The ground state energy of dilute Bose gases

Søren Fournais

Department of Mathematics, Aarhus University, Denmark
and
Institute for Advanced Study, Princeton, NJ, USA

Based on joint work with Jan Philip Solovej, Copenhagen University, Denmark

Caltech & UCLA joint analysis seminar

The dilute Bose gas in 3 dimensions

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

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

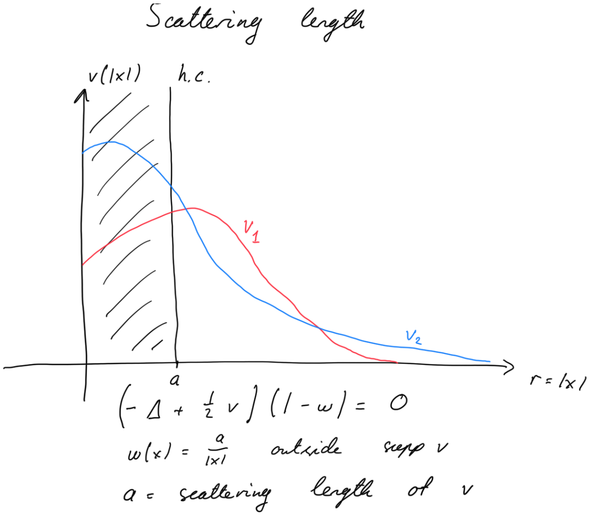
and $0 \leq v$ is radially symmetric with compact support.
The ground state energy of the system is

$$E_0(N, \Lambda) := \inf \mathrm{Spec}\, H_N = \inf_{\Psi \neq 0} \frac{\langle \Psi, H_N \Psi \rangle}{\|\Psi\|^2}.$$

The energy per particle in the thermodynamic limit is

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

The scattering length



Potential v is radial, positive with compact support.
With $g = v(1-\omega)$ the scattering equation can be reformulated as

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

and

$$a = (8\pi)^{-1}\int g < (8\pi)^{-1}\int v$$

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

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

- 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) (and later work by Aaen and Basti-Cenatiempo-Schlein).
- 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 (2017-2021).

The Lee-Huang-Yang formula

Theorem (SF, Solovej 2020)

Given a potential $v \neq 0$, non-negative, radial, L^1, with compact support there exist $C, \eta > 0$ (depending on v) such that for all ρ sufficiently small,

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

- Combined with the upper bound from Yau-Yin (for smooth potentials) this proves the Lee-Huang-Yang formula for the ground state energy.
- Extra work is required for the hard core case (work in progress).

Elements of the proof

- Localize to boxes of size $\ell = K(\rho a)^{-\frac{1}{2}}$, $K \gg 1$. Localization non-standard since need to preserve 'Neumann gap' and algebraic structure. 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.
- 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

Clearly $1 \otimes 1 = P_1 \otimes P_2 + Q_1 \otimes P_2 + P_1 \otimes Q_2 + Q_1 \otimes Q_2$ on $L^2(\text{box}) \otimes L^2(\text{box})$.

$$
\begin{aligned}
w(x_i, x_j) &= P_iP_jwP_jP_i + (Q_iP_jwP_jP_i + P_iQ_jwP_jP_i + h.c.) + \ldots + Q_iQ_jwQ_jQ_i \\
&= \{Q_iQ_j + (P_iP_j + P_iQ_j + Q_iP_j)\omega\}\, w\, \{Q_jQ_i + \omega(P_iP_j + P_iQ_j + Q_iP_j)\} + \ldots
\end{aligned}
$$

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

$$
\begin{aligned}
\mathcal{Q}_3 &:= \sum P_iQ_jw_1(x_i, x_j)Q_jQ_i + h.c. \\
\mathcal{Q}_2 &:= \sum P_iQ_jw_2(x_i, x_j)P_jQ_i + \sum P_iQ_jw_2(x_i, x_j)Q_jP_i \\
&\quad + \frac{1}{2}\sum (P_iP_jw_1(x_i, x_j)Q_jQ_i + h.c.), \\
\mathcal{Q}_1 &:= \sum P_jQ_iw_2(x_i, x_j)P_iP_j + h.c., \qquad \mathcal{Q}_0 := \frac{1}{2}\sum P_iP_jw_2(x_i, x_j)P_jP_i
\end{aligned}
$$

and where $w_1 = w(1 - \omega) \approx g$, $w_2 = w(1 - \omega^2) = w_1(1 + \omega)$.

Elements of proof II

- Discarding the positive $4Q$ term has renormalized the interaction. No "bare" w left.
- Rest of proof in 2nd quantization. In translation invariant setting, $1Q$ 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.

Elements of proof III

- Carry out the Bogoliubov diagonalization of the "idealized" quadratic operator, i.e. with w_2 replaced by w_1 in quadratic terms. The error in this replacement is $\mathcal{Q}_2^{\rm ex} \approx 2\rho \widehat{g\omega}(0) n_+$. This gives

$$E_0 \gtrsim E^{\rm LHY} + \sum \mathcal{D}_k b_k^\dagger b_k + \mathcal{Q}_2^{\rm ex} + \mathcal{Q}_3.$$

- Absorb $\mathcal{Q}_3$ in the positive diagonal operator $\sum \mathcal{D}_k b_k^\dagger b_k$ by a completion-of-the-square argument. This gives rise to many (commutator) terms. The main one of these cancels $\mathcal{Q}_2^{\rm ex}$. The others are small.

THANK YOU FOR YOUR ATTENTION.

Localization

Let $0 \leq \chi \in C_0^\infty((\frac{-1}{2}, \frac{1}{2})^3)$ with $\int \chi^2 = 1$. For $\ell > 0$ and $u \in \mathbb{R}^3$, we define
$B(u) = \ell u + [\frac{-\ell}{2}, \frac{\ell}{2}]^3$ box of sidelength ℓ centered at ℓu.
$\chi_u(x) = \chi(\frac{x}{\ell} - u)$ the localization function χ moved to $B(u)$.
Q_u =the orthogonal projection in $L^2(B(u))$ to functions orthogonal to constants.

Lemma

There exists $b, s > 0$ such that for all $\varphi \in H^1(\mathbb{R}^3)$ and all $\ell > 0$

$$\langle \varphi, -\Delta\varphi \rangle \geq \int_{\mathbb{R}^3} \langle \varphi, Q_u \left[\chi_u \mathcal{K}(-i\nabla)\chi_u + b\ell^{-2}\right] Q_u\varphi \rangle \, du,$$

with $\mathcal{K}(p) = (|p|^2 - \frac{1}{4}(s\ell)^{-2})_+$.