha \\ h \in B_F \cap B_\alpha}} \delta_{p-h,k} a_p^* a_h^*, \quad (5)$$

where a_h^* creates a hole with momentum $-h \in \mathbb{Z}^3$ inside the Fermi ball B_F and a_p^* a particle with momentum p outside the Fermi ball; both h and p are also localized to a patch B_α of the Fermi surface (more precisely, the union of all patches covers a neighborhood of the Fermi surface); $n_{\alpha,k}$ is a normalization constant. The commutator relations of these pair creation and corresponding pair annihilation operators (defined as the adjoint of a pair creation operator) are given by

$$[b_{\alpha,k}, b_{\beta,l}] = 0, \quad [b_{\alpha,k}, b_{\beta,l}^*] = \delta_{\alpha,\beta} (\delta_{k,l} + \mathcal{E}_\alpha(k,l)).$$

If the deviation operator $\mathcal{E}_\alpha(k,l)$ was zero, these pair operators would describe exactly bosonic particles. This can be turned into a rigorous approximation: we bounded the deviation operator in terms of the fermionic number operator \mathcal{N} by

$$\|\mathcal{E}_\alpha(k,l)\psi\| \leq \frac{2}{n_{\alpha,k} n_{\alpha,l}} \|\mathcal{N}\psi\| \quad \text{for all } \psi \text{ in Fock space,}$$

and for large enough patches we have $n_{\alpha,k}^{-1} \rightarrow 0$ as $N \rightarrow \infty$. At the same time, we can adjust the patches to be small enough such that the kinetic energy can be linearized around the patch centers, allowing us to approximate the original interacting fermionic Hamiltonian by a quadratic, approximately bosonic Hamiltonian. We then established an approximate theory of Bogoliubov transformations and quasifree states for collective pairs, and were thus able to construct an approximate ground state. This state, used as a trial state, has energy given by the mean-field analogue of the Gell-Mann–Brueckner formula.

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