Collective Bosonization and the Correlation Energy of a Mean–Field Fermi Gas

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N Spinless Fermions on Fixed Size 3D Torus

Hamilton operator

$$H_N := \sum_{i=1}^{N} (-\Delta_i) + \lambda \sum_{1 \leq i < j \leq N} V(x_i - x_j) \qquad \text{with } V : \mathbb{R}^3 \to \mathbb{R} \,,$$

acting on the L^2–space of antisymmetric wave functions of $3N$ variables:

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

We are interested in the ground state energy

$$E_N := \inf_{\substack{\psi \in L^2_{\mathrm{a}}(\mathbb{T}^{3N}) \\ \|\psi\| = 1}} \langle \psi, H_N \psi \rangle \,.$$

The setting is still too general! We should look at a more specific physical situation.

Mean–Field Scaling Regime

Simplest situation: high density and weak interaction, "close to mean–field".

Mean–Field Scaling Regime [Narnhofer–Sewell '81, Spohn '81]

- high density: fixed volume (the torus) and N particles, with $N \to \infty$.
- weak interation: $\lambda = N^{-1/3}$ because

$$\Big\langle \sum_{i=1}^{N} (-\Delta_i) \Big\rangle \sim N^{5/3} \quad \text{(Fermi energy)}\,, \qquad \Big\langle \lambda \sum_{1 \leq i < j \leq N} V(x_i - x_j) \Big\rangle \sim \lambda N^2\,.$$

Multiply the entire Hamiltonian $\times \hbar^2$, with $\hbar := N^{-1/3}$:

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

Leading Order:
Hartree–Fock Theory

Hartree–Fock Theory = Restriction to Slater Determinants

Convergence to the Hartree–Fock energy [Bach '92, Graf–Solovej '94]:

$$\left|E_N - E_N^{\mathrm{HF}}\right| = o(N)\,, \qquad \text{where } E_N^{\mathrm{HF}} := \inf_{\psi \text{ is Slater}} \langle \psi, H_N \psi \rangle\ ,$$

$$\psi_{\mathrm{Slater}} = \bigwedge_{j=1}^{N} \varphi_j = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \operatorname{sgn}(\pi) \varphi_{\pi(1)} \otimes \cdots \otimes \varphi_{\pi(N)}\ , \qquad \varphi_j \in L^2(\mathbb{T}^3)\ ,$$

The fermionic states with the least possible entanglement are sufficient to obtain the dominant orders of the energy.

Stability: Evolve a Slater determinant in time by $e^{-itH_N/\hbar}$ — it stays close to a Slater determinant but with orbitals $\varphi_{j,t}$ evolved by the time–dependent Hartree–Fock equation [B–Porta–Schlein '14].
HF evolution is optimal in the submanifold of Slater determinants [B–Sok–Solovej '18].

The Minimizing Slater Determinant

Introduce the Slater determinant of N plane waves $f_k(x) := (2\pi)^{-3/2} e^{ik\cdot x}$:

$$\psi_N^{\mathrm{pw}} := \bigwedge_{k \in B_{\mathrm{F}}} f_k \,, \qquad B_{\mathrm{F}} = \text{Fermi ball} := \left\{ k \in \mathbb{Z}^3 : |k| \leq k_{\mathrm{F}} \right\};$$

Under the assumptions $\hat{V}(k) \geq 0$, on the torus and no external potential, with mean–field scaling, with fully filled Fermi ball ($N = |B_{\mathrm{F}}|$) one can show that plane waves are the minimizer among Slater determinants [B–Nam–Porta–Schlein–Seiringer '21, Appendix]:

$$E_N^{\mathrm{pw}} := \langle \psi_N^{\mathrm{pw}}, H_N \psi_N^{\mathrm{pw}} \rangle = E_N^{\mathrm{HF}} \,.$$

[Wigner '34]: How to compute the correlation energy $E_N - E_N^{\mathrm{HF}}$?

Do better than Slater determinants by including non–trivial entanglement!

Next Order:
Random Phase Approximation

Upper Bound on the Correlation Energy

Theorem: [B–Nam–Porta–Schlein–Seiringer '20, B–Porta–Schlein–Seiringer '21]

Let

$$\hat{V}(k) \geq 0 \qquad \text{and} \qquad \sum_{k \in \mathbb{Z}^3} |k| \hat{V}(k)^2 < \infty \, .$$

For $k_{\mathrm{F}} > 0$ let $N := |B_{\mathrm{F}}| = |\{k \in \mathbb{Z}^3 : |k| \leq k_{\mathrm{F}}\}|$. Then

$$E_N \leq E_N^{\mathrm{HF}} + E_N^{\mathrm{RPA}} + o(\hbar) \qquad \text{for } k_{\mathrm{F}} \to \infty$$

with the random phase approximation energy formula

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

Lower Bound on the Correlation Energy

Theorem: [B–Nam–Porta–Schlein–Seiringer '21, B–Porta–Schlein–Seiringer '21]

Let

$$\hat{V}(k) \geq 0 \qquad \text{and} \qquad \sum_{k \in \mathbb{Z}^3} |k| \hat{V}(k) < \infty \,.$$

For $k_{\mathrm{F}} > 0$ let $N := |B_{\mathrm{F}}| = |\{k \in \mathbb{Z}^3 : |k| \leq k_{\mathrm{F}}\}|$. Then

$$E_N \geq E_N^{\mathrm{HF}} + E_N^{\mathrm{RPA}} + o(\hbar) \qquad \text{for } k_{\mathrm{F}} \to \infty \,.$$

Remark: [Hainzl–Porta–Rexze '19] obtained a lower bound to second order in $\hat{V}$,

$$E_N \geq E_N^{\mathrm{HF}} - \hbar \frac{\pi}{2}(1 - \log 2) \sum_{k \in \mathbb{Z}^3} |k| \hat{V}(k)^2 + \mathcal{O}(\hat{V}^3) \,.$$

History of the Random Phase Approximation

- **Macke '50** energy formula by resumming the most divergent term of each order of formal perturbation theory with Coulomb potential
- **Bohm–Pines '53** couple to an auxiliary boson field, introduce a coupling constant to fix # degrees of freedom, invertible transformations, drop phase terms
- **Sawada–Fukuda–Brueckner–Brout '57** treat $a_p^* a_h^*$ as a bosonic particle, keep only quadratic terms and diagonalize
- **Gell-Mann–Brueckner '57** refined resummation of formal perturbation series produces even a further correction

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- **B '20** computation of the one–particle spectrum in the exact bosonic theory
- **B–Nam–Porta–Schlein–Seiringer '21** Fock space norm approximation for the dynamics of particle–hole pair initial data
- **Christiansen–Hainzl–Nam '21** ground state energy and one–particle spectrum by a method similar to Sawada et al.

The Random Phase Approximation as Bosonization

Preparation: Separating the Slater Determinant

Hamiltonian in momentum representation, written with CAR operators:

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

Define the unitary map R ("particle–hole transformation") on fermionic Fock space by

$$R\,\Omega := \psi_N^{\mathrm{pw}}\;, \qquad\qquad R\, a_k^*\, R^* := \begin{cases} a_k^* & k \in B_{\mathrm{F}}^c \\ a_k & k \in B_{\mathrm{F}} \end{cases}$$

Write $\psi_N = R\xi_N$, expand $R^* H_N R$, normal–order: with $e(p) := \left|\hbar^2|p|^2 - (3/4\pi)^{2/3}\right|$ get

$$\langle \psi_N, H_N \psi_N\rangle = E_N^{\mathrm{HF}} + \langle \xi_N, \Big[\underbrace{\sum_{p\in B_{\mathrm{F}}^c} e(p) a_p^* a_p + \sum_{h\in B_{\mathrm{F}}} e(h) a_h^* a_h}_{=:\ H_{\mathrm{kin}}} + \underbrace{Q}_{\text{quartic in operators } a^*,\, a} \Big] \xi_N \rangle$$

Plane–wave slater det. corresponds to $\xi_N = \Omega$: in particular $(H_{\mathrm{kin}} + Q)\,\Omega = 0$.

Collective Particle–Hole Pairs

Key observation: if we introduce collective pair creation operators

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

p "particle" outside the Fermi ball

h "hole" inside the Fermi ball

then

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

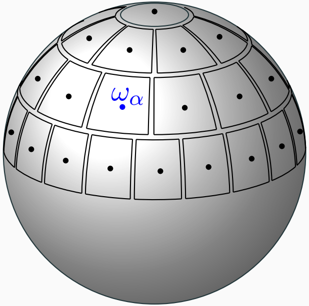
This is convenient because the b_k^* and b_k have approximately bosonic commutators:

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

But how to express H_{kin} through pair operators?

Linearizing the Kinetic Energy Locally in Patches

Fermi ball B_{F}



[Benfatto–Gallavotti '90]
[Haldane '94]
[Fröhlich–Götschmann–Marchetti '95]
[Kopietz et al. '95]

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

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

Linearize kinetic energy around patch center ω_α:

$$\begin{aligned} H_{\mathrm{kin}} b^*_{\alpha,k} \Omega &= \frac{1}{n_{\alpha,k}} \sum_{h,p} \delta_{p-h,k} (p^2 - h^2) a^*_p a^*_h \Omega \\ &= \frac{1}{n_{\alpha,k}} \sum_{h,p} \delta_{p-h,k} \underbrace{(p-h)}_{=k} \cdot \underbrace{(p+h)}_{\simeq 2\omega_\alpha} a^*_p a^*_h \Omega \\ &\simeq 2\hbar |k \cdot \hat{\omega}_\alpha| b^*_{\alpha,k} \Omega \,. \end{aligned}$$

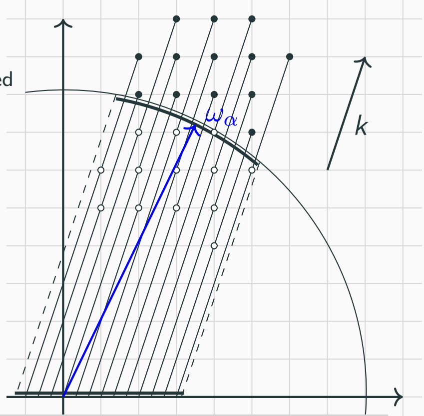
$$H_{\mathrm{kin}} \simeq \sum_{k \in \mathbb{Z}^3} \sum_{\alpha=1}^{M} 2\hbar u_\alpha(k)^2 b^*_{\alpha,k} b_{\alpha,k} \,, \quad u_\alpha(k)^2 := |k \cdot \hat{\omega}_\alpha|$$

(similar to [Lieb–Mattis '65] for 1D Luttinger)

Quadratic Effective Hamiltonian

Recall

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



Decompose

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

Normalization such that $\|b_{\alpha,k}^* \Omega\| = 1$:

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

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

Effective Bosonic Hamiltonian

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

Diagonalization of the Bosonic Hamiltonian

$$H^{\text{eff}} = \hbar \sum_{k \in \mathbb{Z}^3} \left[h^{\text{eff}}(k) - \frac{1}{2} \operatorname{tr}(D(k) + W(k)) \right]$$

$$h^{\text{eff}}(k) = \frac{1}{2} \begin{pmatrix} (b^*)^T & b^T \end{pmatrix} \begin{pmatrix} D + W & \widetilde{W} \\ \widetilde{W} & D + W \end{pmatrix} \begin{pmatrix} b \\ b^* \end{pmatrix} , \qquad \text{(everything depends on } k\text{)}$$

$$D = \begin{pmatrix} \operatorname{diag}(u_\alpha^2) & 0 \\ 0 & \operatorname{diag}(u_\alpha^2) \end{pmatrix}, \quad W = \hat{V} \begin{pmatrix} |u\rangle\langle u| & 0 \\ 0 & |u\rangle\langle u| \end{pmatrix}, \quad \widetilde{W} = \hat{V} \begin{pmatrix} 0 & |u\rangle\langle u| \\ |u\rangle\langle u| & 0 \end{pmatrix} .$$

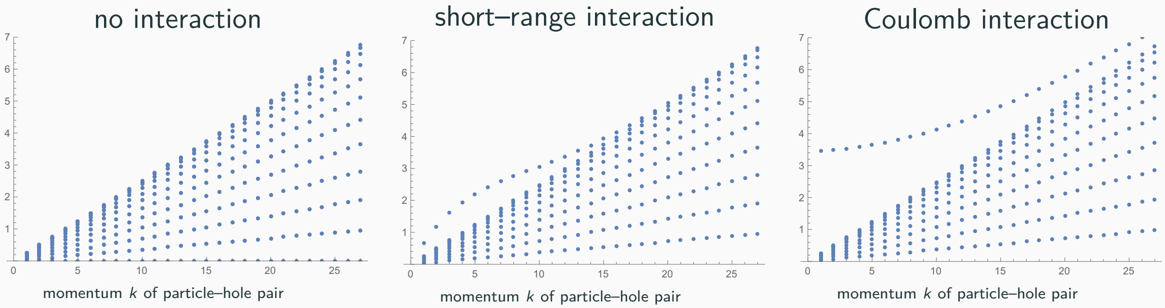
Find a bosonic Bogoliubov transformation such that

$$h^{\text{eff}} = \sum\nolimits_{\gamma=1}^{M} \left(e_\gamma \tilde{b}_\gamma^* \tilde{b}_\gamma + e_\gamma/2 \right) , \quad e_\gamma \in \mathbb{R} .$$

In the limit of large number of patches, $M \to \infty$, the correlation energy becomes

$$\hbar \sum_{k \in \mathbb{Z}^3} \frac{1}{2} \operatorname{tr} \left(E(k) - D(k) - W(k) \right) \to E_N^{\text{RPA}} .$$

Spectrum



- plasmon mode (collective oscillation) emerges
- continuous spectrum qualitatively unchanged

A systematic approach to Bohm–Pines theory.

Proof of the Upper Bound

Trial State

The implementation of the Bogoliubov map makes sense on fermionic Fock space:

$$T = \exp\left(\sum_{k\in\mathbb{Z}^3} \sum_{\alpha,\beta=1}^{M} K(k)_{\alpha,\beta} b^*_{\alpha,k} b^*_{\beta,-k} - \text{h.c.} \right) , \quad K(k) = \log|S_1| \, .$$

We just need to compute the expectation value of $R^* H_N R - E_N^{\text{HF}} = H_{\text{kin}} + Q$ using the "bosonic quasifree state" as trial state in fermionic Fock space

$$\xi_N = T\Omega \, .$$

Error terms:

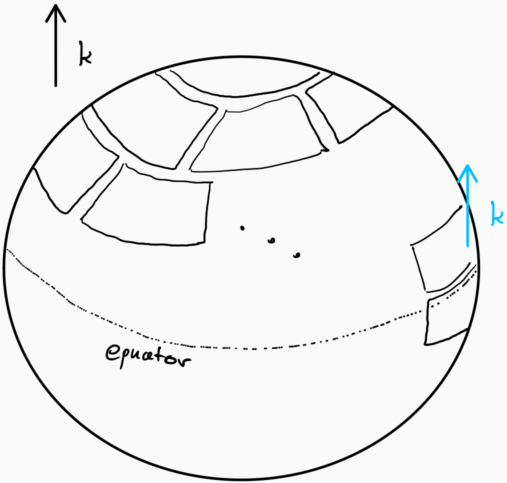
CCR: $$[b_{\alpha,k}, b^*_{\beta,l}] = \delta_{\alpha,\beta}(\delta_{k,l} + \mathcal{E}_\alpha(k,l)) \, , \qquad \|\mathcal{E}_\alpha(k,l)\psi\| \leq \frac{2}{n_\alpha(k) n_\alpha(l)} \|\mathcal{N}\psi\| \, ,$$

Non–bosonizable terms: $$|\langle \psi, Q_{\text{non–pair}}\psi\rangle| \leq N^{-1}\langle\psi, \mathcal{N}^2\psi\rangle \, .$$

Thanks to Grönwall's lemma:

$$\langle T_\lambda\Omega, \mathcal{N}^m T_\lambda\Omega\rangle \leq C_m e^{\lambda c_m} \qquad \forall m \in \mathbb{N} \, .$$

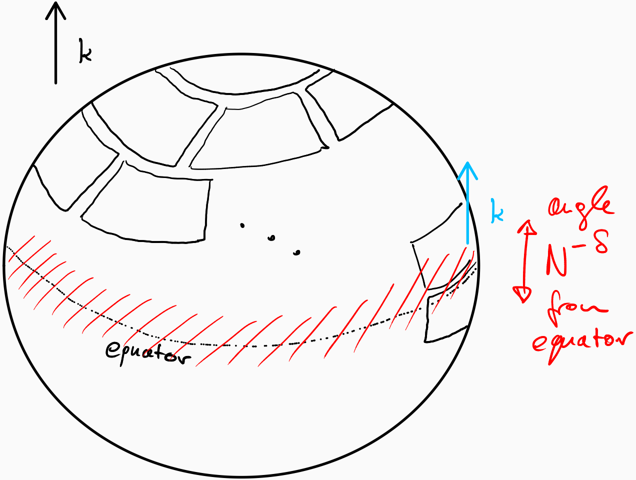
Dangerous Excitations



The energy gap (due to lattice spacing in momentum space) is $\hbar^2$, but we want to compute an energy of order $\hbar$.

The $\hbar^2$ gap still helps a bit, but for getting good bounds the system is to be treated as gapless.

Removing “Gapless” Excitations



Instead of $b_k^* = \sum_{\alpha=1}^{M} n_{\alpha,k} b_{\alpha,k}^*$ consider

$$b_k^* \simeq \sum_{\alpha \in \mathcal{I}_k^+} n_{\alpha,k} b_{\alpha,k}^* \ ,$$

where

$$\mathcal{I}_k^+ := \left\{ \alpha : k \cdot \hat{\omega}_\alpha > N^{-\delta} \right\} .$$

Difference controlled by

$$(\dots) \leq C N^{1/2 - \delta/2} \| H_{\text{kin}}^{1/2} \psi \| \ .$$

Close to the equator, kinetic and excitation energy both vanish like $u_\alpha(k)^2 = |k \cdot \hat{\omega}_\alpha|$.
This permits control of norms and matrix elements of the Bogoliubov kernel $K(k)$.

Proof of the Lower Bound

Two central difficulties compared to the trial state argument:

- How to justify $\mathbb{H}_0 \simeq \mathbb{D}_{\mathrm{B}}$ outside commutators?
- Why is the expectation value of $Q_{\text{no–pair}}$ smaller than order $\hbar$?

Obtain simultaneous diagonalization by choosing a one–particle unitary

$$Z := \exp\left(\sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta=1}^{M} L(k)_{\alpha,\beta} b^*_{\alpha,k} b_{\beta,-k} - \text{h.c.} \right) .$$

such that $T^* Z^* H^{\text{eff}} Z T$ is (almost) completely diagonal.

In fact: write $\psi_{\text{gs}} = TZ\xi$, and obtain

$$\begin{aligned} \langle TZ\xi, (H_{\text{kin}} + Q) TZ\xi \rangle &= \langle TZ\xi, (H_{\text{kin}} - \mathbb{D}_{\mathrm{B}}) TZ\xi \rangle + \langle TZ\xi, (\mathbb{D}_{\mathrm{B}} + Q_{\mathrm{B}}) TZ\xi \rangle + \langle TZ\xi, Q_{\text{no-pair}} TZ\xi \rangle \\ &\simeq \langle \xi, (H_{\text{kin}} - \mathbb{D}_{\mathrm{B}})\xi \rangle + \langle TZ\xi, H^{\text{eff}} TZ\xi \rangle + \langle TZ\xi, (\mathcal{E}_1 + \mathcal{E}_2) TZ\xi \rangle . \end{aligned}$$

Eigenvalues bound the diagonal elements of $-\mathbb{D}_{\mathrm{B}}$.

$\mathcal{E}_1$ can be controlled by gapped number operators and kinetic a–priori estimate.

Specific Technical Tools

1. Kinetic a–priori estimate: $\|b(k)\psi\| \leq CN^{1/2}\|H_{\text{kin}}^{1/2}\psi\|$ [Hainzl–Porta–Rexze '19]. Thus
$$H_{\text{kin}} \leq C(H_{\text{kin}} + Q) \leq \hbar\ .$$
2. Analytic number theory: $|\{\text{lattice points on the sphere}\}| \leq C_\epsilon N^{1/3+\epsilon}$, thus
$$\mathcal{N} := \sum_{i\in\mathbb{Z}^3} a_i^* a_i \leq \sum_{e(i)\leq N^{-\theta}} 1 + \sum_{e(i)>N^{-\theta}} a_i^* a_i \overset{\theta=2/3}{\leq} CN^{1/3+\epsilon} + N^{2/3}H_{\text{kin}} = \mathcal{O}(N^{1/3})\ .$$
3. Gapped number operator wherever possible to avoid low–energy excitations:
$$\|b_{\alpha,k}\psi\| \leq \|\mathcal{N}_\delta^{1/2}\psi\| \qquad \text{where } \mathcal{N}_\delta := \sum\nolimits_{e(i)>\frac{1}{4}N^{-1/3-\delta}} a_i^* a_i\ , \quad \delta \text{ to be optimized.}$$
4. Strong control on the Bogoliubov kernel $K(k)$, e. g.,
$$|K(k)_{\alpha,\beta}| \leq \tfrac{C}{M} \min\left\{\tfrac{u_\alpha(k)}{u_\beta(k)}, \tfrac{u_\beta(k)}{u_\alpha(k)}\right\}\ . \tag{1}$$

Bosonization of Fermionic Dynamics

Effective Bosonic Evolution

The diagonalized effective Hamiltonian is an (approx.) bosonic second quantization:

$$T^* H^{\text{eff}} T \simeq E_N^{\text{RPA}} + \hbar \sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta=1}^{M} E(k)_{\alpha,\beta} b^*_{\alpha,k} b_{\beta,k}$$

$$\simeq E_N^{\text{RPA}} + \mathrm{d}\Gamma_{\text{bosonic}} \Big(\underbrace{\hbar \bigoplus_{k \in \mathbb{Z}^3} E(k)}_{=:\, H_{\mathrm{B}}} \Big) .$$

Consider a one–boson wave function

$$\eta \in \mathfrak{h}_{\mathrm{B}} := \bigoplus_{k \in \mathbb{Z}^3} \mathbb{C}^M .$$

Then

$$\eta_t := e^{-iH_B \tau/\hbar} \eta_0$$

is the time–evolution in the (first quantized) one–boson space $\mathfrak{h}_{\mathrm{B}}$.

Define the boson creation operator $b^*(\eta) := \sum_{k\in\mathbb{Z}^3}\sum_{\alpha=1}^{M} b^*_{\alpha,k}\eta(k)_\alpha$.

Theorem: [B–Nam–Porta–Schlein–Seiringer '21]

Assume that $\hat{V}$ is compactly supported and non–negative. Let

$$\xi_0 := \frac{1}{Z_m} b^*(\eta_1)\cdots b^*(\eta_m)\Omega\,, \qquad \xi_t := \frac{1}{Z_m} b^*(\eta_{1,t})\cdots b^*(\eta_{m,t})\Omega\,.$$

Then in (fermionic) Fock space norm

$$\| e^{-iH_N t/\hbar} RT\xi_0 - e^{-i(E_N^{\mathrm{pw}}+E_N^{\mathrm{RPA}})t/\hbar} RT\xi_t \| \leq C_{m,V}\hbar^{1/15}|t|\,.$$

If $H_{\mathrm{B}}\eta_i = e_i\eta_i$ then we have constructed an approximate eigenstate of the many–body Hamiltonian, evolving up to times $|t| \ll N^{1/45}$ just with a phase:

$$e^{-iH_N t/\hbar} RT\xi_0 \simeq e^{-i\left(E_N^{\mathrm{pw}}+E_N^{\mathrm{RPA}}+\sum_{j=1}^{m} e_j\right)t/\hbar} RT\xi_0\,.$$