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19. Grand-canonical stability
20. Bosonic instability

19. Grand-canonical stability

grand-canonical setting: particle number can change, but not the (finite) volume of the system.

$$H_{M,N} = \sum_{i=1}^{N} (-\Delta_{x_i}) + \sum_{k=1}^{M} (-\Delta_{y_k}) + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} + \sum_{1 \le k < l \le M}' \frac{1}{|y_k - y_l|} - \sum_{i=1}^{N} \sum_{k=1}^{M} \frac{1}{|x_i - y_k|}$$

on $L^2_a(\Omega^N) \otimes L^2_a(\Omega^M)$, Ω- bounded

Df Grand-canonical ground-state energy

$$E(\Omega) := \inf_{M,N} \inf_{\substack{\Psi \in C_c^\infty(\Omega^{M+N}) \\ \|\Psi\| = 1}} \langle \Psi, H_{M,N} \Psi \rangle$$

Thm (grand-canonical stability)

We have

$$\boxed{E(\Omega) \ge - C |\Omega|}$$

Remark

This result holds under more general assumptions, where the masses and charges of the particles can be different.

Proof

By canonical stability we have

$$\sum_{i=1}^{N}\left(-\tfrac{1}{2}\Delta_{x_i}\right) + \sum_{1\le i<j\le N}\frac{1}{|x_i-x_j|} + \sum_{1\le k<l\le M}{}^{'}\frac{1}{|y_k-y_l|} - \sum_{i=1}^{N}\sum_{k=1}^{M}\frac{1}{|x_i-y_k|} \ge -C(M+N)$$

Notice we "borrowed" only half of the electronic kinetic energy. For the rest of the kinetic energy we use the Lieb-Thirring inequality for the following potential:

$$V(x) = \begin{cases} 0 & x\in\Omega \\ \infty & x\notin\Omega. \end{cases}$$

More precisely, we consider the kinetic LT inequality but for a set of orthonormal functions supported on Ω:

$$\operatorname{Tr}(-\Delta\gamma) \ge \sum_{i=1}^{N}\int_\Omega |\nabla u_n|^2 \ge K_d\int_\Omega \rho^{1+\frac{2}{d}} \ge \frac{K}{|\Omega|^{2/d}}\left(\int\rho\right)^{1+\frac{2}{d}}$$

Exercise: proof the last step

here in the last step we used Jensen's inequality

$$\varphi\left(\int_\Omega f\,d\mu\right) \le \int_\Omega \varphi\circ f\,d\mu \quad \text{for } \varphi \text{ convex}$$

and (Ω, A, μ) - probability space. In particular, to make it a prob. space we need to normalize the measure as $\int_\Omega dx = \Omega \Rightarrow \frac{dx}{|\Omega|}$ for Jensen

$$\int_\Omega \rho^{1+\frac{2}{d}}\, dx = |\Omega| \int_\Omega \rho^{1+\frac{2}{d}} \frac{dx}{|\Omega|} \geq |\Omega| \left(\int \rho \frac{dx}{|\Omega|}\right)^{1+\frac{2}{d}} =$$

$$= \frac{|\Omega|}{|\Omega|^{1+2/3}} \left(\int \rho\right)^{1+2/d} = \frac{1}{|\Omega|^{2/3}} \left(\int_\Omega \rho\, dx\right)^{1+2/d}$$

So we have

$$\mathrm{Tr}(-\Delta\gamma) \geq \frac{K}{|\Omega|^{2/d}} \left(\int_\Omega \rho\right)^{1+2/d} = \frac{K\, N^{1+\frac{2}{d}}}{|\Omega|^{2/d}}$$

This implies

$$\sum_{i=1}^{N} \left(-\tfrac{1}{2}\Delta_{x_i}\right) \geq \frac{K\, N^{5/3}}{|\Omega|^{2/3}}, \quad \sum_{k=1}^{M} \left(-\Delta_{y_k}\right) \geq \frac{K}{|\Omega|^{2/3}} N^{5/3}$$

which leads to

$$H_{M,N} \geq \frac{K}{|\Omega|^{2/3}} \left(M^{5/3} + N^{5/3}\right) - C(M+N)$$

Thus

$$E(\Omega) \geq \inf_{M,N} \left(\frac{K}{|\Omega|^{2/3}} \left(M^{5/3} + N^{5/3}\right) - C(M+N)\right) \geq -C|\Omega|$$

$\blacksquare$

Exercise: proof last step

$$\left(\frac{C}{|\Omega|^{2/3}} M^{5/3} - CM\right)' = \frac{5}{3} \frac{C}{|\Omega|^{2/3}} M^{2/3} - C = 0 \Leftrightarrow M^{2/3} = \tilde{C} |\Omega|^{2/3}$$

$$\Rightarrow M = \tilde{C} |\Omega|$$

$\blacksquare$

20. Bosonic instability

We will now show that the fermionic nature of electrons is crucial for stability of matter. Recall

$$H_{N,M} = \sum_{i=1}^{N} (-\Delta_{x_i}) - \sum_{i=1}^{N}\sum_{k=1}^{M} \frac{Z_k}{|x_i - R_k|} + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} + \sum_{1 \le k < \ell \le M} \frac{Z_k Z_\ell}{|R_k - R_\ell|}$$

and let

$$E_B(M,N) = \inf_{\{R_k\}} \inf_{\|\varphi\|_{L^2(\mathbb{R}^{3N})} = 1} \langle \varphi, H_{M,N} \varphi \rangle$$

Remark:

We use the subscript B as for bosons. This is because it is known that the ground state on the full Hilbert space $L^2(\mathbb{R}^{3N})$ is the same as with restriction to bosonic symmetry $L^2_s(\mathbb{R}^{3N})$.

Thm ($N^{5/3}$ instability)

Let $M = N$ and $Z_k = 1$ $\forall k$. Then

$$\boxed{-CN^{5/3} \le E_B(M,N) \le -C^{-1} N^{5/3}}$$

for a constant $C > 0$ independent of N.

Remark:

lower bound: Dyson and Lenard 1967, upper: Lieb 1979.

Proof:

Lower bound

By Baxter's electrostatic inequality

$$-\sum_{i=1}^{N}\sum_{k=1}^{M}\frac{1}{|x_i-R_k|}+\sum_{1\le i<j\le N}\frac{1}{|x_i-x_j|}+\sum_{1\le l<k\le M}\frac{1}{|R_k-R_l|}\ge -\sum_{i=1}^{N}\frac{3}{\mathcal{D}(x_i)}$$

where $\mathcal{D}(x)=\min_{1\le k\le M}|x-R_k|$. Thus

$$H_{M,N}\ge\sum_{i=1}^{N}\left(-\Delta_{x_i}-\frac{3}{\mathcal{D}(x_i)}\right)$$

The desired inequality follows from the estimate

$$(*)\qquad -\Delta-\frac{3}{\mathcal{D}(x)}\ge -CN^{2/3}\quad\text{on } L^2(\mathbb{R}^3)$$

We shall now prove $(*)$. Recall the CLR bound:

$$\mathcal{N}(-\Delta+V)\le C\int_{\mathbb{R}^d}|V_-|^{\frac{d}{2}}$$

where $\mathcal{N}(-\Delta+V)$ is the number of negative eigenvalues of $-\Delta+V(x)$. Thus, if $\mu>0$ is such that

$$\int_{\mathbb{R}^3}\left[\frac{3}{\mathcal{D}(x)}-\mu\right]_+^{3/2}dx\le\varepsilon_0<1$$

then there are no negative eigenvalues and thus

$$-\Delta-\frac{3}{\mathcal{D}(x)}+\mu\ge 0.$$

By the definition of $\mathcal{D}(x)$ we have

$$\int_{\mathbb{R}^3}\left[\frac{3}{\mathcal{D}(x)}-\mu\right]_+^{3/2}dx\le\sum_{k=1}^{N}\int_{\mathbb{R}^3}\left[\frac{3}{|x-R_k|}-\mu\right]_+^{3/2}dx=$$

$$= N \int_{\mathbb{R}^3} \left(\frac{3}{|x|} - \mu\right)_+^{3/2} dx = C N \mu^{-3/2}$$

Exercise: check last equality

$$\int_{\mathbb{R}^3} \left(\frac{3}{|x|} - \mu\right)_+^{3/2} = \left\| \begin{array}{c} \frac{3}{|x|} - \mu > 0 \\ |x| < \frac{\mu}{3} \end{array} \right\| = 4\pi \int_0^{\frac{\mu}{3}} r^2 \left(\frac{3}{r} - \mu\right)^{3/2} dr$$

$$= 4\pi \int_0^{\mu/3} r^2 \mu^{3/2} \left(\frac{3}{r\mu} - 1\right)^{3/2} dr = \left\| \begin{array}{c} r\mu = t \\ dr = \frac{dt}{\mu} \end{array} \right\| =$$

$$= 4\pi \int_0^{\frac{t}{3}} \frac{t^2}{\mu^2} \mu^{3/2} \left(\frac{3}{t} - 1\right)^{3/2} \frac{dt}{\mu} = C \mu^{-3/2}.$$

$\square$

Thus the condition $CN\mu^{-3/2} \leq \varepsilon_0$ is satisfied when $\mu \sim N^{2/3}$ which proves $(*)$.

Upper bound

We take a product trial function

$$\psi(x_1, \dots, x_N) = u(x_1) \dots u(x_N)$$

when $u \in L^2(\mathbb{R}^3)$ is normalized. Then

$$E_B(M,N) \leq \langle u^{\otimes N}, H_{M,N} u^{\otimes N} \rangle \overset{(*)}{=} N \int_{\mathbb{R}^3} |\nabla u|^2 +$$

$$+ \frac{N(N-1)}{2} \iint_{\mathbb{R}^3\,\mathbb{R}^3} \frac{|u(x)|^2 |u(y)|^2}{|x-y|} dx dy - N \sum_{k=1}^{N} \int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x - R_k|} + \sum_{l<k} \frac{1}{|R_l - R_k|}$$

Exercise: Show $(*)$.

Solution:

First term:

$$\langle u^{\otimes N}, (\sum_i -\Delta_i) u^{\otimes N}\rangle = N\langle u(x_1)\dots u(x_N), (-\Delta_{x_1} u(x_1))\, u(x_2)\dots u(x_N)\rangle$$

$$= N\int \bar{u}(x_1)(-\Delta) u(x_1)\ |u(x_2)|^2 \cdots |u(x_N)|^2\, dx_1\, dx_2 \dots dx_N =$$

$$= N\int \bar{u}(x_1) -\Delta u(x_1) = N\int |\nabla u|^2$$

Second term:

$$\langle u^{\otimes N}, \sum_{i<j} \frac{1}{|x_i - x_j|} u^{\otimes N}\rangle = \sum_{i<j} \langle u^{\otimes N}, \frac{1}{|x_i - x_j|} u^{\otimes N}\rangle =$$

$$= \frac{N(N-1)}{2} \int dx_1 \int dx_2\ \frac{|u(x_1)|^2\, |u(x_2)|^2}{|x_1 - x_2|} \iiint |u(x_3)|^2 \cdots |u(x_N)|^2\, dx_3 \dots dx_N$$

$$= \frac{N(N-1)}{2} \iint \frac{|u(x)|^2\, |u(y)|^2}{|x-y|}\, dx\, dy$$

and so on.

This upper bound holds for any choice of nuclear positions $\{R_k\}_{k=1}^N$. Hence, we can average over $\{R_k\}$.

<u>First try</u>

Integrate the inequality (*) against

$$|u(R_1)|^2\, |u(R_2)|^2 \cdots |u(R_N)|^2\, dR_1 \dots dR_N, \quad R_k \in \mathbb{R}^3.$$

We obtain

$$E_B(M,N) \le N\int |\nabla u|^2 + \frac{N(N-1)}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|u(x)|^2\, |u(y)|^2}{|x-y|}\, dx\, dy$$

$$- N^2 \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|u(x)|^2\, |u(R)|^2}{|x-R|}\, dx\, dR + \frac{N(N-1)}{2} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|u(R_1)|^2\, |u(R_2)|^2}{|R_1 - R_2|}\, dR_1\, dR_2.$$

$$= N \left(\int_{\mathbb{R}^3} |Du|^2 - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|u(x)|^2 \, |u(y)|^2}{|x-y|} \, dx\, dy \right)$$

This leads to the upper bound $E_B(M,N) \leq -CN$.

Second try

We divide the support of u into N disjoint sets $\{\Omega_k\}_{k=1}^{N}$ such that $\int_{\Omega_k} |u|^2 = \frac{1}{N}$ $\forall k = 1, \dots, N$

We then integrate $(*)$ against

$$(N|u(R_1)|^2) \cdots (N|u(R_N)|^2) \, dR_1 \cdots dR_N \quad , \; R_k \in \Omega_k$$

to obtain

$$E_B(M,N) \leq N \int_{\mathbb{R}^3} |\nabla u|^2 + \frac{N(N-1)}{2} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|u(x)|^2 \, |u(y)|^2}{|x-y|} \, dx\, dy$$

$$- N^2 \sum_{k=1}^{N} \int_{\mathbb{R}^3} dx \int_{\Omega_k} \frac{|u(x)|^2 \, |u(R_k)|^2}{|x-R_k|} \, dR_k + \frac{N^2}{2} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|u(R_1)|^2 \, |u(R_2)|^2}{|R_1-R_2|} \, dR_1 \, dR_2$$

$\sum_k \sum_j$ all k and j

$$- \frac{N^2}{2} \sum_{k=1}^{N} \int_{\Omega_k}\int_{\Omega_k} \frac{|u(R_1)|^2 \, |u(R_2)|^2}{|R_1-R_2|} \, dR_1 \, dR_2$$

minus diagonal ones

$$\leq N \int_{\mathbb{R}^3} |\nabla u|^2 - N^2 \sum_{k=1}^{N} \int_{\Omega_k}\int_{\Omega_k} \frac{|u(x)|^2 \, |u(y)|^2}{|x-y|} \, dx\, dy$$

We choose the support of u to be a cube $[0,L]^3$. Then any set Ω_k has diameter $\sim L/N^{1/3}$. This gives

$$N^2 \int_{\Omega_k} \int_{\Omega_k} \frac{|u(x)|^2 |u(y)|^2}{|x-y|} dx\, dy \geq N^2 \int_{\Omega_k} \int_{\Omega_k} \frac{|u(x)|^2 |u(y)|^2}{(CL/N^{1/3})} dx\, dy = \frac{N^{1/3}}{CL}$$

Moreover, if u behaves as a constant inside its support, then $\|\nabla u\|_{L^2}^2 \sim L^{-2}$ (the spectral gap of the Laplacian). Thus

$$E_B(M,N) \leq N \int_{\mathbb{R}^3} |\nabla u|^2 - N^2 \sum_{k=1}^{N} \int_{\Omega_k} \int_{\Omega_k} \frac{|u(x)|^2 |u(y)|^2}{|x-y|} dx\, dy$$

$$\leq C^{-1} \frac{N}{L^2} - C \frac{N^{4/3}}{L} \underset{\substack{\uparrow \\ \text{choose } L \sim N^{-1/3}}}{\leq} -C^{-1} N^{5/3}$$

$\boxtimes$

Note that the theorem above we ignored the kinetic energy of the nuclei. Since this is a positive term, in principle this could help and give stability. It turns out that in that case we don't have stability either. Indeed, for

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i}) + \sum_{k=1}^{N} (-\Delta_{y_k}) - \sum_{i=1}^{N} \sum_{k=1}^{N} \frac{1}{|x_i - y_k|} + \sum_{i<j} \frac{1}{|x_i - x_j|} + \sum_{l<k} \frac{1}{|y_l - y_k|}$$

on $L^2(\mathbb{R}^{6N})$ we define

$$E_B(N) = \inf_{\|\varphi\|=1} \langle \varphi, H_N \varphi \rangle .$$

Then the following theorem holds:

Thm ($N^{7/5}$ instability)

We have

$$\lim_{N\to\infty} \frac{E_B(N)}{N^{7/5}} = \inf_{\|u\|_{L^2(\mathbb{R}^3)}=1} \int_{\mathbb{R}^3} \left(2|\nabla u|^2 - I_0 |u(x)|^{5/2} \right) dx$$

where

$$I_0 = \left(\frac{2}{\pi}\right)^{3/4} \int_0^\infty \frac{1}{1+t^4+t^2\sqrt{t^4+2}}\, dt = \frac{4^{5/4}\, \Gamma\left(\frac{3}{4}\right)}{5\pi^{1/4}\, \Gamma\left(\frac{5}{4}\right)}$$

$\boxed{\diagup}$

Remarks

- clearly $\frac{5}{3} > \frac{7}{5}$
- upper bound $-CN^{7/5}$ – Dyson (1966)
- lower bound $-\tilde{C}N^{7/5}$ – Conlon, Lieb, Yau (1988)
- exact constant by Lieb-Solovej (2004, lower) and Solovej (2006, upper) using Bogoliubov theory.