Bosonization of Fermionic Many-Body Systems

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Model Reduction in Quantum Mechanics

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Bosonic systems

Statistics: we distinguish between

Bosons: described by symmetric wave functions, ie.

$$\psi_N(x_{\pi 1}, x_{\pi 2}, \dots, x_{\pi N}) = \psi_N(x_1, x_2, \dots, x_N)$$
 for all $\pi \in S_N$

Fermions: described by antisymmetric wave functions, ie.

$$\psi_N(x_{\pi 1}, x_{\pi 2}, \dots, x_{\pi N}) = \sigma_{\pi} \psi_N(x_1, x_2, \dots, x_N)$$
 for all $\pi \in S_N$

Bosonic mean-field regime: N particles in torus $\Lambda = [0; 2\pi]^3$, with Hamiltonian

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \frac{1}{N} \sum_{i< j}^N V(x_i - x_j) \qquad \text{acting on } L_s^2(\Lambda^N)$$

Goals: ground state energy, excitations, time-evolution.

Bogoliubov theory

Fock space: describe bosons on

$$\mathcal{F}_s = \bigoplus_{n \ge 0} L_s^2(\Lambda^n)$$

For $p \in \mathbb{Z}^3$, we introduce a_p^*, a_p satisfying **CCR**

$$[a_p, a_q^*] = \delta_{pq}, \qquad [a_p, a_q] = [a_p^*, a_q^*] = 0$$

Then

 $a_p^* a_p =$ number of particles with momentum p

In particular, $\sigma(a_p^*a_p) = \mathbb{N}$.

Hamilton operator: in second quantized form, we find

$$H_N = \sum_{p \in \mathbb{Z}^3} p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q,r \in \mathbb{Z}^3} \widehat{V}(r) a_{p+r}^* a_q^* a_{q+r} a_p$$

BEC: low-energy states exhibit Bose-Einstein condensation, ie.

$$a_0^*, a_0 \simeq \sqrt{N} \gg 1 = [a_0, a_0^*]$$

Hence,

$$H_{N} \simeq \frac{(N-1)\hat{V}(0)}{2} + \sum_{p \neq 0} \left[p^{2} + \hat{V}(p) \right] a_{p}^{*} a_{p} + \frac{1}{2} \sum_{p \neq 0} \hat{V}(p) \left[a_{p}^{*} a_{-p}^{*} + a_{p} a_{-p} \right]$$

$$+ \frac{1}{\sqrt{N}} \sum_{p,r \neq 0} \hat{V}(r) \left[a_{p+r}^{*} a_{-r}^{*} a_{p} + \text{h.c.} \right]$$

$$+ \frac{1}{2N} \sum_{p,q,r \neq 0} \hat{V}(r) a_{p+r}^{*} a_{q}^{*} a_{q+r} a_{p}$$

Neglect cubic and quartic terms: we find

$$H_N \simeq \frac{(N-1)\widehat{V}(0)}{2} + \sum_{p \neq 0} \left[p^2 + \widehat{V}(p) \right] a_p^* a_p + \frac{1}{2} \sum_{p \neq 0} \widehat{V}(p) \left[a_p^* a_{-p}^* + a_p a_{-p} \right]$$

Bogoliubov transformations: let

$$T = \exp\left[\frac{1}{2} \sum_{p \neq 0} \tau_p \left(a_p^* a_{-p}^* - a_p a_{-p}\right)\right]$$

Then

$$T^* a_p^* T = (\cosh \tau_p) a_p^* + (\sinh \tau_p) a_{-p}$$

 $T^* a_p T = (\cosh \tau_p) a_p + (\sinh \tau_p) a_{-p}^*$

Diagonalization: with appropriate choice of τ_p , we obtain

$$T^*H_NT \simeq \frac{(N-1)\widehat{V}(0)}{2} - \frac{1}{2} \sum_{p \neq 0} \left[p^2 + \widehat{V}(p) - \sqrt{|p|^4 + 2p^2}\widehat{V}(p) \right]$$
$$+ \sum_{p \neq 0} \sqrt{|p|^4 + 2p^2}\widehat{V}(p) \cdot a_p^* a_p$$

From this expression, we can read off ground state energy and excitations.

Mean-field fermions

Mean-field regime: consider N fermions in torus $\Lambda = [0; 2\pi]^3$. System described on

$$L_a^2(\Lambda^N) = \{ \psi \in L^2(\Lambda^N), \text{ antisymmetric w.r.t. permutations} \}$$

On
$$L_a^2(\Lambda^N)$$
, we have $\sum_{j=1}^N -\Delta_{x_j} \simeq N^{5/3}$.

Hamilton operator: given by

$$H_N = \sum_{j=1}^{N} -\varepsilon^2 \Delta_{x_j} + \frac{1}{N} \sum_{i < j}^{N} V(x_i - x_j)$$

with semiclassical parameter $\varepsilon = N^{-1/3}$. We assume $\hat{V} \geq 0$.

We are interested in ground state energy

$$E_N = \min_{\psi \in L_a^2(\Lambda^N): \|\psi\| = 1} \langle \psi, H_N \psi \rangle$$

Hartree-Fock theory: consider Slater determinants

$$\psi_{\text{slater}}(x_1,\ldots,x_N) = C \det \left[f_i(x_j) \right]_{1 \le i,j \le N}$$

with $\{f_1,\ldots,f_N\}$ an orthonormal system in $L^2(\Lambda)$.

They are characterized by one-particle reduced density

$$\omega = N \operatorname{tr}_{2,\dots,N} |\psi_{\operatorname{slater}}\rangle \langle \psi_{\operatorname{slater}}| = \sum_{j=1}^{N} |f_j\rangle \langle f_j|$$

Their energy is given by Hartree-Fock functional

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

The Hartree-Fock energy is defined by

$$E_N^{\mathsf{HF}} = \min_{0 \le \omega \le 1: \operatorname{tr} \omega = N} \mathcal{E}_{\mathsf{HF}}(\omega)$$

Fermi sea: If V = 0, Hartree-Fock energy minimized by

$$\omega_F = \frac{1}{(2\pi)^3} \sum_{p \in \mathbb{Z}^3 : |p| \le p_F} |e^{ip \cdot x}\rangle \langle e^{ip \cdot x}|$$

with Fermi momentum

$$p_F \simeq (3/4\pi)^{1/3} N^{1/3} =: \kappa_0 N^{1/3}$$

Here, we assume that Fermi ball is completely filled.

Then ω_F also minimizes Hartree-Fock functional if $V \neq 0$. Hence

$$E_N^{\mathsf{HF}} = \mathcal{E}_{\mathsf{HF}}(\omega_F) = \sum_{|p| \le p_F} \varepsilon^2 p^2 + \frac{N\hat{V}(0)}{2} - \frac{1}{2N} \sum_{|p|,|p'| \le p_F} \hat{V}(p - p')$$

Remark: in general, [Gontier-Hainzl-Lewin, 19] proved that $E_N^{\mathsf{HF}} - \mathcal{E}_{\mathsf{HF}}(\omega_F)$ is sub-exponentially small in N.

Remark: justification of Hartree-Fock theory by [Bach, 92], [Graf-Solovej, 94] for Coulomb interaction.

Correlation energy

Theorem [Benedikter, Porta, S., Seiringer]: let $|k|\hat{V} \in \ell^1(\mathbb{Z}^3)$, $\hat{V} > 0$. Then

$$\begin{split} &\lim_{N \to \infty} \left[E_N - \mathcal{E}_{\mathsf{HF}}(\omega_F) \right] / \varepsilon \\ &= \kappa_0 \sum_{k \in \mathbb{Z}^3} |k| \bigg\{ \frac{1}{\pi} \int_0^\infty \log \left[1 + 2\pi \kappa_0 \hat{V}(k) \left(1 - \lambda \mathrm{arctan} \left(\frac{1}{\lambda} \right) \right) \right] d\lambda - \frac{\pi}{2} \kappa_0 \hat{V}(k) \bigg\} \end{split}$$

Remark 1: for upper bound, only need $\sum_{k \in \mathbb{Z}^3} |k| \hat{V}^2(k) < \infty$.

Remark 2: Result agrees with formula first predicted by Gell-Mann-Brueckner, through random phase approximation.

Remark 3: for small V, theorem proven by [Benedikter-Nam-Porta-S.-Seiringer, 20].

[Christiansen-Hainzl-Nam] proved similar result, with different approach.

Some ideas from proof

To estimate energy, it is convenient to factor out Fermi sea and focus on its excitations.

Fock space representation: on

$$\mathcal{F}_a = \bigoplus_{n \ge 0} L_a^2(\Lambda^n)$$

we introduce creation, annihilation operators satisfying canonical anticommutation relations

$$\{a_p, a_q^*\} = \delta_{p,q}, \qquad \{a_p, a_q\} = \{a_p^*, a_q^*\} = 0$$

We consider the Hamilton operator

$$\mathcal{H}_{N} = \sum_{p \in \mathbb{Z}^{3}} \varepsilon^{2} p^{2} a_{p}^{*} a_{p} + \frac{1}{2N} \sum_{p,q,r \in \mathbb{Z}^{3}} \hat{V}(r) a_{p+r}^{*} a_{q}^{*} a_{q+r} a_{p}$$

Particle-hole transformation: on \mathcal{F}_a , define unitary R with

$$R\Omega = \prod_{|p| \le p_F} a_p^* \Omega = \text{Fermi sea}$$

and

$$Ra_p^*R^* = \begin{cases} a_p^*, & \text{if } |p| > p_F \\ a_p, & \text{if } |p| \le p_F \end{cases}$$

After conjugation, a_p^* creates a hole in the Fermi sea, if $|p| \leq p_F$.

Observe:
$$R: \chi(\mathcal{N}_h = \mathcal{N}_p)\mathcal{F}_a \to L_a^2(\Lambda^N)$$
, where

$$\mathcal{N}_h = \sum_{|p| \le p_F} a_p^* a_p, \qquad \mathcal{N}_p = \sum_{|p| > p_F} a_p^* a_p$$

count number of **holes** and of excited **particles**.

Excitation Hamiltonian: we define

$$\mathcal{L}_N = R^* \mathcal{H}_N R$$

Conjugation of kinetic energy: we compute

$$\sum_{p \in \mathbb{Z}^3} \varepsilon^2 p^2 R^* a_p^* a_p R$$

$$= \sum_{|p| \le p_F} \varepsilon^2 p^2 a_p a_p^* + \sum_{|p| > p_F} \varepsilon^2 p^2 a_p^* a_p$$

$$= \sum_{|p| \le p_F} \varepsilon^2 p^2 - \sum_{|p| \le p_F} \varepsilon^2 p^2 a_p^* a_p + \sum_{|p| > p_F} \varepsilon^2 p^2 a_p^* a_p$$

$$= \operatorname{tr} \left[-\varepsilon^2 \Delta \right] \omega_F + \mathbb{H}_0$$

with the kinetic energy of excitations:

$$\mathbb{H}_0 = \sum_{p \in \mathbb{Z}^3} |\varepsilon^2 p^2 - \varepsilon^2 p_F^2| \, a_p^* a_p$$

Conjugation of potential energy: we find

$$\frac{1}{2N} \sum_{p,q,r} \hat{V}(r) R^* a_{p+r}^* a_q^* a_{q+r} a_p R = \frac{N\hat{V}(0)}{2} - \frac{1}{2N} \sum_{|p|,|p'| \le p_F} \hat{V}(p-p') + Q_B + \text{corrections}$$

where

$$Q_{B} = \frac{1}{2N} \sum_{|p|,|q| \le p_{F},|p+r|,|q+r| > p_{F}} \hat{V}(r) a_{p+r}^{*} a_{p}^{*} a_{q+r} a_{q}$$

$$+ \frac{1}{2N} \sum_{|p|,|q+r| \le p_{F},|p+r|,|q| > p_{F}} \hat{V}(r) \left[a_{p+r}^{*} a_{p}^{*} a_{q+r}^{*} a_{q}^{*} + a_{q} a_{q+r} a_{p} a_{p+r} \right]$$

$$= \frac{1}{2N} \sum_{r \in \mathbb{Z}^{3}} \hat{V}(r) \left[b_{r}^{*} b_{r} + \frac{1}{2} (b_{r}^{*} b_{-r}^{*} + b_{r} b_{-r}) \right]$$

in terms of particle-hole pair creation operators

$$b_r^* = \sum_{|p| \le p_F, |p+r| > p_F} a_{p+r}^* a_p^*$$

satisfying (after normalization) approximately bosonic relations

$$[b_r^*, b_k^*] = [b_r, b_k] = 0,$$
 $[b_r, b_k^*] = \operatorname{const} \cdot \delta_{r,k} + \operatorname{corrections}$

Conclusion: excitation Hamiltonian is given by

$$\mathcal{L}_N = \mathcal{E}_{HF}(\omega_F) + \mathbb{H}_0 + Q_B + \text{corrections}$$

where

$$\mathbb{H}_{0} = \sum_{p \in \mathbb{Z}^{3}} |\varepsilon^{2} p^{2} - \varepsilon^{2} p_{F}^{2}| a_{p}^{*} a_{p}$$

$$Q_{B} = \frac{1}{2N} \sum_{r \in \mathbb{Z}^{3}} \hat{V}(r) \left[b_{r}^{*} b_{r} + \frac{1}{2} (b_{r}^{*} b_{-r}^{*} + b_{r} b_{-r}) \right]$$

and where corrections are small on states with few excitations.

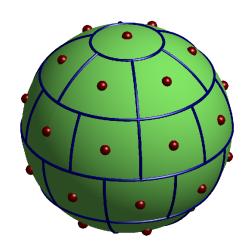
Question: can \mathbb{H}_0 be expressed through operators b, b^* ?

$$\mathbb{H}_{0} b_{r}^{*} \Omega = \sum_{\substack{|q| \leq p_{F}, |q+r| > p_{F}}} \mathbb{H}_{0} a_{q+r}^{*} a_{q}^{*} \Omega$$

$$= \sum_{\substack{|q| \leq p_{F}, |q+r| > p_{F}}} \left[\varepsilon^{2} (q+r)^{2} - \varepsilon^{2} q^{2} \right] a_{q+r}^{*} a_{q}^{*} \Omega$$

$$\simeq \sum_{\substack{|q| \leq p_{F}, |q+r| > p_{F}}} 2\varepsilon^{2} q \cdot r a_{q+r}^{*} a_{q}^{*} \Omega \neq \epsilon(r) b_{r}^{*} \Omega$$

Localized bosonic modes: we decompose Fermi sphere into $M = N^{\delta}$ patches $\{B_{\alpha}\}_{\alpha=1,...,M}$, and define modes



$$b_{k,\alpha}^* = \frac{1}{n_{\alpha}(k)} \sum_{\substack{p \in B_{\alpha}, \\ |p| \le p_F, |p+k| > p_F}} a_{p+k}^* a_p^*$$

with $n_{\alpha}(k)$ chosen so that

$$\left[b_{\alpha,k},b_{\beta,q}^*\right] \simeq \delta_{\alpha,\beta}\delta_{k,q}$$

Now, we find, with w_{α} the center of B_{α} ,

$$\mathbb{H}_0 b_{r,\alpha}^* \Omega \simeq \sum_{\substack{q \in B_\alpha, \\ |q| \leq p_F, |q+r| > p_F}} 2\varepsilon^2 q \cdot r a_{q+r}^* a_q^* \Omega \simeq 2\varepsilon^2 (w_\alpha \cdot r) b_{r,\alpha}^* \Omega$$

suggesting

$$\mathbb{H}_0 \simeq 2\kappa_0 \varepsilon \sum_{r \in \mathbb{Z}^3} (\widehat{w}_{\alpha} \cdot r) b_{r,\alpha}^* b_{r,\alpha}$$

Quadratic Hamiltonian: combining modes with momenta k and -k, we arrive at

$$\mathcal{L}_N = \mathcal{E}_{HF}(\omega_F) + \sum_{k \in \Gamma^{nor}} 2\varepsilon \kappa_0 |k| \mathfrak{h}(k) + \text{corrections}$$

with

$$\mathfrak{h}(k) = \sum_{\alpha,\beta=1}^{M} (D(k) + W(k))_{\alpha,\beta} b_{k,\alpha}^* b_{k,\beta}$$

$$+ \frac{1}{2} \sum_{\alpha,\beta=1}^{M} \widetilde{W}(k)_{\alpha,\beta} \left[b_{k,\alpha}^* b_{k,\beta}^* + b_{k,\beta} b_{k,\alpha} \right]$$

where the $M \times M$ matrices $D(k), W(k), \widetilde{W}(k)$ have entries

$$D(k)_{\alpha,\beta} = \delta_{\alpha,\beta} | \hat{k} \cdot \hat{\omega}_{\alpha} |,$$

$$W(k)_{\alpha,\beta} = \frac{\hat{V}(k)}{2\hbar\kappa_0 N|k|} \times \begin{cases} n_{\alpha}(k)n_{\beta}(k) & \text{if } \alpha,\beta \in \mathcal{I}_k^+ \text{ or } \alpha,\beta \in \mathcal{I}_k^- \\ 0 & \text{otherwise,} \end{cases}$$

$$\widetilde{W}(k)_{\alpha,\beta} = \frac{\hat{V}(k)}{2\hbar\kappa_0 N|k|} \times \begin{cases} 0 & \text{if } \alpha,\beta \in \mathcal{I}_k^+ \text{ or } \alpha,\beta \in \mathcal{I}_k^- \\ n_{\alpha}(k)n_{\beta}(k) & \text{otherwise.} \end{cases}$$

Bogoliubov theory: let

$$T = \exp\left[\frac{1}{2} \sum_{k \in \Gamma^{\mathsf{nor}}} \sum_{\alpha,\beta} K(k)_{\alpha,\beta} \, b_{k,\alpha}^* b_{k,\beta}^* - \mathsf{h.c.}\right]$$

Up to small corrections,

$$T^*b_{k,\alpha}T\simeq\sum_{\beta}\cosh(K(k))_{\alpha,\beta}\,b_{k,\beta}+\sum_{\beta}\sinh(K(k))_{\alpha,\beta}\,b_{k,\beta}^*$$

With appropriate choice of K, we find

$$\begin{split} T^*\mathcal{L}_N T &= \mathcal{E}_{\mathsf{HF}}(\omega_F) + 2\varepsilon\kappa_0 \sum_{k\in\Gamma^{\mathsf{nor}}} |k| \operatorname{tr} \big[E(k) - D(k) - W(k) \big] \\ &+ \sum_{k\in\Gamma^{\mathsf{nor}}} \sum_{\alpha,\beta} \mathfrak{K}(k)_{\alpha,\beta} \, b_{k,\alpha}^* b_{k,\beta} + \text{corrections} \end{split}$$

Finally, explicit computation shows that

$$\operatorname{tr} \big[E(k) - D(k) - W(k) \big] \\ \simeq \frac{1}{\pi} \int_0^\infty \log \left[1 + 2\pi \kappa_0 \hat{V}(k) (1 - \lambda \operatorname{arctan}(1/\lambda)) \right] d\lambda - \frac{\pi}{2} \kappa_0 \hat{V}(k)$$

An additional challenge: From

$$\mathbb{H}_0 b_{r,\alpha}^* \Omega \simeq 2\kappa_0 \varepsilon \left(\widehat{w}_{\alpha} \cdot r \right) b_{r,\alpha}^* \Omega \quad \Rightarrow \quad \mathbb{H}_0 \simeq 2\kappa_0 \varepsilon \sum_{r \in \mathbb{Z}^3} (\widehat{w}_{\alpha} \cdot r) b_{r,\alpha}^* b_{r,\alpha} =: \mathbb{D}_B$$

Instead, we only obtain that

$$\left[\mathbb{H}_{0}-\mathbb{D}_{B},b_{r,\alpha}\right],\left[\mathbb{H}_{0}-\mathbb{D}_{B},b_{r,\alpha}^{*}\right]\simeq0\quad\Rightarrow\quad T^{*}(\mathbb{H}_{0}-\mathbb{D}_{B})T\simeq(\mathbb{H}_{0}-\mathbb{D}_{B})$$

Therefore,

$$\mathcal{L}_N \simeq \mathcal{E}_{\mathsf{HF}}(\omega_F) + \mathbb{H}_0 + Q_B$$

 $\simeq \mathcal{E}_{\mathsf{HF}}(\omega_F) + (\mathbb{H}_0 - \mathbb{D}_B) + 2\kappa_0 \varepsilon \sum_{k \in \mathsf{\Gamma}^\mathsf{nor}} |k| \mathfrak{h}(k)$

and

$$T^*\mathcal{L}_N T \simeq \mathcal{E}_{\mathsf{HF}}(\omega_F) + 2\kappa_0 \varepsilon \sum_{k \in \Gamma^{\mathsf{nor}}} |k| \operatorname{tr} \left[E(k) - D(k) - W(k) \right] + (\mathbb{H}_0 - \mathbb{D}_B) + 2\kappa_0 \varepsilon \sum_{k \in \Gamma^{\mathsf{nor}}} |k| \sum_{\alpha, \beta} \mathfrak{K}(k)_{\alpha, \beta} \, b_{k, \alpha}^* b_{k, \beta}$$

To control $-\mathbb{D}_B$, we use a **second** almost bosonic **Bogoliubov transformation**, diagonalizing \mathfrak{K} .

Dynamics of excitations

Time evolution of almost bosonic excitations can be described by **Bogoliubov Hamiltonian** $\mathfrak{K}(k)$.

Schrödinger equation: consider solution of

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

with initial data of the form $\psi_{N,0} = RT\xi \in L_a^2(\Lambda^N)$, with

$$\xi = \frac{1}{Z} b^*(\varphi_1) \dots b^*(\varphi_m) \Omega, \qquad \text{with } b^*(\varphi) = \sum_{k \in \Gamma^{\mathsf{nor}}} \sum_{\alpha \in \mathcal{I}_k} \varphi_\alpha(k) b_{k,\alpha}^*$$

Then

$$T^*R^*\psi_{N,t} = T^*R^*e^{-iH_Nt/\varepsilon}RT\xi$$
$$= e^{-iT^*R^*H_NRTt/\varepsilon}\xi = e^{-iT^*\mathcal{L}_NTt/\varepsilon}\xi$$

From approximation

$$T^*\mathcal{L}_N T = \mathcal{E}_{\mathsf{HF}}(\omega_F) + 2\varepsilon\kappa_0 \sum_{k \in \Gamma^{\mathsf{nor}}} |k| \operatorname{tr} \left[E(k) - D(k) - W(k) \right]$$
$$+ (\mathbb{H}_0 - \mathbb{D}_B) + 2\kappa_0 \varepsilon \sum_{k \in \Gamma^{\mathsf{nor}}} |k| \sum_{\alpha, \beta} \mathfrak{K}(k)_{\alpha, \beta} \, b_{k, \alpha}^* b_{k, \beta}$$

we are led to excitation dynamics

$$\xi_t = \frac{1}{Z} b^*(\varphi_{1,t}) \dots b^*(\varphi_{m,t}) \Omega$$

where

$$\varphi_t = e^{-ih_B t/\varepsilon} \varphi$$
, with $h_B = 2\kappa_0 \varepsilon \bigoplus_{k \in \Gamma^{\text{nor}}} |k| \mathfrak{K}(k)$

Theorem [Benedikter, Nam, Porta, S., Seiringer]: many-body evolution can be approximated in norm by

$$||e^{-iH_N t/\varepsilon}RT\xi - e^{-i(\mathcal{E}_{\mathsf{HF}}(\omega_F) + E_{\mathsf{corr}})t/\varepsilon}RT\xi_t|| \le C|t|\varepsilon^{1/15}$$