Rigorous Results on the energy and structure of ground states of large many-body systems
II. Approximate models

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List of Slides

Equivalence of canonical and grand canonical pictures

If the system is stable of the 2nd kind we may define the **grand canonical pressure** for $\mu \in [C, \infty)$ for some $C > 0$

$$P(\mu) = \inf_{\|\Psi\|=1,\ \Psi \in \mathcal{F}} (\Psi, (H + \mu N)\Psi).$$

The parameter μ is called the chemical potential.

In fact P is the **Legendre transform** of the energy function $N \mapsto E_N$

$$P(\mu) = \inf_N (E_N + \mu N)$$

Thus if $N \mapsto E_N$ is convex we may reconstruct E_N from P

$$E_N = \sup_\mu (P(\mu) - \mu N).$$

The bosonic Hartree approximation

In the following we will consider mainly the case where

$$h = -\tfrac{1}{2}\Delta + V, \qquad W_{ij} = W(x_i - x_j)$$

In the **bosonic Hartree approximation** one restricts attention to wave functions of the non-interacting form $\Psi = \underbrace{\psi \otimes \cdots \otimes \psi}_{N}$.

Then

$$\mathcal{E}_N^{\mathrm{H}}(\psi) := (\Psi, H_N \Psi) =$$

$$\tfrac{1}{2}N \int |\nabla\psi|^2 + N \int |\psi|^2 V + \tfrac{1}{2}N(N-1) \iint |\psi(x)|^2 W(x-y) |\psi(y)|^2 dxdy.$$

$$E_N^{\mathrm{H}} = \inf_{\psi \in \mathfrak{h},\ \|\psi\|=1} \mathcal{E}^{\mathrm{H}}(\psi) \geq E_N^{\mathrm{B}}$$

Or we may use the density $\rho = N|\psi|^2$. If W is positive type (i.e., $\widehat{W} \geq 0$) then $\mathcal{E}^{\mathrm{H}}$ is convex and the minimizer ψ is unique (up to a constant phase).

Is this a good approximation? Certainly not if W is a hard core.

The Hartree-Fock model

In the **Hartree-Fock approximation** we do the same for fermions and restrict to Slater determinants $\Psi = \psi_1 \wedge \cdots \wedge \psi_N$. The energy expectation can be expressed entirely from the 1-particle density matrix γ, which is the projection onto the space spanned by $\psi_1, \ldots, \psi_N$:

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma) \quad := \quad & (\Psi, H_N \Psi) = \mathrm{Tr}[-\tfrac{1}{2}\Delta\gamma] + \int \rho_\gamma V \\ & +\tfrac{1}{2}\iint \rho_\gamma(x) W(x-y) \rho_\gamma(y) dx dy \\ & -\tfrac{1}{2}\iint \mathrm{Tr}_{\mathbb{C}^q} |\gamma(x,y)|^2 W(x-y) dx dy\end{aligned}$$

The last two terms are called respectively the direct term and the exchange term. ρ_γ is the density of γ

$$\gamma(x,y) = \sum_{k=1}^{N} \psi_k(x)\psi_k(y)^*, \qquad \rho_\gamma(x) = \mathrm{Tr}_{\mathbb{C}^q}\gamma(x,x) = \sum_{k=1}^{N} |\psi_k(x)|^2.$$

Properties of the Hartree-Fock model

$$E_N^{\rm HF} = \inf\{\mathcal{E}^{\rm HF}(\gamma) \mid \gamma \text{ projection } {\rm Tr}\gamma = N\} \geq E_N^{\rm F}$$

THEOREM 1 (Self-consistency, Bach-Lieb-Loss-Sol.). *If γ is an HF minimizer then γ is the unique projection onto the N "lowest" eigenvectors of the* **mean field** *operator*

$$H_{\rm MF} = -\tfrac{1}{2}\Delta + V + \rho_\gamma * W - \mathcal{K}_\gamma, \quad \mathcal{K}_\gamma\phi(x) = \int \gamma(x,y)^* W(x-y)\phi(y)dy.$$

The *uniqueness* means that there are no degeneracies. Put differently: **There are no unfilled shells in Hartree-Fock theory**. Minimizer are not necessarily unique. The approximation is again very bad for hard core.

THEOREM 2 (Lieb's variational principle).

$$E_N^{\rm HF} = \inf\{\mathcal{E}^{\rm HF}(\gamma) \mid 0 \leq \gamma \leq \mathbf{1},\ {\rm Tr}\gamma = N\}.$$

Semiclassics

We want next to approximate the fermionic energy by a functional of the density alone. We will ignore the exchange term. We make the semiclassical approximations for a non-interacting system

$$\rho(x) = (2\pi)^{-3} \int_{\frac{1}{2}p^2+V(x)<0} 1 dp = C_{\rm d}|V(x)|_-^{3/2},$$

for the density and for the energy

$$(2\pi)^{-3} \int_{\frac{1}{2}p^2+V(x)<0} (\tfrac{1}{2}p^2 + V(x)) dp dx = -C_{\rm cl} \int |V|_-^{5/2} = C_{\rm TF} \int \rho^{5/3} + \int \rho V.$$

THEOREM 3 (semiclassics).

$$\lim_{h\to 0} (2\pi h)^3 \mathrm{Tr}[-|-h^2\Delta + V|_-] = -C_{\rm cl} \int |V|_-^{5/2}.$$

Here $\mathrm{Tr}[-|-h^2\Delta + V|_-]$ *is the sum of the negative eigenvalues of* $-h^2\Delta + V$*, i.e., the minimal fermionic energy.*

The Thomas-Fermi approximation

Motivated by semiclassics we define the **Thomas-Fermi functional**

$$\mathcal{E}^{\mathrm{TF}}(\rho) := C_{\mathrm{TF}} \int \rho^{5/3} + \int \rho V + \tfrac{1}{2} \int\int \rho(x) W(x-y) \rho(y) dx dy$$

$$E_N^{\mathrm{TF}} = \inf\{\mathcal{E}^{\mathrm{TF}}(\rho) |\ \rho \geq 0,\ \int \rho = N\}.$$

If V, W tend to zero at infinity and W is positive type ($\widehat{W} \geq 0$) then the minimzing ρ is unique and $N \mapsto E_N^{\mathrm{TF}}$ is convex and non-increasing. There is N_c^{TF} (possibly$= \infty$) such that $N \mapsto E_N^{\mathrm{TF}}$ is strictly decreasing for $N \leq N_c^{\mathrm{TF}}$ and constant otherwise. For $N < N_c^{\mathrm{TF}}$ a minimizing ρ exists Lieb-Simon).

In many cases one can prove that the TF approximation is good using semiclassical techniques.

Quasi-free fermionic states

We shall now see that we may improve Hartree-Fock theory by considering a grand canonical generalization.

We generalize from Slater determinants to ground states Ψ of general **quadratic** Hamiltonians

$$\sum_{\alpha\beta} A_{\alpha\beta}a_\alpha^* a_\beta + B_{\alpha\beta}a_\alpha a_\beta - \overline{B}_{\alpha\beta}a_\alpha^* a_\beta^*$$

(Slater determinants correspond to $B = 0$). If we introduce

$$\gamma_{ij} = (\Psi, a_i^* a_j \Psi), \quad \alpha_{ij} = (\Psi, a_i a_j \Psi)$$

then $\gamma^2 + \alpha\alpha^* = \gamma, \quad [\gamma, \alpha] = 0$. In particular, $0 \leq \gamma \leq \mathbf{1}$.

$$\text{Slater: } a(\psi_1)^* \cdots a(\psi_N)^* |0\rangle$$

$$\text{BCS: } [\sigma_1 + \tau_1 a(\psi_1)^* a(\psi_2)^*][\sigma_2 + \tau_2 a(\psi_3)^* a(\psi_4)^*] \cdots |0\rangle, \quad \sigma_i, \tau_i \in \mathbb{C}$$

BCS theory

The BCS approximation to the pressure is

$$P^{\mathrm{BCS}}(\mu) := (\Psi, (H + \mu N)\Psi) = \mathcal{E}^{\mathrm{HF}}(\gamma) + \mu \mathrm{Tr}\gamma + \frac{1}{2}\iint |\mathrm{Tr}_{\mathbb{C}^q}\alpha(x,y)| W(x-y)\,dx\,dy$$

From Lieb's variational principle we see that if $W \geq 0$ the best choice is $\alpha = 0$. Otherwise $\alpha \neq 0$ may be better. This has been analyzed in great detail by Bach-Lieb-Sol. for the Hubbard model: $\mathbb{R}^3 \to \mathbb{Z}^3$, $-\Delta$ discrete, $V = 0$, $W(x) = 0$ unless $x = 0$.

The BCS mean field operator is a quadratic Hamiltonian.

The Bogolubov approximation

Quadratic Hamiltonians are also important in the Bogolubov approximation for bosons. Let us write the 2nd quantized Hamiltonian in an eigenbasis for the one-particle operator

$$H = \sum_{\alpha} h_\alpha a_\alpha^* a_\alpha + \tfrac{1}{2} \sum_{\alpha\beta\mu\nu} W_{\alpha\beta\mu\nu} a_\alpha^* a_\beta^* a_\nu a_\mu$$

The Bogolubov approximation is based on the assumption that $\alpha = 0$ corresponds to a condensate.

Bogolubov approximation: (1) $a_0^*, a_0 \to \sqrt{N}$, (2) keep only quartic terms with at least two α, β, μ, ν being 0. The Hamiltonian becomes quadratic plus linear

$$\sum_{\alpha} h_\alpha a_\alpha^* a_\alpha + \tfrac{1}{2} N \sum_{\alpha\beta\neq 0} W_{\alpha 0 \beta} a_\alpha^* a_\beta + W_{\alpha\beta 00} a_\alpha^* a_\beta^* + \ldots$$

$$+ \tfrac{1}{2} N^{3/2} \sum_{\alpha} W_{\alpha 000} a_\alpha^* + \ldots + \tfrac{1}{2} N^2 W_{0000}.$$