Rigorous Results on the energy and structure of ground states of large many-body systems III. Specific many body systems

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List of Slides

The thermodynamic limit

We now restrict to a box $\Omega = [0, L]^3$, i.e., consider the Hilbert space $\mathfrak{h} = L^2(\Omega; \mathbb{C}^q)$ and introduce suitable boundary condition for the Laplacian (Dirichlet, Neumann or periodic). $|\Omega| = L^3$, we write $\Omega \to \infty$ for $L \to \infty$.

Allow the 1-particle potential V_Ω to depend on the domain.

$$H_{N,\Omega} = \sum_{i=1}^{N} (-\tfrac{1}{2}\Delta_i + V_\Omega(x_i)) + \sum_{1 \le i < j \le N} W(x_i - x_j).$$

We say that the ground state energy $E_N(\Omega)$ has a **thermodynamic limit** if for fixed $\rho > 0$ there is $e(\rho)$ such that

$$\frac{E_N(\Omega)}{|\Omega|} \to e(\rho)$$

as $N \to \infty$, $\Omega \to \infty$ with $N/|\Omega| = \rho$.

Existence of thermodynamic limit requires **stability of the 2nd kind**.

Short range Fermi and Bose systems

Now $V = 0$ and $W \geq 0$ with finite range and **scattering length**:

$$a = \lim_{R\to\infty} \frac{R^3}{3} \inf \left\{ \int_{|x|<R} |\nabla\phi|^2 + \int_{|x|<R} W|\phi|^2 \;\middle|\; \int_{|x|<R} |\phi|^2 = 1 \right\}.$$

(no 1/2 in front of the kinetic energy; reduced mass).

In particular, we may have a hard core with diameter a: $W(x) = \infty$ if $|x| < a$ and 0 otherwise. In this case Hartree and Hartree-Fock are very bad.

For both fermions and bosons the thermodynamic limits exist.

THEOREM 1 (Low density Bose and Fermi gas). *For* $\rho \to 0$

$$e^{\mathrm{B}}(\rho) = 2\pi a\rho^2 + o(\rho^2) \qquad \textit{Lieb-Yngvason}$$

$$e^{\mathrm{F}}(\rho) = C_{\mathrm{TF}}\rho^{5/3} + 2\pi(1-q^{-1})a\rho^2 + o(\rho^2) \quad \textit{Lieb-Seiringer-Sol. (in prep.)}$$

A modification of Bogolubov is supposed to give next Bose term.

Charged systems I: Atoms and molecules

Atoms and Molecules: Two types of particles N electrons and K nuclei.

$$
\begin{aligned}
H_{N,K} \quad = \quad & \sum_{i=1}^{N} -\tfrac{1}{2}\Delta_i - \sum_{i=1}^{N}\sum_{k=1}^{K} Z_k |x_i - R_k|^{-1} + \sum_{1\leq i<j\leq N} |x_i - x_j|^{-1} \\
& + \sum_{1\leq k<\ell\leq K} Z_k Z_\ell |R_k - R_\ell|^{-1}
\end{aligned}
$$

The electrons are fermions. The nuclei are classical particles at positions $R_1, \ldots, R_K \in \mathbb{R}^3$ and nuclear charges. $Z_1, \ldots, Z_K > 0$. Since we look for the ground state we have ignored the kinetic energy of the nuclei. We simply look for the energetically best positions. From the point of view of stability this is the worst case. Recall: **Stable of 1st kind by Sobolev.**

$$
E^{\mathrm{F}}_{N,K} = \inf_{R_1,\ldots,R_K} \inf_{\Psi, \|\Psi\|=1} (\Psi, H_{N,K}\Psi) > -\infty.
$$

Charged systems II: Matter

Fermionic Matter: As above, but confined to box Ω with Dirichlet b.c. and with $Z_1 = \ldots = Z_K = Z$. We consider the thermodynamic limit of $E^{\mathrm{F}}_{N,K}(\Omega)$ with $N/|\Omega| = \rho$ and $N = ZK$ (neutrality).

Bosonic Matter: We have two species of opposite charge. We will show that bosonic matter is unstable even if we keep the kinetic energy of both positive and negative particles:

$$H_N = \sum_{i=1}^{N} -\tfrac{1}{2}\Delta_i + \sum_{1\le i<j\le N} z_i z_j |x_i - x_j|^{-1}, \qquad z_i = 1 \text{ or } z_i = -1$$

$$E^{\mathrm{B}}_N = \inf_{z_i=\pm 1} \inf_{\Psi, \|\Psi\|=1} (\Psi, H_N \Psi).$$

Charged systems II: One component plasma

One component plasma (jellium): This is again a charged system confined to a box Ω, but instead of nuclei we have a uniform background of density ρ.

$$\begin{aligned} H_N &= \sum_{i=1}^{N} -\tfrac{1}{2}\Delta_i - \rho \int_{\Omega} |x_i - y|^{-1} dy + \sum_{1\leq i<j\leq N} |x_i - x_j|^{-1} \\ &\quad + \tfrac{1}{2}\rho^2 \iint_{\Omega\times\Omega} |x-y|^{-1} dx dy. \end{aligned}$$

We consider thermodynamics for the neutral system $N = \rho|\Omega|$. The neutral system has ground state energy E_N.

In the physics literature one finds a different formulation on a torus. We discuss this later.

Results on Atoms

For neutral atoms $N = Z$

$$\lim_{Z\to\infty} \frac{E_Z}{E_Z^{\mathrm{TF}}} = 1, \quad E_Z^{\mathrm{TF}} = c_{\mathrm{TF}} Z^{7/3} \quad \text{Lieb-Simon}$$

For neutral quantum density $\rho(x) = \mathrm{Tr}\gamma_\Psi(x,x)$:

$$Z^{-2}\rho(Z^{-1/3}x) \to \rho_{Z=1}^{\mathrm{TF}}(x),\ L^1_{\mathrm{loc}} \text{ as } Z\to\infty$$

Improved asymptotics:

$$E_Z^{\mathrm{F}} - E_Z^{\mathrm{HF}} = o(Z^{5/3}) \text{ as } Z \to \infty \quad \text{Bach, Fefferman-Seco}$$

$$E_Z^{\mathrm{F}} = c_{\mathrm{TF}} Z^{7/3} + C_{\mathrm{S}} Z^2 + C_{\mathrm{DS}} Z^{5/3} + o(Z^{5/3}) \quad \text{Siedentop-Weikards, Fefferman-Seco}$$

TF has minimizer iff $N \leq Z$. HF has a minimizer for $N < Z + 1$ (Lieb-Simon) and no minimizer for $N > Z + Q$ for some constant Q (Sol.). The quantum theory has stable ground state for $N < Z + 1$ (Zhislin) and no ground state for $N > 2Z + 1$ (Lieb) or for $N \gg Z$ when Z large.

Foldy's use of Bogolubov aprox. to jellium like system

Bosons on Ω; translation invariant Hamiltonian periodic b.c ("jellium")

$$H = \sum_k \tfrac{1}{2} k^2 a_k^* a_k + \tfrac{1}{2}\Omega^{-1} \sum_{k\neq 0} \frac{4\pi}{k^2} \sum_{p,q} a_p^* a_q^* a_{p+k} a_{q-k}$$

The sum is over momenta. After Bogolubov approximation ($\rho = N/\Omega$)

$$\tfrac{1}{2} \sum_{k\neq 0} \tfrac{1}{2} k^2 (a_k^* a_k + a_{-k}^* a_{-k}) + \frac{4\pi\rho}{k^2} (a_k^* a_k + a_{-k}^* a_{-k} + a_k^* a_{-k}^* + a_{-k}^* a_k^*)$$

$$= \sum_{k\neq 0} D_k (a_k^* + \alpha_k a_{-k})(a_k^* + \alpha_k a_{-k})^* + D_k (a_{-k}^* + \alpha_k a_k)(a_{-k}^* + \alpha_k a_k)^*$$

$$-\sum_{k\neq 0} D_k \alpha_k^2 ([a_k, a_k^*] + [a_{-k}, a_{-k}^*]), \quad 4D_k\alpha_k^2 = (\tfrac{1}{2}k^2 + 4\pi\rho k^{-2}) - \sqrt{\tfrac{1}{4}k^4 + 4\pi\rho}$$

Thus the ground state energy per volume for $\Omega \to \infty$ (thermod. limit)

$$-(2\pi)^{-3} \int 2D_k \alpha_k^2 dk = -J\rho^{5/4}, \quad J \text{ explicit.}$$

Results for the one-component plasma

The termodynamic limits exist (Lieb-Narnhofer) for both fermionic ($e^{\rm F}(\rho) = \lim_{\Omega\to\infty} E_N^{\rm F}/|\Omega|$) and bosonic ($e^{\rm B}(\rho)$) neutral ($\rho = N/|\Omega|$) jellium.

For large ρ we have

$$e^{\rm B}(\rho) = -J\rho^{5/4} + o(\rho^{5/4}) \quad \text{Lieb-Sol } (\geq), \text{ Sol. } (\leq)$$

and

$$e^{\rm F}(\rho) = e^{\rm HF}(\rho) + o(\rho^{4/3}) \quad \text{Graf-Sol.}$$

$$e^{\rm HF}(\rho) = C_{\rm TF}\rho^{5/3} - C_{\rm D}\rho^{4/3} + o(\rho^{4/3}) \quad \text{Graf-Sol. based on Dirac.}$$

For small ρ

$$e^{\rm B}(\rho) = c_{\rm cl}\rho^{4/3} + o(\rho^{4/3}), \quad e^{\rm F}(\rho) = c_{\rm cl}\rho^{4/3} + o(\rho^{4/3}),$$

where $e^{\rm classical}(\rho) = c_{\rm cl}\rho^{4/3}$. Conjecture: *Optimal classical configuration is a Body Centered Cubic lattice.*