Rigorous Results on the energy and structure of ground states of large many-body systems I: Elementary formalism

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List of Slides

Program for next lectures

Lecture II: **Approximate models:**

- Hartree and Hartree-Fock models

- Semiclassics and the Thomas-Fermi model

- The BCS approximation

- The Bogolubov approximation

Lecture III: **Specific many-body systems :**

- Short range Bose and Fermi systems

- Charged systems: atoms, molecules, one component plasma (jellium), matter

Lecture IV: **Stability and instability of matter:**

- Correlation estimates

- Stability of fermionic matter

- Instability of bosonic matter

Formulation of many-body quantum mechanics

We consider Hamiltonians with two-body interactions

$$H_N = \sum_{i=1}^{N} h_i + \sum_{1 \leq i < j \leq N} W_{ij}$$

h_i: the one-body Hamiltonian describing particle i; acts on the **Hilbert space** $\mathfrak{h}_i$ of particle i; Normally $h_i = T_i + V_i$, $T_i =$kinetic energy $V_i =$potential energy.

W_{ij}: Interaction of particles i and j; Operator on $\mathfrak{h}_i \otimes \mathfrak{h}_j$.

Hilbert space H_N acts on: $\mathcal{H}_N = \bigotimes_{i=1}^{N} \mathfrak{h}_i$.

Of special importance is the situation of identical particles

$$h_1 = \ldots = h_N = h, \qquad \mathfrak{h}_1 = \ldots = \mathfrak{h}_N = \mathfrak{h}, \qquad W_{ij} = W_{ji} = W$$

$$\textbf{Fermions:} \quad \mathcal{H}_N^F = \bigwedge^{N} \mathfrak{h} \subset \mathcal{H}_N \qquad \textbf{Bosons:} \quad \mathcal{H}_N^B = \bigotimes_{\text{sym}}^{N} \mathfrak{h} \subset \mathcal{H}_N.$$

The grand canonical picture

The previous situation where the particle number N is given is called the **canonical picture**. In the **grand canonical picture** we consider all particle numbers at the same time:

$$H = \bigoplus_{N=0}^{\infty} H_N, \qquad \mathcal{H} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N$$

($H_0 = 0$ and $\mathcal{H}_0 = \mathbb{C}$).

The corresponding (**fermionic Fock space:**)

$$\mathcal{F}^{\mathrm{F}}(\mathfrak{h}) = \bigoplus_{N=0}^{\infty} \bigwedge^{N} \mathfrak{h}.$$

and (**bosonic Fock space:**)

$$\mathcal{F}^{\mathrm{B}}(\mathfrak{h}) = \bigoplus_{N=0}^{\infty} \bigotimes_{\mathrm{sym}}^{N} \mathfrak{h}.$$

Fermions and bosons and their second quantizations

In the grand canonical picture it is convenient for bosons and fermions to introduce the notion of **creation** and *annihilation* operators on the Fock spaces. The operator that creates a particle in the one-particle state $f \in \mathfrak{h}$:

$$(a(f)^* \Psi_N)_{\alpha_1 \ldots \alpha_{N+1}} = \frac{1}{\sqrt{N+1}} \sum_{j=1}^{N} \overbrace{(-1)^j}^{\text{fermion}} f_{\alpha_j} (\Psi_N)_{\alpha_1 \ldots \widehat{\alpha}_j \ldots \alpha_{N+1}}$$

(using coordinates in an orthonormal basis). The adjoint annihilates

$$(a(f) \Psi_{N+1})_{\alpha_1 \ldots \alpha_N} = \sqrt{N+1} \sum_{\alpha_{N+1}} \overbrace{(-1)^{N+1}}^{\text{fermion}} \overline{f_{\alpha_{N+1}}} (\Psi_{N+1})_{\alpha_1 \ldots \alpha_{N+1}}.$$

The algebras ($[A, B] = AB - BA$, $\{A, B\} = AB + BA$)

Fermions CAR: $\{a(f), a(g)\} = \{a(f)^*, a(g)^*\} = 0, \quad \{a(f), a(g)^*\} = (f, g)$

Bosons CCR: $[a(f), a(g)] = [a(f)^*, a(g)^*] = 0, \quad [a(f), a(g)^*] = (f, g).$

Expressing operators using second quantization

We may write the grand canonical operator

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

where $a_\alpha = a(u_\alpha)$ and u_α, $\alpha = 0, \ldots$ is an orthonormal basis for the one-particle space $\mathfrak{h}$. Here

$$h_{\alpha\beta} = (u_\alpha, h u_\beta), \quad W_{\alpha\beta\mu\nu} = (u_\alpha \otimes u_\beta, W u_\mu \otimes u_\nu).$$

In particular, the particle number is $N = \sum_\alpha a_\alpha^* a_\alpha$ (now an operator).

For any normalized Ψ we define the **1-particle density matrix** γ_Ψ on the one-particle space $\mathfrak{h}$ by

$$(f, \gamma_\Psi g) = (\Psi, a(g)^* a(f) \Psi).$$

Then $0 \leq \gamma_\Psi \leq (\Psi, N\Psi)\mathbf{1}$ (as operators) and $\mathrm{Tr}\gamma_\Psi = (\Psi, N\Psi)$.

Properties of bosonic and fermionic states

For normalized *fermionic* Ψ we have

$$(f, \gamma_\Psi f) = (\Psi, a(f)^* a(f) \Psi) \leq (\Psi, \{a(f)^*, a(f)\} \Psi) \leq \|f\|^2$$

Thus for fermions

$$0 \leq \gamma_\Psi \leq \mathbf{1}.$$

For bosons however γ_Ψ may have an eigenvalue N (see slide on non-interacting systems). We will say that our system satisfies **Bose-Einstein condensation** if for large N, γ_Ψ has an eigenvalue of order N.

The 1-particle density matrix can be expressed without 2nd quantization as the operator γ_Ψ such that

$$\left(\Psi, \sum_i X_i \Psi \right) = \mathrm{Tr}(X \gamma_\Psi)$$

for all operators X on the one-particle space $\mathfrak{h}$.

Stability and self-adjointness

The system is said to satisfy **Stability (of the first kind)** if

$$E_N := \inf\big\{(\Psi, H_N\Psi) \,\big|\, \Psi \in \mathcal{D}(\mathcal{H}_N) \subset \mathcal{H}_N, \|\Psi\| = 1\big\} > -\infty$$

(H_N is bounded below)

EXPLANATION: Often H_N is an **unbounded operator** not defined on all of $\mathcal{H}_N$, but on some dense domain $\mathcal{D}(\mathcal{H}_N) \subset \mathcal{H}_N$. If stability holds then the symmetric operator $\mathcal{H}_N$ has a special self-adjoint extension, the **Friedrichs extension**.

For this extension the **variational principle** states that E_N is the bottom of the spectrum.

We say that the system has **a (stable) ground state** if E_N is a (discrete) eigenvalue. E_N is the **ground state energy**.

A **ground state** is a corresponding normalized eigenfunction (it is not necessarily unique).

Stability of the second kind

Stability of the second kind is a grand canonical notion of stability. We say that the system satisfies stability of the second kind if there exists a constant $C > 0$ such that for all N

$$E_N > -CN,$$

i.e., if the grand canonical operator

$$H + CN > 0$$

Stability of the first kind means that the energy cannot be arbitrarily negative.

Stability of the second kind means that the energy per particle cannot be arbitrarily negative.

Non-interacting systems

If $W_{ij} = 0$ the system is *non-interacting* $H_N = \sum_{i=1}^{N} h_i$. The ground state energy (or bottom of spec) for such a system is

$$E_N = \sum_{i=1}^{N} e_1^{(i)} \qquad \text{Ground state: } \Psi_N = \psi_1^{(1)} \otimes \cdots \otimes \psi_1^{(N)}$$

$e_1^{(i)}$ is the lowest eigenvalue (or bottom of spec) for h_i, $\psi_1^{(i)}$ corresponding normalized eigenfunction .

For *bosons*: $E_N^{\mathrm{B}} = Ne_1$. Ground state: $\Psi_N = \psi_1 \otimes \cdots \otimes \psi_1$; e_1 is lowest eigenvalue for h with eigenfunction ψ_1; $\gamma_\Psi = N|\psi_1\rangle\langle\psi_1|$

For *fermions*: $E_N^{\mathrm{F}} = e_1 + \cdots + e_N$. Ground state: $\Psi_N = \psi_1 \wedge \cdots \wedge \psi_N$; $e_1 \leq e_2, \leq \ldots$ eigenvalues of h, with orthonormal eigenfunctions $\psi_1, \ldots, \psi_N$; γ_Ψ is the projection onto the space spanned by $\psi_1, \ldots, \psi_N$.

Schrödinger operators and the Sobolev inequality

The *Schrödinger operator* on $\mathbb{R}^3$

$$h = -\tfrac{1}{2}\Delta + V(x), \qquad \mathfrak{h} = L^2(\mathbb{R}^3, \mathbb{C}^q)$$

describes a particle (with q internal degrees of freedom) moving in 3-dimensional space in an external potential $V(x)$. For electrons $q = 2$; using atomic units ($\hbar = m = e = 1$, V electric potential)

The uncertainty principle (Sobolev inequality) :

$$(\psi, -\Delta\psi) = \int_{\mathbb{R}^3} |\nabla\psi|^2 \geq C_{\mathrm{S}} \left(\int |\psi|^6\right)^{1/3}.$$

$$\tfrac{1}{2}\int |\nabla\psi|^2 + \int V|\psi|^2 \quad \geq \quad \tfrac{1}{2}C_{\mathrm{S}}\left(\int \psi^6\right)^{1/3} - \left(\int |V|_-^{5/2} \int |\psi|^2\right)^{2/5} \left(\int |\psi|^6\right)^{1/5}$$

$$\geq \quad -C\int |V|_-^{5/2} \int |\psi|^2. \qquad [|V|_- = \max\{-V, 0\}]$$

The Lieb-Thirring inequality

Hence

$$e_1 = \inf_{\psi, \|\psi\|=1} (\psi, h\psi) \geq -C \int |V|_-^{5/2}.$$

This proves **stability of the first kind** for many potentials. The bosonic energy satisfies

$$E_N^{\mathrm{B}} \geq -CN \int |V|_-^{5/2}.$$

The **Lieb-Thirring inequality** (Lieb-Thirring '76) generalizes this to fermions

$$E_N^{\mathrm{F}} = e_1 + \cdots e_N \geq -C_{\mathrm{LT}} \int |V|_-^{5/2}.$$

One should compare this to the classical phase space integral

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

Lieb-Thirring conjecture: The LT inequality holds with $C_{\mathrm{LT}} = C_{\mathrm{cl}}$.