Effective Theories for Many–Body Quantum Systems

Niels Benedikter

based on joint work with Vojkan Jakšić, Phan Thành Nam, Gustavo de Oliveira, Marcello Porta, Chiara Saffirio, Benjamin Schlein, Robert Seiringer, Jérémy Sok, and Jan Philip Solovej

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Università degli Studi di Milano

Free Quantum Particle in $\mathbb{R}^3$

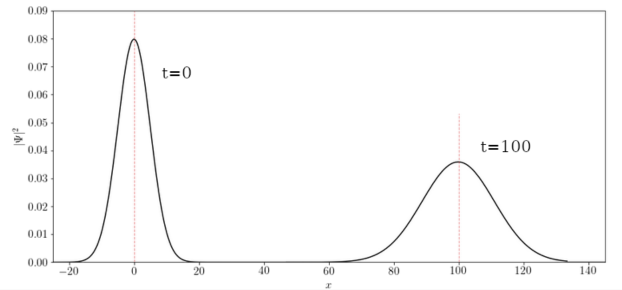
A single free quantum particle in $\mathbb{R}^3$

Time evolution defined by the Cauchy problem of the Schrödinger equation:

$$i\partial_t \psi(t) = -\Delta_x \psi(t) \,, \qquad \psi(0) \in L^2(\mathbb{R}^3) \,.$$

Explicitly solvable by a Fourier transform from position x to momentum k.

Typical behavior is dispersive:



http://www.astro.utoronto.ca/~mahajan/notebooks/quantum_tunnelling.html

Particle in External Potential

A single particle in an external potential

Hamilton operator $H = H^* : H^2(\mathbb{R}^3) \subset L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ defined by

$$H := -\Delta_x + V_{\text{ext}}(x) \,, \qquad V_{\text{ext}} : \mathbb{R}^3 \to \mathbb{R}$$

and time evolution given by the Schrödinger equation

$$i\partial_t \psi(t) = H\psi(t) \,, \qquad \psi(0) \in L^2(\mathbb{R}^3) \,.$$

There may now be solutions that do not disperse, called bound states and described by eigenvectors of the Hamilton operator:

$$H\psi = E\psi \quad \text{with } E \in \mathbb{R} \qquad \Leftrightarrow \qquad \psi(t) = e^{-iEt}\psi(0) \,.$$

In particular, if

$$E_{\text{gs}} := \inf \operatorname{spec}(H) = \inf_{\|\psi\|=1} \langle \psi, H\psi \rangle$$

is an eigenvalue, it is called the ground state energy.

Example: hydrogen atom

One electron attracted by the Coulomb potential of a proton, in relative coordinates:

$$H = -\Delta_x - \frac{1}{|x|} \, .$$

The spectrum is

$$\mathrm{spec}(H) = \mathrm{spec}_{\mathrm{ess}}(H) \cup \mathrm{spec}_{\mathrm{pp}}(H)$$

where scattering solutions (i. e., with dispersive behavior) correspond to

$$\mathrm{spec}_{\mathrm{ess}}(H) = [0, +\infty)$$

and bound states to

$$\mathrm{spec}_{\mathrm{pp}}(H) = \left\{ -\frac{1}{4n^2} \mid n \in \mathbb{N} \right\} \, .$$

Non–Interacting N–body System

Non–Interacting N–body System

The Hilbert space of an N–particle system is the tensor product $\bigotimes_{i=1}^{N} L^2(\mathbb{R}^3) \simeq L^2(\mathbb{R}^{3N})$. Non–interacting Hamiltonian on this space

$$H = \sum_{i=1}^{N} h_i \ , \qquad h_i = 1 \otimes \cdots \otimes h \otimes \cdots \otimes 1 \ , \qquad h = -\Delta_x + V_{\text{ext}} \ .$$

Solutions are trivial: given initial data

$$\psi(0) = \sum_{k=1}^{\infty} \lambda_k \, \varphi_{k,1} \otimes \cdots \otimes \varphi_{k,N}$$

the solution is

$$\psi(t) = \sum_{k=1}^{\infty} \lambda_k \, \varphi_{k,1}(t) \otimes \cdots \otimes \varphi_{k,N}(t)$$

where each factor of the tensor product solves the one–particle Schrödinger equation

$$i\partial_t \varphi_{k,i}(t) = h \, \varphi_{k,i}(t) \ .$$

Interacting N–body system

Interacting N–body system

The Hilbert space is still $\bigotimes_{i=1}^{N} L^2(\mathbb{R}^3) \simeq L^2(\mathbb{R}^{3N})$, but H contains a pair interaction:

$$H = \sum_{i=1}^{N} h_i + \lambda \sum\sum_{1 \leq i < j \leq N} V(x_i - x_j)\,, \qquad h = -\Delta_x + V_{\text{ext}}\,.$$

With $N \simeq 10^{23}$ not even numerically tractable.

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With $N \simeq 10^{23}$ not even numerically tractable.

Quantum statistics: for indistinguishable particles the wave function is symmetric

$$\psi(x_1, \ldots, x_N) = \psi(x_{\sigma(1)}, \ldots, x_{\sigma(N)}) \qquad \forall \sigma \in S_N \qquad \text{(bosons)}$$

or antisymmetric

$$\psi(x_1, \ldots, x_N) = \operatorname{sgn}(\sigma) \psi(x_{\sigma(1)}, \ldots, x_{\sigma(N)}) \qquad \forall \sigma \in S_N \qquad \text{(fermions)}$$

Examples: cold atomic gases (bosons & fermions), electrons in a metal (fermions).

Now what is an effective theory?

Example 1: time–dependent Hartree equation

N bosons in a mean–field regime: $N \to \infty$ and coupling constant $\lambda = N^{-1}$.

Assume that at $t = 0$ we start in a Bose–Einstein condensate:

$$\psi(0) = \bigotimes_{i=1}^{N} \varphi \qquad \Leftrightarrow \qquad \psi(0)(x_1, \ldots, x_N) = \prod_{i=1}^{N} \varphi(x_i) \,, \qquad \varphi \in L^2(\mathbb{R}^3) \,.$$

The solution of the Schrödinger equation does not remain factorized:

$$\psi(t) \neq \bigotimes_{i=1}^{N} \varphi(t) \,,$$

but if we project on the sub–manifold of such product states, the best possible approximation to $\psi(t)$ is obtained by assuming that $\varphi(t)$ solves the Hartree equation:

$$\boxed{i\partial_t \varphi(t) = h\varphi(t) + \left(V * |\varphi(t)|^2\right) \varphi(t) \,, \qquad \varphi(0) = \varphi \in L^2(\mathbb{R}^3) \,.}$$

The problem has been reduced from $L^2(\mathbb{R}^{3N})$ to $L^2(\mathbb{R}^3)$.

Example 2: Hartree energy functional

Can the same idea be used to predict the ground state energy of N bosons?

Take $\psi = \bigotimes_{i=1}^{N} \varphi$ and compute

$$\boxed{\langle \psi, H\psi \rangle =: \mathcal{E}^{\text{Hartree}}(\varphi)\ .}$$

We can minimize over the set of product states to define the Hartree energy

$$E^{\text{Hartree}} := \inf_{\varphi \in L^2(\mathbb{R}^3),\ \|\varphi\|=1} \mathcal{E}^{\text{Hartree}}(\varphi)\ .$$

Since the Hartree energy originates from a trial state it follows that

$$E^{\text{Hartree}} \geq E_{\text{gs}}\ .$$

In the mean–field regime $\lambda = N^{-1}$ one can prove more than that, namely:

$$\frac{E^{\text{Hartree}}}{N} - \frac{E_{\text{gs}}}{N} \to 0 \qquad \text{as } N \to \infty\ .$$

Fermionic mean–field regime

Recall: N interacting fermions on the torus $\mathbb{R}^3/2\pi\mathbb{Z}^3$

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

$$\psi(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(N)}) = \mathrm{sgn}(\sigma)\psi(x_1, x_2, \ldots, x_N) \qquad \forall \sigma \in S_N .$$

Again the simplest possibility: gas at high density with weak interaction.

- High density: N fermions on fixed–size torus and $N \to \infty$
- What λ do we intend by "weak interaction"?

Let's construct a trial state. We start from the plane waves

$$f_k(x) := (2\pi)^{-3/2} e^{ik\cdot x} , \quad k \in \mathbb{Z}^3$$

which constitute a basis of eigenfunctions for the Laplacian: $-\Delta f_k = |k|^2 f_k$.

Now we build an N–particle state:

Fermionic mean–field regime

Consider a totally antisymmetric tensor product (Slater determinant) of plane waves:

$$\psi = \frac{1}{N!} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma)\, f_{k_{\sigma(1)}} \otimes \cdots \otimes f_{k_{\sigma(N)}} \qquad \Rightarrow \qquad \langle \psi, \sum_{j=1}^{N} (-\Delta_j) \psi \rangle = \sum_{j=1}^{N} |k_j|^2 \,.$$

Minimization by occupying the Fermi ball $\mathcal{B}_{\mathrm{F}} := \{k \in \mathbb{Z}^3 : |k| \leq (3/4\pi)^{1/3} N^{1/3}\}$.

$$\sum_{k \in \mathcal{B}_F} |k|^2 \sim N^{5/3} \qquad \text{c. f.} \qquad \langle \psi, \lambda \sum_{1 \leq i < j \leq N} V(x_i - x_j) \psi \rangle = \lambda N^2 \,.$$

mean–field scaling regime: $\lambda := N^{-1/3}$

Introduce an effective Planck constant $\hbar := N^{-1/3}$ and multiply by $\hbar^2$:

$$H = \sum_{j=1}^{N} -\hbar^2 \Delta_{x_j} + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j) \,.$$

Hartree–Fock energy functional

For ψ the Slater determinant constructed from the $\varphi_i \in L^2(\mathbb{R}^3)$, $i = 1, \ldots, N$, we set

$$\boxed{\langle \psi, H\psi \rangle =: \mathcal{E}^{\mathrm{HF}}(\varphi_1, \ldots, \varphi_N)} \qquad \text{(Hartree–Fock energy functional)}$$

In the mean–field scaling regime and for $\hat{V} \geq 0$, this has an explicit minimizer:

$$E^{\mathrm{HF}} := \inf_{(\varphi_i)_{i=1}^N \, , \, \|\varphi_i\|=1} \mathcal{E}^{\mathrm{HF}}(\varphi_1, \ldots, \varphi_N) = \mathcal{E}^{\mathrm{HF}}(f_{k_i} : k_i \in \mathcal{B}_{\mathrm{F}}) \, .$$

In general the plane waves are only a stationary point, not a minimizer. This is special to the mean–field scaling regime.

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Hartree and Hartree–Fock theory are of mean–field type: only (anti–symmetrized) tensor products — minimal entanglement/avoiding linear combinations.

New: construct a refined theory that adds entanglement to the plane wave state.

Beyond Hartree–Fock: from the Fermi Gas to a Bosonic Effective Theory

Preparation: particle–hole transformation

The N–particle Hamiltonian in Fock space representation

$$H = \hbar^2 \sum_{k\in\mathbb{Z}} |k|^2 a_k^* a_k + \frac{1}{2N} \sum_{k\in\mathbb{Z}^3} \hat{V}(k) \sum_{p,q\in\mathbb{Z}^3} a_{p+k}^* a_{q-k}^* a_q a_p \; .$$

Consider the particle–hole transformation $R : \mathcal{F} \to \mathcal{F}$ such that

$$R\, a_k^*\, R^* := \begin{cases} a_k^* & k \in \mathcal{B}_{\mathrm{F}}^c \\ a_k & k \in \mathcal{B}_{\mathrm{F}} \; . \end{cases}$$

Expand $R^* H_N R$ and normal–order to separate Hartree–Fock energy

$$R^* H_N R = E^{\mathrm{HF}} + \underbrace{\hbar^2 \sum_{p\in\mathcal{B}_{\mathrm{F}}^c} p^2 a_p^* a_p - \hbar^2 \sum_{h\in\mathcal{B}_{\mathrm{F}}} h^2 a_h^* a_h}_{=:\; H^{\mathrm{kin}}} + \underbrace{Q}_{\text{quartic in operators } a^*,\, a}$$

Goal: a quadratic approximation to the excitation Hamiltonian $H^{\mathrm{kin}} + Q$.

Bosonization of the interaction

Observation: if we introduce collective pair operators

$$b_k^* := \sum_{\substack{p \in \mathcal{B}_F^c \\ h \in \mathcal{B}_F}} \delta_{p-h,k} a_p^* a_h^*$$

p "particle" outside the Fermi ball

h "hole" inside the Fermi ball

then

$$Q = \frac{1}{N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \Big(2 b_k^* b_k + b_k^* b_{-k}^* + b_{-k} b_k \Big) + \mathcal{O}\Big(\frac{\mathcal{N}^2}{N} \Big) .$$

This is convenient because the b_k^* and b_k have approximately bosonic commutators:

$$[b_k^*, b_l^*] = 0 \quad , \qquad [b_l, b_k^*] = \delta_{k,l} n_k^2 + \mathcal{E}(k,l) .$$

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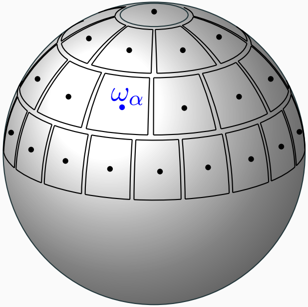
But how to express H^{kin} through pair operators?

Bosonization of the kinetic energy

Fermi ball $\mathcal{B}_\mathrm{F}$



[Benfatto–Gallavotti '90]
[Haldane '94]
[Fröhlich–Götschmann–Marchetti '95]

Localize to $M = M(N)$ patches near the Fermi surface,

$$b^*_{\alpha,k} := \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in \mathcal{B}_\mathrm{F}^c \cap B_\alpha \\ h \in \mathcal{B}_\mathrm{F} \cap B_\alpha}} \delta_{p-h,k} a^*_p a^*_h$$

with $n_{\alpha,k}$ chosen to normalize $\|b^*_{\alpha,k}\Omega\| = 1$.

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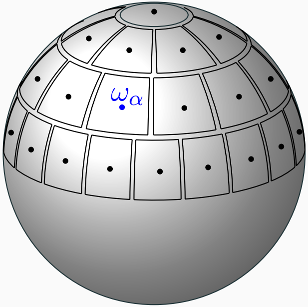

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Linearize kinetic energy around patch center ω_α:

$$[H^\mathrm{kin}, b^*_{\alpha,k}] \simeq 2\hbar|k \cdot \hat{\omega}_\alpha| b^*_{\alpha,k} \ ,$$

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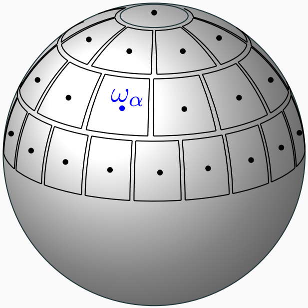

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Linearize kinetic energy around patch center ω_α:

$$[H^{\mathrm{kin}}, b^*_{\alpha,k}] \simeq 2\hbar |k \cdot \hat{\omega}_\alpha| b^*_{\alpha,k} \; ,$$

same as with the approximation

$$H^{\mathrm{kin}} \simeq \sum_{k \in \mathbb{Z}^3} \sum_{\alpha=1}^{M} 2\hbar u_\alpha(k)^2 b^*_{\alpha,k} b_{\alpha,k} \; , \quad u_\alpha(k)^2 := |k \cdot \hat{\omega}_\alpha| \, .$$

Quadratic effective Hamiltonian

Recall

$$Q = \frac{1}{N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \left(2 b_k^* b_k + b_k^* b_{-k}^* + b_{-k} b_k\right) \ .$$

Decompose

$$b_k^* = \sum_{\alpha=1}^{M} n_{\alpha,k} b_{\alpha,k}^* + \text{lower order} \ .$$

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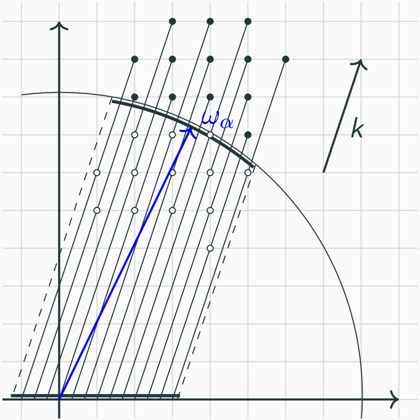
Normalization:

$$n^2_{\alpha,k} = \#\text{p-h pairs in patch } B_\alpha \text{ with momentum } k$$

$$\simeq \frac{4\pi N^{2/3}}{M} |k \cdot \hat{\omega}_\alpha| \ .$$



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Decompose

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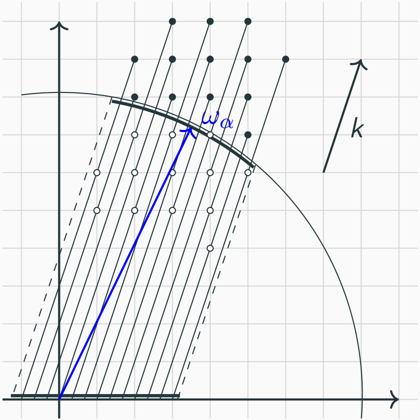
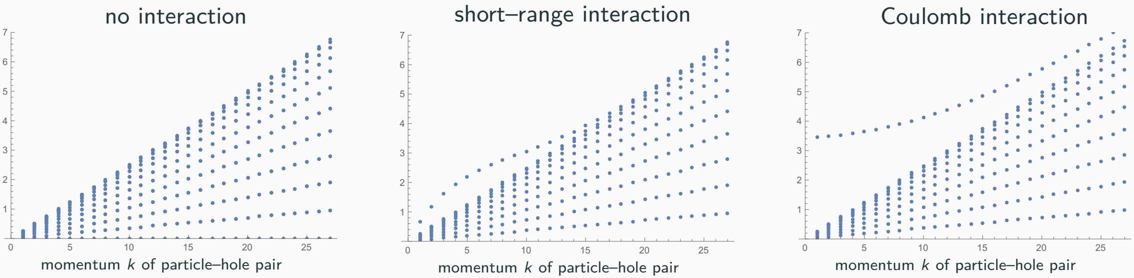


$$H^{\text{RPA}} = \hbar \sum_{k \in \mathbb{Z}^3} \left[\sum_\alpha u_\alpha(k)^2 b_{\alpha,k}^* b_{\alpha,k} + \frac{\hat{V}(k)}{M} \sum_{\alpha,\beta} \left(u_\alpha(k) u_\beta(k) b_{\alpha,k}^* b_{\beta,k} + u_\alpha(k) u_\beta(k) b_{\alpha,k}^* b_{\beta,-k}^* + \text{h.c.} \right) \right]$$

Spectrum of the effective Hamiltonian

H^{RPA} can be diagonalized—in the bosonic approximation—by a bosonic Bogoliubov transformation, yielding the following spectrum:



- plasmon mode (observable collective oscillation)
- continuous bulk of the spectrum only weakly renormalized

indicates a non–perturbative approach to Fermi liquid theory

A rigorous result: the ground state energy

Theorem: [B–Nam–Porta–Schlein–Seiringer, Inventiones Mathematicae **225**(3) p.885 (2021) and B-Porta–Schlein–Seiringer arXiv:2106.13185]

Let $\hat{V} \geq 0$ and $\sum_{k\in\mathbb{Z}^3} \hat{V}(k)|k| < \infty$. Then there exists $\epsilon > 0$ such that for $N \to \infty$ we have

$$E_N = E_N^{\mathrm{pw}} + E_N^{\mathrm{RPA}} + \mathcal{O}(N^{-1/3-\epsilon}) \,,$$

where

$$E_N^{\mathrm{RPA}} := N^{-1/3} \sum_{k\in\mathbb{Z}^3} |k| \left[\int_0^\infty \log\Big(1 + \hat{V}(k)\Big(1 - \lambda \arctan \lambda^{-1}\Big)\Big)\, \mathrm{d}\lambda - \frac{1}{4}\hat{V}(k) \right]$$

is the continuum approximation ($M \to \infty$) to $\inf \operatorname{spec}(H^{\mathrm{RPA}})$.

Thank you!