(Upper bound for) the free energy of the dilute Bose gas at low temperature

j.w.w. F. Haberberger, C. Hainzl, B. Schlein

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Arnaud Triay

Mathematical setting

$$H_N = \sum_{i=1}^{N} -\Delta_{x_i} + \sum_{1 \leq i < j \leq N} V(x_i - x_j)$$

- Acting on $\bigotimes_s^N L^2([0, L]^3)$
- $0 \leq V$ compactly supported
- Thermodynamic limit $N/L^3 = \rho \ll 1$ (dilute regime)

Low density expansion (Lee-Huang-Yang 1957)

- $E_0 = \inf \sigma(H_N)$: Ground state energy
- $\mathfrak{a}$: scattering length of V

LEE, HUANG, AND YANG

x I that the eigen- or

$$E_0 = 4\pi a N\rho\left[1 + \frac{128}{15\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}}\right], \qquad (25)$$

$4y^2)^{\frac{1}{2}}$, (18) a result which was first obtained in reference 4 by the

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Two-body problem:

$$4\pi\,\mathfrak{a} = \inf\left\{\int_{\mathbb{R}^3} |\nabla f|^2 + \frac{1}{2}\int_{\mathbb{R}^3} V|f|^2,\ f(x) \underset{|x|\to\infty}{\longrightarrow} 1\right\}$$

Mathematical setting

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(28) nonvanishing momentum. This is discussed in detail in Appendix I. The eigenvalues for these states can be shown to be

$$E = E_0 + \sum_{\mathbf{k} \neq 0} m_{\mathbf{k}} k (k^2 + 16\pi a \rho)^{\frac{1}{2}}, \tag{34}$$

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Diagonalizing the Bose gas

Theorem: Free energy expansion

Let $0 \leq V \in L^2$, non-increasing, with compact support

$$-\frac{T}{L^3} \log \operatorname{tr} e^{-H_N/T} \simeq 4\pi\,\mathfrak{a}\,\rho^2 + 4\pi \times \frac{128}{15\sqrt{\pi}}(\rho\,\mathfrak{a})^{5/2} + T^{5/2}\int_{\mathbb{R}^3} \log\left(1 - e^{-\sqrt{p^4 + 16\pi\frac{\mathfrak{a}\,\rho}{T}p^2}}\right)\mathrm{d}p + o((\rho\,\mathfrak{a})^{5/2})$$

for $T \lesssim \rho a = \ell_{GP}^{-2}$

- Upper bound: [Yau-Yin '09] [Basti-Cenatiempo-Schlein '21], Lower bound: [Fournais-Solovej '19 '20]
- Lower bound: [Haberberger-Hainzl-Nam-Seiringer-T '23] [Fournais-Girardot-Junge-Morin-Olivieri-T 24+], Upper bound [Haberbeger-Hainzl-Schlein-T '24]

Gibbs Variational problem:

$$-\frac{T}{L^3} \log \operatorname{tr} e^{-H_N/T} = \inf\left\{\operatorname{tr} H_N\Gamma + T \operatorname{tr}\Gamma\log\Gamma, \Gamma \geq 0, \operatorname{tr}\Gamma = 1\right\}$$

Quasi-Free states

In second quantization

$$H_N = \sum_{p\in 2\pi\mathbb{Z}^3/L} p^2 a_p^* a_p + \frac{1}{2L^3}\sum_{p,q,r}\widehat{V}(r) a_{p+r}^* a_q^* a_p a_{q+r}$$

First guess: Try quasi-free states

$$\Gamma = Z^{-1}\mathcal{W}^*\mathbb{U}^* e^{-T^{-1}\mathrm{d}\Gamma(E_{\mathrm{Bog}})}\mathbb{U}\mathcal{W}, \qquad \mathrm{d}\Gamma(E_{\mathrm{Bog}}) = \sum_{p\neq 0}(p^4 + 16\pi\,\mathfrak{a}\,\rho p^2)^{1/2} a_p^* a_p$$

with $\mathcal{W} = e^{\sqrt{N}a_0^* - \mathrm{h.c.}}$ a Weyl transform $\mathcal{W}^* a_0^* \mathcal{W} = a_0^* + \sqrt{N}$
and $\mathbb{U} = \exp(\mathcal{B})$, $\mathcal{B} = \sum_r \eta_r a_r^* a_{-r}^* - \mathrm{h.\,c.}$ a Bogoliubov rotation
Good news: easy to compute (Wicks rule)

$$\mathbb{U}^* a_p^* \mathbb{U} = a_p^* + \int_0^1 e^{-t\mathcal{B}}[a_p^*, \mathcal{B}]e^{t\mathcal{B}}\mathrm{d}t = \sum_{k\geq 0}\frac{1}{k!}(-1)^k \mathrm{ad}_{\mathcal{B}}^{(k)}(a_p^*)$$
$$= \gamma_p a_p^* + \sigma_p a_{-p}$$

Bad news: Wrong second order [Erdös-Schlein-Yau '09]

$$\mathrm{tr}\, H_N\Gamma \geq 4\pi\rho\,\mathfrak{a}\, N(1 + C_{\mathrm{Wrong}}\sqrt{\rho\,\mathfrak{a}^3} + o(\sqrt{\rho\,\mathfrak{a}^3}))$$

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Soft pairs

The Quasi-Free states only sees terms of the form $a_0^* a_0^* a_0 a_0$, $a_r^* a_r a_0^* a_0$

$$a_r^* a_{-r}^* a_0 a_0 \qquad \text{or} \qquad a_0^* a_0^* a_r a_{-r}$$

But the LHY term is also sensitive to processes involving soft-pairs

$$a_{r+p}^* a_{-r}^* a_p a_0 \qquad \text{or} \qquad a_0^* a_p^* a_{p+r} a_{-r}$$

and it is enough to consider r "very large" and p "small"

Bad news: hard to compute, no closed formula for cubic transformations, we can try a perturbative expansion

$$e^{-\mathcal{B}_c} a_p^* e^{\mathcal{B}_c} \stackrel{?}{=} \sum_{k \geq 0} \frac{1}{k!} (-1)^k \operatorname{ad}_{\mathcal{B}_c}^{(k)}(a_p^*)$$

with $\mathcal{B}_c = \sum_{p,r} \eta_r a_{p+r}^* a_{-r}^* a_p - \mathrm{h.c.}$ which requires

$$\langle \mathcal{B}_c \rangle \ll 1.$$

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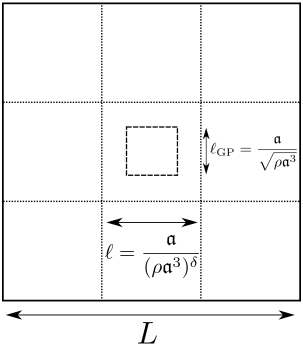
Dirichlet bracketing

To make the expansion converge, we consider subsystems where excitations are much fewer

$$H_N = \sum_{i=1}^{N} -\Delta_{x_i} + \sum_{1\le i<j\le N} N^{2(1-\kappa)} V(N^{1-\kappa}(x_i - x_j))$$

on $[0,1]^3$ where $0 \le \kappa \le 2/3$ interpolates between Gross-Pitaevskii and Thermodynamic limit, $\langle \mathcal{N}_+ \rangle \simeq N^{3\kappa/2}$

- trial state on $[0,L]^3 \longrightarrow$ patching subsystems with Dirichlet boundary conditions
- border effects $\ll$ Lee-Huang-Yang: if $\kappa > 1/2$ ($\ell \gg \rho^{-1}$)
- $\langle \mathcal{B}_c \rangle = N^{9\kappa/2-2} \ll 1$ for $\kappa < 4/9$



Fermionization: non unitary

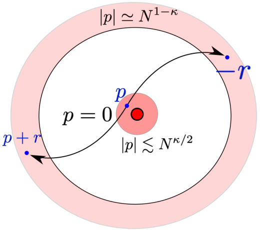
[Basti-Cenatiempo-Schlein '21]: non-unitary transformation with cut-offs $\Theta_{r,p}$ allowing to compute the cubic transformation

$$\Psi = \mathbb{U}_{Bog} e^{\widetilde{\mathcal{B}}_c} |\Omega\rangle$$

with

$$\widetilde{\mathcal{B}}_c^* = \sum_{p \in L, r \in H} \eta_{r,p} \Theta_{r,p} a^*_{p+r} a^*_{-r} a^*_{-p}$$

- role of $\Theta_{r,p}$ is to make the "p-connection" excitation $(-r, p+r)$ "fermionic"
- create a p-connection if there is not already one
- don't create any q-connection for $q \neq p$
- use simplification from $|\Omega\rangle$



$$\frac{\langle \Psi, H_N \Psi\rangle}{\|\Psi\|^2} = \frac{1}{\|\Psi\|^2} \sum_{m,n \geq 0} \frac{1}{n!} \frac{1}{m!} \langle (\widetilde{\mathcal{B}}_c)^m \mathbb{U}^*_{Bog} H_N \mathbb{U}_{Bog} (\widetilde{\mathcal{B}}_c^*)^n \rangle_\Omega$$

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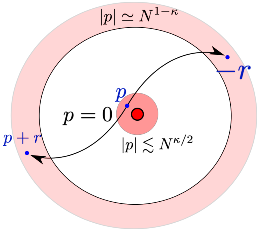

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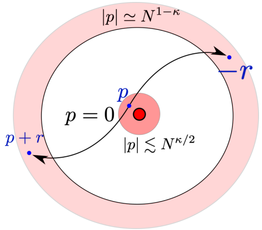

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Fermionization: unitary

- To compute the spectrum of H_N we need a unitary version of $e^{\widetilde{\mathcal{B}}_c}$
- We need to dress the Gibbs state instead of the vacuum

$$|\Omega\rangle \longmapsto Z^{-1} e^{-T^{-1}\sum_p E_{\mathrm{Bog}}(p) a_p^* a_p}$$

- We define for $p \in L$

$$\mathcal{B}_p^* = \sum_{r \in H} \eta_r \Theta_{r,p} a_{-r}^* a_{r+p}^* a_p$$

which acts as a fermionic creation operator $(\mathcal{B}_p^*)^2 = 0$

- and define the unitary transformation

$$T_p = e^{\mathcal{B}_p^* - \mathcal{B}_p} = \cos(X_p) + (\mathcal{B}_p^* \frac{\sin(X_p)}{X_p} - \mathrm{h.c.}) + \mathcal{B}_p^* \frac{\cos(X_p) - 1}{X_p^2} \mathcal{B}_p$$

with $X_p = \sqrt{\mathcal{B}_p \mathcal{B}_p^*}$ ($\ll 1$ on the trial state).

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Trial state

We take for trial state

$$\Gamma = \mathcal{W}\mathbb{U}_H T_c \mathbb{U}_L \mathbb{1}_{\mathcal{F}(L)} \frac{1}{Z} e^{-T^{-1}\mathrm{d}\Gamma(E_{\mathrm{Bog}})} \mathbb{U}_L^* T_c^* \mathbb{U}_H^* \mathcal{W}^*$$

with $\mathcal{F}(L) = \mathcal{F}(\{|p| \lesssim N^{\kappa/2}\})$.

- $\Gamma_{\mathbb{H}} := Z^{-1}\mathbb{U}_L \mathbb{1}_{\mathcal{F}(L)} \frac{1}{Z} e^{-T^{-1}\mathrm{d}\Gamma(E_{\mathrm{Bog}})} \mathbb{U}_L^*$ is the Gibbs state of

$$\mathbb{H}_{Bog} = \sum_p (p^2 + 8\pi\,\mathfrak{a}\,N^\kappa) a_p^* a_p + \sum_{|p| \lesssim N^{\kappa/2}} 4\pi\,\mathfrak{a}\,N^\kappa (a_p^* a_{-p}^* + \mathrm{h.\,c.})$$

- $\mathbb{U}_H T_c$ is responsible for the high-momenta renormalization $a_r^* a_{-r}^* a_0 a_0$ and $a_{r+p}^* a_{-r}^* a_p a_0$ for $|r| \gtrsim N^{1-\kappa}$ and $|p| \lesssim N^{\kappa/2}$, $\widehat{V}(0) \mapsto 8\pi\,\mathfrak{a}$
- $\mathcal{W}$ accounts for the particles in the condensate

and on $\mathrm{Ran}\Gamma_{\mathbb{H}}$

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Thank you for your attention!

Bogoliubov's strategy

$$H_N = \sum_{p\in 2\pi\mathbb{Z}^3/L} p^2 a_p^* a_p + \frac{1}{2L^3}\sum_{p,q,r}\widehat{V}(r) a_{p+r}^* a_q^* a_p a_{q+r}$$

$$\simeq \frac{\widehat{V}(0)}{2}\rho N + \sum_p (p^2 + \rho\widehat{V}(p)) a_p^* a_p + \frac{\rho}{2}\sum_p \widehat{V}(p)\left(a_p^* a_{-p}^* + a_p a_{-p}\right)$$

$$a_0^* \simeq a_0 \simeq \sqrt{N}, \quad \text{(Bogoliubov's approximation: c-number substitution)}$$

$$\widehat{V}(p) \longmapsto 8\pi\,\mathfrak{a} \qquad \text{(Landau's correction: high momenta renormalization)}$$

$$\simeq 4\pi\,\mathfrak{a}\,\rho N + \sum_p (p^4 + 16\pi\rho\,\mathfrak{a}\,p^2)^{1/2}(\gamma_p a_p^* + \sigma_p a_{-p})(\gamma_p a_p + \sigma_p a_{-p}^*) + C_{LHY}^{(2)}$$

(Bogoliubov diagonalization)

$$\simeq 4\pi\,\mathfrak{a}\,\rho N + C_{LHY}^{(2)} + \sum_p (p^4 + 16\pi\rho\,\mathfrak{a}\,p^2)^{1/2} b_p^* b_p$$

$$[b_p, b_q^*] = \delta_{p,q} \qquad \text{(Canonical Commutation Relations)}$$

- $\operatorname{tr} e^{-\frac{E}{T}b^* b} = \sum_{n\geq 0} e^{-\frac{E}{T}n} = (1 - e^{-\frac{E}{T}})$

$$-\frac{T}{L^3}\log \operatorname{tr} e^{-H_N/T} \simeq 4\pi\,\mathfrak{a}\,\rho^2 + 4\pi \times \frac{128}{15\sqrt{\pi}}(\rho\,\mathfrak{a})^{5/2}$$

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$a_0^* \simeq a_0 \simeq \sqrt{N}$, (Bogoliubov's approximation: c-number substitution)

$\widehat{V}(p) \longmapsto 8\pi\mathfrak{a}$ (Landau's correction: high momenta renormalization)

$$\simeq 4\pi\mathfrak{a}\rho N + \sum_p (p^4 + 16\pi\rho\mathfrak{a} p^2)^{1/2} (\gamma_p a_p^* + \sigma_p a_{-p})(\gamma_p a_p + \sigma_p a_{-p}^*) + C_{LHY}^{(2)}$$

(Bogoliubov diagonalization)

$$\simeq 4\pi\mathfrak{a}\rho N + C_{LHY}^{(2)} + \sum_p (p^4 + 16\pi\rho\mathfrak{a} p^2)^{1/2} b_p^* b_p$$

$[b_p, b_q^*] = \delta_{p,q}$ (Canonical Commutation Relations)

- $\operatorname{tr} e^{-\frac{E}{T} b^* b} = \sum_{n \geq 0} e^{-\frac{E}{T} n} = (1 - e^{-\frac{E}{T}})$

$$-\frac{T}{L^3} \log \operatorname{tr} e^{-H_N/T} \simeq 4\pi\mathfrak{a}\rho^2 + 4\pi \times \frac{128}{15\sqrt{\pi}} (\rho\mathfrak{a})^{5/2}$$

Bogoliubov's strategy

$$H_N = \sum_{p\in 2\pi\mathbb{Z}^3/L} p^2 a_p^* a_p + \frac{1}{2L^3}\sum_{p,q,r} \widehat{V}(r) a_{p+r}^* a_q^* a_p a_{q+r}$$

$$\simeq 4\pi\,\mathfrak{a}\,\rho N + \sum_p (p^2 + 8\pi\rho\,\mathfrak{a}) a_p^* a_p + \sum_p 4\pi\rho\,\mathfrak{a}\left(a_p^* a_{-p}^* + a_p a_{-p}\right) + C_{LHY}^{(1)}$$

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