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The Lee-Huang-Yang formula for the ground state energy of Bose gases

Søren Fournais

QMATH and University of Copenhagen

**Based on joint work with Jan Philip Solovej,
and Théotime Girardot, Lukas Junge, Leo Morin and Marco Olivieri**

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The dilute Bose gas

Consider N interacting, non-relativistic bosons in a box $\Lambda := [-L/2, L/2]^3$.
Let $N \in \mathbb{N}$, $\rho := N/|\Lambda| = N/L^3$.
The Hamiltonian of the system is, on the symmetric (bosonic) space $\otimes_s^N L^2(\Lambda)$,

$$H_N := \sum_{i=1}^{N} -\Delta_i + \sum_{i<j} v(x_i - x_j),$$

and $0 \leq v$ is radially symmetric with compact support.

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The energy density in the thermodynamic limit is

$$e(\rho) = \lim_{L\to\infty, N/|\Lambda|=\rho} E_0(N,\Lambda)/L^3.$$

The scattering length

Scattering equation

$$(-\Delta + \frac{1}{2}v(x))(1-\omega(x)) = 0, \qquad \text{with } \omega \to 0, \text{ as } |x| \to \infty.$$

Scattering length

$$a := \lim_{|x|\to\infty} |x|\omega(x) = \frac{1}{8\pi}\int v(1-\omega) < \frac{1}{8\pi}\int v = \frac{1}{8\pi}\widehat{v}(0).$$

With $g = v(1-\omega)$ the scattering equation can be reformulated as

$$-\Delta\omega = \frac{1}{2}g, \qquad \text{i.e.} \qquad \widehat{\omega}(k) = \frac{\widehat{g}(k)}{2k^2}.$$

The two-term formula

We study $e(\rho)$ in the dilute limit $\rho a^3 \to 0$. The following formula is expected to be true

$$e(\rho) = 4\pi\rho^2 a(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}) + \rho^2 a\, o((\rho a^3)^{1/2}).$$

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- Lenz (1929), Bogoliubov (1947), Lee-Huang-Yang (1957).
- Rigorous proof of leading term Dyson (1957, upper), Lieb-Yngvason (1998).
- Upper bounds giving second order term: Erdős-Schlein-Yau (2008), Yau-Yin (2009).
- Study of the limit for v becoming 'soft' as $\rho \to 0$: Lieb-Solovej, Giuliani-Seiringer (2008), Brietzke-Solovej (2018).
- Bogoliubov theory for confined Bose gases (Gross-Pitaevskii limit) Boccato, Brennecke, Cenatiempo, Schlein, Basti, Olgiati, Seiringer, Morris, Nam, Hainzl, Triay, Deuchert,....

The Lee-Huang-Yang formula

Theorem (SF, Solovej 2019&21)

Given a potential $v \neq 0$, non-negative, radial, with compact support there exist $C, \eta > 0$ (depending on v) such that for all ρ sufficiently small,

$$e(\rho) \geq 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{\frac{1}{2}}\right) - C\rho^2 a(\rho a^3)^{\frac{1}{2}+\eta}.$$

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Combined with the upper bound from Yau-Yin this proves the Lee-Huang-Yang formula for the ground state energy.
Neumann approach by Boccato-Seiringer and Hainzl-Nam-Triay.

The Bogoliubov Approach

In second quantization, i.e. with $a_k, a_k^\dagger$ standard creation/annihilation operators, $[a_k, a_p^\dagger] = \delta_{k,p}$, we have

$$H = \sum_k k^2 a_k^\dagger a_k + \frac{1}{2|\Lambda|} \sum_{r+s=p+q} \widehat{v}(p-s) a_r^\dagger a_s^\dagger a_p a_q = \mathcal{K}_0 + \cdots + \mathcal{K}_4 \approx \mathcal{K}_0 + \mathcal{K}_1 + \mathcal{K}_2.$$

Replace a_0 and $a_0^\dagger$ by $\sqrt{N}$. This is based on the assumption of (complete) BEC. Then,

$$\mathcal{K}_0 = \frac{1}{2} N\rho\widehat{v}(0), \quad \mathcal{K}_1 = 0, \quad \mathcal{K}_2 = \sum_{k\neq 0} (k^2 + \rho\widehat{v}(k)) a_k^\dagger a_k + \rho \frac{\widehat{v}(k)}{2} (a_k^\dagger a_{-k}^\dagger + a_k a_{-k}).$$

The quadratic operator $\mathcal{K}_2$ can be diagonalized explicitly. This gives an energy formula of the correct structure but with $\frac{1}{2}\widehat{v}(0)$ instead of the smaller $4\pi a$.

Strategy of proof of rigorous lower bound

- Localize to boxes of size $\ell \gg (\rho a)^{-\frac{1}{2}}$. Localization non-standard since need to preserve 'Neumann gap'. To get a priori information localize to smaller boxes of size $\lesssim (\rho a)^{-\frac{1}{2}}$. Here Neumann gap can be used to control errors. Rest of analysis carried out on large box. Loss of translation invariance - which we will ignore in the rest of this talk.
- Condensation. Let P projection on constant function, Q orthogonal complement.

$$n_0 = \sum P_i, \qquad n_+ = \sum Q_i.$$

A priori bounds control expected values $\langle n_0 \rangle$ and $\langle n_+ \rangle$. Energy error negligible if localizing to subspace where $n_+ \leq \mathcal{M}$, where $\mathcal{M}$ is of the order of the bound on $\langle n_+ \rangle$.

2-particle terms/The 4Q term

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$$v(x_i - x_j) = P_iP_jvP_jP_i + (Q_iP_jvP_jP_i + P_iQ_jvP_jP_i + h.c.) + \ldots + Q_iQ_jvQ_jQ_i$$
$$= \{Q_iQ_j + (P_iP_j + P_iQ_j + Q_iP_j)\omega\}\, v\, \{Q_jQ_i + \omega(P_iP_j + P_iQ_j + Q_iP_j)\} + \ldots$$

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So (all sums over $i \neq j$): $\frac{1}{2} \sum v(x_i, x_j) \geq \mathcal{Q}_0 + \mathcal{Q}_1 + \mathcal{Q}_2 + \mathcal{Q}_3'$,

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So (all sums over $i \neq j$): $\frac{1}{2} \sum v(x_i, x_j) \geq \mathcal{Q}_0 + \mathcal{Q}_1 + \mathcal{Q}_2 + \mathcal{Q}_3'$, where

$$\mathcal{Q}_3' := \sum P_i Q_j v_1(x_i, x_j) Q_j Q_i + h.c.$$
$$\mathcal{Q}_2 := \sum P_i Q_j v_2(x_i, x_j) P_j Q_i + \sum P_i Q_j v_2(x_i, x_j) Q_j P_i + \frac{1}{2} \sum (P_i P_j v_1(x_i, x_j) Q_j Q_i + h.c.),$$
$$\mathcal{Q}_1 := \sum P_j Q_i v_2(x_i, x_j) P_i P_j, \qquad \mathcal{Q}_0 := \frac{1}{2} \sum P_i P_j v_2(x_i, x_j) P_j P_i$$

and where $v_1 = v(1 - \omega) = g$, $v_2 = v(1 - \omega^2) = g(1 + \omega)$.

Strategy of proof II

- Discarding the positve $4Q$ term has renormalized the interaction. No "bare" v appears.
- Rest of proof in 2nd quantization. For simplicity of presentation, we will assume periodic boundary conditions. Then $1Q$ terms disappear. In the real proof, $1Q$ terms are present and the cancelation of the $1Q$ terms has to be done carefully.

Strategy of proof II

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- Rest of proof in 2nd quantization. For simplicity of presentation, we will assume periodic boundary conditions. Then $1Q$ terms disappear. In the real proof, $1Q$ terms are present and the cancelation of the $1Q$ terms has to be done carefully. Standard bosonic creation/annihilation operators $a_k, a_k^\dagger$, $k \in (2\pi\ell^{-1})\mathbb{Z}^3$.
$$[a_k, a_{k'}] = 0, \qquad [a_k, a_{k'}^\dagger] = \delta_{k,k'}.$$
- c-number substitution. Replace all $a_0, a_0^\dagger$ by $\sqrt{n}$.
Expect $n_0 \approx n \approx \rho\ell^3 = K^3(\rho a^3)^{-\frac{1}{2}}$. So $1/n_0 \ll (\rho a^3)^{\frac{1}{2}}$.
- Localize $3Q$-term: A preliminary analysis allows cut-offs in the $3Q$-term to soft-pair interactions only.

Diagonalizing the operator

Let $\mathcal{K}$ be the Hamiltonian on a periodic box, after c-number substitution

$$\mathcal{K} = \frac{1}{2}\rho^2\ell^3\widehat{g}(0) + \frac{1}{2}\rho^2\ell^3\widehat{g\omega}(0) + \mathcal{K}^{\mathrm{Bog}} + \mathcal{Q}_2^{\mathrm{ex}} + \mathcal{Q}_3.$$

Here, with $\mathcal{A}(k) := k^2 + \rho\widehat{g}(k), \quad \mathcal{B}(k) := \rho\widehat{g}(k).$

$$\mathcal{K}^{\mathrm{Bog}} := \frac{1}{2}\sum_k \Big(\mathcal{A}(k)(a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + \mathcal{B}(k)(a_k^\dagger a_{-k}^\dagger + a_k a_{-k}\Big),$$

and (with P_L being low momenta $\leq \sqrt{\rho a}$, P_H high momenta $\approx a^{-1}$)

$$\mathcal{Q}_2^{\mathrm{ex}} := \rho\sum_k \big(\widehat{g\omega}(0) + \widehat{g\omega}(k)\big)a_k^\dagger a_k \approx 2\rho\widehat{g\omega}(0)n_+$$

$$\mathcal{Q}_3 := \ell^{-3}\sqrt{n}\sum_{k\in P_H, s\in P_L}\widehat{g}(k)(a_s^\dagger a_{s-k}a_k + a_k^\dagger a_{s-k}^\dagger a_s).$$

Diagonalizing $\mathcal{K}^{\mathrm{Bog}}$ (The idealized Bogoliubov calculation)

$$(a_k^\dagger + \alpha_k a_{-k})(a_k + \alpha_k a_{-k}^\dagger) = a_k^\dagger a_k + \alpha_k^2 a_{-k}^\dagger a_{-k} + \alpha_k (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger) - \alpha_k^2 [a_{-k}, a_{-k}^\dagger].$$

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$$\begin{aligned}\mathcal{K}^{\mathrm{Bog}} &= \frac{1}{2}\sum_k \Big(\mathcal{A}(k)(a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + \mathcal{B}(k)(a_k^\dagger a_{-k}^\dagger + a_k a_{-k})\\ &= \sum_k \Big(\mathcal{D}_k b_k^\dagger b_k - (\mathcal{A}_k - \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2})\Big)\end{aligned}$$

where $b_k := a_k + \alpha_k a_{-k}^\dagger$, $\mathcal{D}_k = \frac{1}{2}(\mathcal{A}_k + \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2}) \approx k^2$, and

$\alpha_k = \mathcal{B}_k^{-1}(\mathcal{A}_k - \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2}) \approx \frac{\mathcal{B}_k}{2\mathcal{A}_k} \approx \rho\frac{\widehat{g}(k)}{2k^2} = \rho\widehat{\omega}(k)$ ($\approx$ valid for $|k|$ near a^{-1}).

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where $b_k := a_k + \alpha_k a_{-k}^\dagger$, $\mathcal{D}_k = \frac{1}{2}(\mathcal{A}_k + \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2}) \approx k^2$, and
$\alpha_k = \mathcal{B}_k^{-1}(\mathcal{A}_k - \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2}) \approx \frac{\mathcal{B}_k}{2\mathcal{A}_k} \approx \rho\frac{\widehat{g}(k)}{2k^2} = \rho\widehat{\omega}(k)$ ($\approx$ valid for $|k|$ near a^{-1}).
The constant term $\sum(\mathcal{A}_k - \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2})$ joins the constant $\frac{1}{2}\rho^2\ell^3\widehat{g}(0) + \frac{1}{2}\rho^2\ell^3\widehat{g\omega}(0)$ from $\mathcal{K}$ to give the right energy to LHY precision.

Treating $\mathcal{Q}_3 = \ell^{-3}\sqrt{n}\sum_{k\in P_H, s\in P_L} \widehat{g}(k)(a_s^\dagger a_{s-k} a_k + a_k^\dagger a_{s-k}^\dagger a_s)$

$$a_{s-k} a_k = \frac{1}{1-\alpha_k^2}\frac{1}{1-\alpha_{s-k}^2}\Big(b_{s-k} b_k - \alpha_k b_{-k}^\dagger b_{s-k} - \alpha_{s-k} b_{k-s}^\dagger b_k + \alpha_k \alpha_{s-k} b_{k-s}^\dagger b_{-k}^\dagger - \alpha_k [b_{s-k}, b_{-k}^\dagger]\Big).$$

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So,

$$\sum_{k\in P_H}\mathcal{D}_k b_k^\dagger b_k + \mathcal{Q}_3 \approx \sum_{k\in P_H}\mathcal{D}_k b_k^\dagger b_k + \ell^{-3}\sqrt{n}\sum_{k\in P_H, s\in P_L}\widehat{g}(k)(a_s^\dagger b_{s-k}b_k + b_k^\dagger b_{s-k}^\dagger a_s)$$

$$= \sum_{k\in P_H}\mathcal{D}_k\Big(b_k^\dagger + \ell^{-3}\sqrt{n}\frac{\widehat{g}(k)}{\mathcal{D}_k}\sum_{s\in P_L}a_s^\dagger b_{s-k}\Big)\Big(b_k + \ell^{-3}\sqrt{n}\frac{\widehat{g}(k)}{\mathcal{D}_k}\sum_{s'\in P_L}b_{s'-k}^\dagger a_{s'}\Big)$$

$$-2\frac{n}{\ell^6}\sum_{k\in P_H}\frac{\widehat{g}(k)^2}{2\mathcal{D}_k}\sum_{s\in P_L}a_s^\dagger b_{s-k}\sum_{s'\in P_L}b_{s'-k}^\dagger a_{s'}.$$

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$a_{s-k}a_k =$
$\frac{1}{1-\alpha_k^2}\frac{1}{1-\alpha_{s-k}^2}\Big(b_{s-k}b_k - \alpha_k b^\dagger_{-k}b_{s-k} - \alpha_{s-k}b^\dagger_{k-s}b_k + \alpha_k\alpha_{s-k}b^\dagger_{k-s}b^\dagger_{-k} - \alpha_k[b_{s-k}, b^\dagger_{-k}]\Big).$
So,

$$\sum_{k\in P_H}\mathcal{D}_k b_k^\dagger b_k + \mathcal{Q}_3 \approx \sum_{k\in P_H}\mathcal{D}_k b_k^\dagger b_k + \ell^{-3}\sqrt{n}\sum_{k\in P_H, s\in P_L}\widehat{g}(k)(a_s^\dagger b_{s-k}b_k + b_k^\dagger b_{s-k}^\dagger a_s)$$
$$= \sum_{k\in P_H}\mathcal{D}_k\Big(b_k^\dagger + \ell^{-3}\sqrt{n}\frac{\widehat{g}(k)}{\mathcal{D}_k}\sum_{s\in P_L}a_s^\dagger b_{s-k}\Big)\Big(b_k + \ell^{-3}\sqrt{n}\frac{\widehat{g}(k)}{\mathcal{D}_k}\sum_{s'\in P_L}b^\dagger_{s'-k}a_{s'}\Big)$$
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Notice that $\ell^{-3}\sum_{k\in P_H}\frac{\widehat{g}(k)^2}{2\mathcal{D}_k} \approx \widehat{g\omega}(0)$ and $[b_{s-k}, b^\dagger_{s'-k}] \approx \delta_{s,s'}$. Therefore, this term takes out $\mathcal{Q}_2^{\mathrm{ex}}$.
Normal ordered 4th order term requires the bound on $\mathcal{M}$.

Comments

- **Hard core**. We used a bound on $\int v$ to get the bound on $\mathcal{M}$. Need to replace v_{hc} by a softer potential with $0 < v < v_{hc}$ and $a(v_{hc}) - a(v) \ll \sqrt{\rho a^3}$. This forces $\int v \gg (\rho a^3)^{-\frac{1}{2}}$. In this case the window for localizing n_+ closes. But it turns out to be possible and sufficient to localize the low-momentum part of n_+.
- In the **2D** case, the energy becomes - with $Y = |\log(\rho a^2)|^{-1}$ -

$$e^{\mathrm{2D}}(\rho) = 4\pi\rho^2 Y\Big(1 - Y|\log Y| + \Big(2\Gamma + \frac{1}{2} + \log(\pi)\Big)Y\Big) + o(\rho^2 Y^2),$$

as $\rho a^2 \to 0$. Notice that the leading order term is a factor of the expansion parameter Y smaller than $4\pi\rho^2 \int v$ even for soft v. Therefore, $2D$ presents the same difficulties as the the $3D$ hardcore case - plus specific $2D$ complications. Joint work with Girardot, Junge, Morin, and Oliviera.