Asymptotics of the Energy of the Bose Gas

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Interacting Bose Gas

- N particles in a box of length L: $\Lambda_L = \left[-\frac{L}{2}, \frac{L}{2}\right]^3$
- One-particle Hilbert space $\mathcal{H} = L^2\left(\Lambda_L\right)$
- N particles: $\mathcal{H}^{\otimes_s N} = P_+\mathcal{H}^{\otimes N}$, P_+ projection onto symmetric states
- interaction V, Hamiltonian

$$H_N^L = -\mu \sum_{i=1}^{N} \Delta_i^L + \sum_{1 \leqslant i < j \leqslant N} V(x_i - x_j), \quad \mu = \frac{\hbar^2}{2m}$$

- ground state energy

$$E_0(N, L) := \inf_{\psi \in \mathcal{H}^{\otimes_s N}} \left\langle \psi, H_N^L \psi \right\rangle$$

- density $\rho = \frac{N}{L^3}$ fixed
- thermodynamic limit

$$e_0(\rho) := \lim_{N \to \infty, L^3 = \rho N} \frac{E_0(N, L)}{N}$$

Asymptotic Expressions

With appropriate conditions on V

- high density

$$\lim_{\rho \to \infty} \frac{e_0(\rho)}{\rho} = \frac{1}{2} \int_{\mathbb{R}^3} V$$

- low density: Lee-Huang-Yang formula

$$e_0(\rho) = 4\pi\mu\rho a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho})\right) \text{ for } \rho \to 0$$

- scattering length a describes range of the potential

High Density

Theorem (Lieb, 1963)

Let V satisfy $\widehat{V} \geqslant 0$ and $V, \widehat{V} \in L^1$. Then

$$\frac{1}{2}\rho \int V > e_0(\rho) > \frac{1}{2}\rho \int V - \frac{V(0)}{2}$$

Proof: Upper bound:

$$\frac{E_0(N,L)}{N} = \frac{1}{N} \inf_{\psi \in \mathcal{H}^{\otimes_s N}} \langle \psi, H_N^L \psi \rangle \leqslant \frac{1}{N} \langle \psi_0, H_N^L \psi_0 \rangle \text{ for any } \psi_0$$

Choose $\psi_0 = L^{-3N/2}$, then

$$\langle \psi_0, H_N^L \psi_0 \rangle = \frac{1}{L^{3N}} \int_{\Lambda_L^N} dx_1 \dots dx_N \sum_{1 \leqslant i < j \leqslant N} V(x_i - x_j) = \frac{N(N-1)}{2L^6} \int_{\Lambda_L \times \Lambda_L} V(x_1 - x_2)$$

$$\Rightarrow e_0(\rho) \leqslant \lim_{N \to \infty, L^3 = N\rho} \frac{1}{N} \langle \psi_0, H_N^L \psi_0 \rangle = \frac{1}{2}\rho \int_{\mathbb{R}^3} V$$

Lower bound:

$$\frac{E_0(N,L)}{N} \geqslant \frac{1}{N} \min_{x_1,\ldots,x_N\in\Lambda_L} \sum_{1\leqslant i<j\leqslant N} V(x_i - x_j)$$

Minimum attained at $x_i = a_i$. Define $\varphi(x) = \sum_{i=1}^{N} \delta(x - a_i)$. Then

$$\begin{aligned}\frac{1}{N}\sum_{1\leqslant i<j\leqslant N} V(a_i - a_j) &= \frac{1}{2N}\int_{\Lambda_L}\int_{\Lambda_L} \bar{\varphi}(x)V(x-y)\varphi(y)dxdy - \frac{1}{2}V(0) \\ &= \frac{1}{2NL^3}\sum_k |\widehat{\varphi}(k)|^2\,\widehat{V}(k) - \frac{1}{2}V(0) \\ &\geqslant \frac{1}{2}\rho\int_{\Lambda_L} V - \frac{1}{2}V(0)\end{aligned}$$

using $\widehat{\varphi}(0) = N$

Low Density

Book: The Mathematics of the Bose Gas and its Condensation (Lieb, Seiringer, Solovej, Yngvason)

Definition (Scattering length)

Let $V \geqslant 0$ radial, $V(r) = 0$ for $r > R_0$. Then define the scattering energy

$$8\pi\mu a = \inf\left\{\int_{\mathbb{R}^3} 2\mu\left|\nabla\psi\right|^2 + V\left|\psi\right|^2, \lim_{|x|\to\infty}\psi(x) = 1\right\}.$$

where a is the scattering length. There is a unique minimizer $0 \leqslant \psi_0 \leqslant 1$ with

$$\psi_0(x) = 1 - \frac{a}{|x|} \text{ for } |x| \geqslant R_0.$$

$$-2\mu\Delta\psi_0 + V\psi_0 = 0$$

Example: Hard sphere $V(x) = \infty$ for $|x| \leqslant R$, $V(x) = 0$ for $|x| \geqslant 0$: then $a = R$

- describes two particle energy
- a: effective range
- low density: high interparticle distance, two-particle contributions important

Theorem (Lieb-Yngvason, 1998)

Let $V \geqslant 0$ *radial,* $V(r) = 0$ *for* $r > R_0$*. Define* $Y = 4\pi\rho a^3/3$*. Then*

$$e_0(\rho) \geqslant 4\pi\rho\mu a(1 - CY^{1/17}).$$

- $\rho^{-1/3}$: average interparticle distance
- Y small if $\rho^{-1/3} \gg a$

Proof: main steps

- split box of length L into boxes of length l, consider $L \to \infty$ while l fixed
- reduce to nearest-neighbour interaction
- replace the potential by a smeared-out version

Proof of the Theorem:

- N particles in a box of length L
- split box into smaller cubes (cells) of fixed length l
- choose $N = kM$: $k \in \mathbb{N}$, $M^{1/3} \in \mathbb{N}$
- define l via $\rho l^3 = k \Leftrightarrow L^3 = Ml^3$
- M boxes with k particles per box on average
- take $M \to \infty$, l fixed
- want lower bound for the energy: Neumann boundary conditions on the boxes

$$H_N^L = -\mu \sum_{i=1}^{N} \Delta_i^L + \sum_{1 \leqslant i < j \leqslant N} V(x_i - x_j), \quad \mu = \frac{\hbar^2}{2m}$$

Idea:

- distribute particles in the cells: Mc_n cells with n particles
- drop interactions between different cells ($V \geqslant 0$)
- impose Neumann boundary conditions on cells
- minimize over distributions

$$E_0(N, L) \geqslant M \min_{\{c_n\}} \sum_{n=0}^{N} c_n E_0(n, l) \quad \text{with} \ \sum_{n=0}^{N} c_n = 1, \quad \sum_{n=0}^{N} nc_n = k$$

- superadditivity: $E_0(n+n',l) \geqslant E_0(n,l) + E_0(n',l)$ (ignore interactions)
- assume $E_0(n,l) \geqslant K(l)n(n-1)$ for $0 \leqslant n \leqslant 4k$
- assume $K(l) \geqslant 4\pi\mu a l^{-3}(1 - C'Y^{1/17})$ for ρ small enough

$$\begin{aligned}
\sum_{n=0}^{N} c_n E_0(n,l) &= \sum_{n=0}^{4k} c_n E_0(n,l) + \sum_{n=4k+1}^{N} c_n E_0(n,l) \\
&\geqslant K(l) \sum_{n=0}^{4k} c_n n(n-1) + \sum_{n=4k+1}^{N} c_n \left\lfloor \frac{n}{4k} \right\rfloor E_0(4k,l) \\
&\geqslant K(l) \sum_{n=1}^{4k} c_n n(n-1) + \sum_{n=4k+1}^{N} c_n \frac{n}{8k} E_0(4k,l) \\
&\geqslant K(l) \sum_{n=1}^{4k} c_n n \sum_{m=1}^{4k} c_m(m-1) + \frac{K(l)(4k-1)}{2} \sum_{n=4k+1}^{N} c_n n \\
&\geqslant K(l)\left(t(t-1) + \frac{4k-1}{2}(k-t)\right) \qquad \text{where } t = \sum_{n=0}^{4k} c_n n \leqslant k \\
&\geqslant K(l)k(k-1)
\end{aligned}$$

$$\sum_{n=0}^{N} c_n E_0(n,l) \geqslant K(l)k(k-1), \quad K(l) \geqslant 4\pi\mu a l^{-3}(1 - C' Y^{1/17})$$

$$\begin{aligned}\Rightarrow E_0(N,L) &\geqslant M \min_{\{c_n\}} \sum_{n=0}^{N} c_n E_0(n,l) \\ &\geqslant NK(l)(\rho l^3 - 1) \\ &\geqslant 4\pi\mu a\rho(1 - C' Y^{1/17})(1 - \frac{1}{\rho l^3}) \\ &\geqslant 4\pi\mu a\rho(1 - C Y^{1/17}) \text{ if } \rho l^3 > C'' Y^{-1/17}\end{aligned}$$

The claim follows by choosing l large in comparison to the interparticle distance.
Left to show: bound for cells

Lemma (first version by Dyson, 1957)

Let $U(r) \geqslant 0$ be such that $\int_{\mathbb{R}} r^2 U(r) \leqslant 1$, $U(r) = 0$ for $r \leqslant R_0$ and let $B \subset \mathbb{R}^3$ be star-shaped with respect to 0. Then for all differentiable ψ

$$\int_B 2\mu \left|\nabla\psi\right|^2 + V\left|\psi\right|^2 \geqslant 2\mu a \int_B U\left|\psi\right|^2$$

Proof: Consider radial integral with fixed angles and write $\psi(x) = \frac{u(r)}{r}$, $u(0) = 0$ along this line.
Take $U(r) = \frac{1}{R^2}\delta(r - R)$ for $R \geqslant R_0$. Using $\left|\nabla\psi\right|^2 \geqslant \left|\partial_r\psi\right|^2$ the claim follows if

$$\int_0^{R_1} 2\mu \left|u' - \frac{u}{r}\right|^2 + V\left|u\right|^2 \geqslant 2\mu a \left|u(R)\right|^2 / R^2$$

where $R_1 \geqslant R$ is the length of the radial line ($R_1 < R$ is trivial).

$$\int_0^{R_1} 2\mu \left|u' - \frac{u}{r}\right|^2 + V\left|u\right|^2 \geqslant \int_0^{R} 2\mu \left|u' - \frac{u}{r}\right|^2 + V\left|u\right|^2$$

Minimize RHS with $u(0) = 0$, $u(R) = R - a$ (possible since everything is homogeneous) $\rightarrow$ related to scattering equation

Minimizer $u_0(r)$ of $\int_0^R 2\mu \left|u' - \frac{u}{r}\right|^2 + V|u|^2$ with $u(0) = 0$, $u(R) = R - a$ satisfies Euler-Lagrange equation

$$-2\mu u_0''(r) + V(r)u_0(r) = 0.$$

Compare to scattering equation:

$$-2\mu\Delta\psi_0 + V\psi_0 = 0, \quad \psi_0(x) = \psi_0(|x|) = 1 - \frac{a}{|x|} \text{ for } |x| \geqslant R_0.$$

$u_0(r) = r\psi_0(r)$ solves the EL equation and satisfies boundary conditions.
EL equations plus integration by parts using $u_0(r) = r - a$ for $r > R_0$:

$$\begin{aligned}
\int_0^R 2\mu \left|u' - \frac{u}{r}\right|^2 + V|u|^2 &\geqslant \int_0^R 2\mu \left|u_0' - \frac{u_0}{r}\right|^2 + V|u_0|^2 \\
&= 2\mu \int_0^R (u_0')^2 - \frac{2u_0u_0'}{r} + \frac{u_0^2}{r^2} + u_0''u_0 \\
&= 2\mu \left(u_0'u_0|_0^R - \frac{u_0^2}{r}|_0^R \right) \\
&= 2\mu \left(R - a - \frac{(R-a)^2}{R} \right) \\
&= 2\mu a \frac{R-a}{R} \geqslant 2\mu a \frac{(R-a)^2}{R^2} = 2\mu a \frac{u(R)^2}{R^2}
\end{aligned}$$

General U: decompose

$$U(r) = \int_{R_0}^{\infty} dR \frac{1}{R^2} \delta(r - R) U(R) R^2$$

Know for a radial line with $R_1 \geqslant R$

$$\int_0^{R_1} dr 2\mu \left| u' - \frac{u}{r} \right|^2 + V |u|^2 \geqslant 2\mu a \int_0^{R_1} dr \frac{1}{R^2} \delta(r - R) |u|^2$$

Integrate

$$\begin{aligned}\int_0^{R_1} dr 2\mu \left| u' - \frac{u}{r} \right|^2 + V |u|^2 &\geqslant \int_{R_0}^{\infty} dR U(R) R^2 \int_0^{R_1} dr 2\mu \left| u' - \frac{u}{r} \right|^2 + V |u|^2 \\ &\geqslant 2\mu a \int_{R_0}^{\infty} dR U(R) R^2 \int_0^{R_1} dr \frac{1}{R^2} \delta(r - R) |u(r)|^2 \\ &= 2\mu a \int_0^{R_1} dr U(r) |u(r)|^2\end{aligned}$$

Need to show the lower bound for a cell of fixed size:

- $E_0(n,l) \geqslant K(l)n(n-1)$ for $0 \leqslant n \leqslant 4k$
- $K(l) \geqslant 4\pi\mu a l^{-3}(1 - C' Y^{1/17})$ for ρ small enough

For particles $X := x_1, \ldots, x_n$ define nearest-neighbour potential

$$W_V(X) = \frac{1}{2}\sum_{i=1}^{n} V(x_i - x_{j(i)}), \quad j(i) = \text{ nearest neighbour of } i$$

$$H_n^l(X) = \underbrace{-\mu\sum_{i=1}^{n}\Delta_i^l}_{T} + \sum_{1\leqslant i<j\leqslant n} V(x_i - x_j) \geqslant T + W_V(X) = \widetilde{H}_n^l(X)$$

Define U_R for $R \gg R_0$ via $U_R(r) = \frac{3}{R^3 - R_0^3}\mathbb{1}(R_0 < r < R)$.
Recall Dyson-Lemma:

$$\int_B 2\mu\left|\nabla\psi\right|^2 + V\left|\psi\right|^2 \geqslant 2\mu a\int_B U\left|\psi\right|^2$$

for $U(r) \geqslant 0$ such that $\int_{\mathbb{R}} r^2 U(r) \leqslant 1$, $U(r) = 0$ for $r \leqslant R_0$. Want to show:

$$\widetilde{H}_n^l(X) \geqslant \mu a W_{U_R}$$

$$\left\langle \psi, \widetilde{H}_n^l \psi \right\rangle = \mu \sum_i \int_{\Lambda_L^n} dX \, |\nabla_i \psi(X)|^2 + \frac{1}{2} \sum_i \int_{\Lambda_L^n} dX \, V(x_i - x_{j(i)}) \, |\psi(X)|^2$$

- consider x_1 integral
- view $x_2, \ldots, x_n$ as fixed
- $\psi, x_{j(i)}$ functions of x_1
- split Λ_l into Voronoi cells: $B_k = \{x \in \Lambda_l | \min_{2 \leqslant j \leqslant n} |x - x_j| = |x - x_k|\}$, $k \geqslant 2$
- $\widetilde{X} = x_2 \ldots x_n$

Apply Dyson-Lemma in the cells

$$\mu \int_{\Lambda_L^{n-1}} d\widetilde{X} \int_{B_k} dx_1 \left(|\nabla_1 \psi(X)|^2 + \frac{1}{2} V(x_1 - x_k) \, |\psi(X)|^2 \right) \geqslant \int_{\Lambda_L^{n-1}} d\widetilde{X} \int_{B_k} dx_1 \, \mu a U_R(x_1 - x_k) \, |\psi(X)|^2$$

Sum over Voronoi cells:

$$\mu \int_{\Lambda_L^n} dX \, |\nabla_1 \psi(X)|^2 + \frac{1}{2} \int_{\Lambda_L^n} dX \, V(x_1 - x_{j(1)}) \, |\psi(X)|^2 \geqslant \int_{\Lambda_L^n} dX \, \mu a U_R(x_1 - x_{j(1)}) \, |\psi(X)|^2$$

Summing over i gives the result.

$$H_n^l \geqslant \epsilon T + (1-\epsilon) H_n^l \geqslant \epsilon T + (1-\epsilon)\mu a W_{U_R} =: H_{\epsilon,R}$$

- view ϵT as unperturbed operator, $(1-\epsilon)\mu a W_{U_R}$ as perturbation
- ground state of ϵT: $\psi_0 = \frac{1}{l^{3n/2}}$, $\langle \psi_0, T\psi_0 \rangle = 0$
- $E_0^{\epsilon,R} < E_1^{\epsilon,R}$ lowest eigenvalues of $H_{\epsilon,R}$
- Temple's inequality: $\left\langle \psi_0, (H_{\epsilon,R} - E_0^{\epsilon,R})(H_{\epsilon,R} - E_1^{\epsilon,R})\psi_0 \right\rangle \geqslant 0$ implies

$$\begin{aligned} E_0^{\epsilon,R} &\geqslant \langle \psi_0, H_{\epsilon,R}\psi_0 \rangle - \frac{\left\langle \psi_0, H_{\epsilon,R}^2 \psi_0 \right\rangle - \langle \psi_0, H_{\epsilon,R}\psi_0 \rangle^2}{E_1^{\epsilon,R} - \langle \psi_0, H_{\epsilon,R}\psi_0 \rangle} \\ &\geqslant \langle \psi_0, H_{\epsilon,R}\psi_0 \rangle - \frac{\left\langle \psi_0, H_{\epsilon,R}^2 \psi_0 \right\rangle}{E_1^{\epsilon T} - \langle \psi_0, H_{\epsilon,R}\psi_0 \rangle} \\ &\geqslant \langle \psi_0, (1-\epsilon)\mu a W_{U_R}\psi_0 \rangle - \frac{\langle \psi_0, ((1-\epsilon)\mu a W_{U_R})^2 \psi_0 \rangle}{E_1^{\epsilon T} - \langle \psi_0, (1-\epsilon)\mu a W_{U_R}\psi_0 \rangle} \end{aligned}$$

$E_1^{\epsilon T}$: second eigenvalue of ϵT. Necessary: $E_1^{\epsilon T} = \epsilon\mu\pi^2/l^2 \geqslant \langle \psi_0, H_{\epsilon,R}\psi_0 \rangle$.

$$W_{U_R}(X) = \frac{1}{2}\sum_{i=1}^{n} U_R(x_i - x_{j(i)}), \quad U_R(r) = \frac{3}{R^3 - R_0^3}\mathbb{1}(R_0 < r < R)$$

Want bounds on $\langle \psi_0, W_{U_R}\psi_0\rangle$:

$$\langle \psi_0, W_{U_R}\psi_0\rangle = \frac{1}{l^{3n}}\int_{\Lambda_l^n} dx_1 \dots dx_n \sum_{i=1}^{n} \frac{3}{2(R^3 - R_0^3)}\mathbb{1}(R_0 < \left|x_i - x_{j(i)}\right| < R)$$

$$= \frac{n}{l^{3n}}\int_{\Lambda_l^n} dx_1 \dots dx_n \frac{3}{2(R^3 - R_0^3)}\mathbb{1}(R_0 < \left|x_1 - x_{j(1)}\right| < R)$$

- lower bound: integrate only over $x_1 \in [l - R, l + R]^3$
- probability that $R_0 < |x_j - x_1| < R$ is $Q = \frac{4\pi(R^3 - R_0^3)}{3l^3}$

$$\Rightarrow \langle \psi_0, W_{U_R}\psi_0\rangle \geqslant \frac{3n}{R^3 - R_0^3}\frac{(l - 2R)^3}{l^3}(1 - (1 - Q)^{n-1})$$

$$\geqslant \frac{3n}{R^3 - R_0^3}\left(1 - \frac{2R}{l}\right)^3\left(1 - \frac{1}{1 + Q(n-1)}\right)$$

$$= \frac{4\pi n(n-1)}{l^3}\left(1 - \frac{2R}{l}\right)^3\frac{1}{1 + Q(n-1)}$$

similarly

$$\begin{aligned}\langle \psi_0, W_{U_R}\psi_0\rangle &\leqslant \frac{3n}{R^3 - R_0^3}(1-(1-Q)^{n-1}) \\ &\leqslant \frac{3n}{R^3 - R_0^3}Q(n-1) \\ &= \frac{4\pi n(n-1)}{l^3}\end{aligned}$$

and $U_R^2 = \frac{4\pi}{Ql^3}U_R$ implies

$$\left\langle \psi_0, W_{U_R}^2\psi_0\right\rangle \leqslant \frac{4\pi n}{Ql^3}\left\langle \psi_0, W_{U_R}\psi_0\right\rangle$$

Put together:

$$E_0(n,l) \geqslant E_0^{\epsilon,R} \geqslant (1-\epsilon)\mu a \left\langle \psi_0, W_{U_R}\psi_0\right\rangle \left(1 - \frac{4\pi a n}{Ql^3}\frac{1}{\epsilon\pi^2 - al^2\left\langle \psi_0, W_{U_R}\psi_0\right\rangle}\right)$$

$\rightarrow$ correct leading order
Corrections are $O(Y^{1/17})$ if $\epsilon = R/l = Y^{1/17}$, $Q = O(Y^{1/17})$, $\rho R^3 = Y^{2/17}$.
Length scales: $a \ll R \ll \rho^{-1/3} \ll l \ll (\rho a)^{-1/2}$

Theorem (Dyson, 1957)

For a hard-sphere potential with range a we have for small $Y = 4\pi\rho a^3/3$

$$e_0(\rho) \leqslant 4\pi\mu\rho a \frac{1+2Y^{1/3}}{(1-Y^{1/3})^2}$$

Idea of the proof:

- trial state for upper bound of $E_0(N, L)$
- can drop symmetry condition for ground state energy
- $\psi(x_1, \dots x_N) = F_1(x_1)F_2(x_1, x_2)\dots F_N(x_1, \dots x_N)$
- idea: insert particles one after the other
- when adding j only consider particles $1, \dots, j-1$
- $F_1 = 1$, $i > 1 : F_i(x_1, \dots, x_i) = f(t_i)$ with $t_i = \min(|x_i - x_j|, j = 1, \dots, i-1)$
- define nearest-neighbour distance b via $\frac{4}{3}\pi\frac{b^3}{L^3}(N-1) = 1$
- choose

$$f(r) = \begin{cases} 0 & \text{if } r \leqslant a \\ \frac{b}{b-a}\left(1 - \frac{a}{x}\right) & \text{if } a \leqslant r \leqslant b \\ 1 & \text{if } b \leqslant r \end{cases}$$

- related to scattering solution
- calculation yields the desired bound