A variational approach to computing the ground state energy of the Lieb–Liniger model

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General setting

N particle Hamiltonian in a d-dimensional box Λ of sidelength L

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

- acting on symmetric (bosonic) part of $\bigotimes_{i=1}^{N} L^2(\Lambda)$
- ground state energy:

$$E_0(N, L) = \inf \operatorname{spec}(H_N), \;\; e(\rho) = \lim_{\substack{N, L \to \infty \\ N/L^d = \rho}} L^{-d} E_0(N, L),$$

,

Ground state energy of Bose gases - short overview

d=3

- dilute case: $e(\rho) = 4\pi a\rho^2 \left(1 + \frac{128}{15\pi}(\rho a^3)^{1/2} + o((\rho a^3)^{1/2}\right)$ (LHY formula) [Dyson '57, Lieb–Yngvason '98, Yau–Yin '09, Fournais–Solovej '20]
- weak coupling – high density: LHY (Giuliani–Seiringer '09)
- full density range: 'simplified equation' (Carlen–Jauslin–Lieb '19)

d=2

- dilute case:
  $e(\rho) = 4\pi\rho^3 ab\,(1 + b\log b + 2\gamma + \log\pi)b + o(b))$ with $b = \log\left(\rho a^2\right)|^{-1}$
  [Schick '71, Lieb–Yngvason '01, Fournais–Girardot–Junge–Morin–Olivieri '22]
- high density – charged particles [Lieb–Solovej '02,'04, Solovej '06]

Ground state energy of Bose gases - short overview

Here: d=1

- dilute case, certain class of potentials with support in $[-R_0, R_0]$:

$$\frac{E_0(N,L)}{L} = \frac{\pi^2}{3}\rho^3\left(1 + 2\rho a + \mathcal{O}\left((\rho|a|)^{6/5} + (\rho R_0)^{6/5} + N^{-2/3}\right)\right)$$

  (Agerskov–Reuvers–Solovej '22)

- our analysis based on a variational approach restricting to Bogoliubov (quasi-free) states is mainly interesting for the **high density regime**

Bogoliubov theory (Bogoliubov 1947)

- generic transl.-inv. Hamiltonian in 2nd quant. on $[0, L)^d$

$$H = \sum_p \varepsilon(p) a_p^* a_p + \frac{1}{2L^d} \sum_{k,p,q} v(p) a_{k+p}^* a_{q-p}^* a_k a_q$$

- for small T, weak coupling:
  1. neglecting terms of higher order than quadratic in annihilation/creation operators $a_{p\neq 0}^{(*)}$
  2. $[a_0^*, a_0] = 1 \ll N_0$, setting $a_0^* = a_0 = \sqrt{N_0}$ ('c-number substitution')
- approximation of the Hamiltonian $H \approx H_{\mathrm{Bog}}$ (quadr. Hamiltonian)
- H_{Bog} is minimised by *Bogoliubov variational states*

Bogoliubov variational states

Bogoliubov Hamiltonian H_{Bog} = quadr. terms + const N_0

- Quadratic part: minimised by *quasi-free states*.
- Quasi-free states ψ given by *generalised one-particle density matrix*

$$\omega_{\gamma,\alpha}(\psi) = \begin{pmatrix} \gamma_\psi & \alpha_\psi \\ \alpha_\psi^* & 1 + J\gamma_\psi J^* \end{pmatrix} \text{ on } \mathcal{H} \oplus \mathcal{H}', \qquad J : \mathcal{H} \to \mathcal{H}' \text{ isometric isom.}$$

$$\langle g, \gamma_\psi h\rangle = \langle \psi, a^*(g)a(h)\psi\rangle, \ \langle g, \alpha_\psi h\rangle = \langle \psi, a(g)a(h)\psi\rangle \text{ for } g, h \in \mathcal{H}.$$

- altogether: $\psi_{Bog} = U_{N_0}\omega_{\gamma,\alpha} \mathrel{\widehat{=}} (\gamma, \alpha, N_0)$ with $U_{N_0}^* a_p U_{N_0} = a_p + \sqrt{N_0}\delta_{p,0}$

Bogoliubov variational principle

$\mathcal{D}_{\text{Bog}} = \{\psi \mid \psi \text{ is a Bogoliubov variational state}\}$

- exact ground state energy $E_0 = \inf_{\substack{\psi \in D(H) \\ \psi \neq 0}} \frac{\langle \psi, H\psi \rangle}{\|\psi\|^2}$
- ground state energy according to Bogoliubov's theory

$$E_0^{\text{Bog}} = \inf_{\substack{\psi \in \mathcal{D}_{\text{Bog}} \subset D(H) \\ \psi \neq 0}} \frac{\langle \psi, H_{\text{Bog}}\psi \rangle}{\|\psi\|^2}$$

- ground state energy from *Bogoliubov variational principle*

$$E_0^{approx} = \inf_{\substack{\psi \in \mathcal{D}_{Bog} \subset D(H) \\ \psi \neq 0}} \frac{\langle \psi, H\psi \rangle}{\|\psi\|^2} \geq E_0$$

The Bogoliubov energy functional

$$\mathcal{E}(\gamma,\alpha,\varrho_0)=\lim_{N,L\to\infty}\langle\psi_{\text{Bog}},H\psi_{\text{Bog}}\rangle L^{-d}=\frac{1}{2\pi}\int_{\mathbb{R}^d}p^2\gamma(p)\mathrm{d}p-\frac{\widehat{V}(0)}{2}\rho^2+$$
$$\frac{1}{8\pi^2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\widehat{V}(p-q)\left(\gamma(p)\gamma(q)+\alpha(p)\alpha(q)\right)\mathrm{d}p\mathrm{d}q+\frac{1}{2\pi}\int_{\mathbb{R}^d}\widehat{V}(p)\left(\gamma(p)+\gamma(q)\right)\mathrm{d}p$$

plane wave representation, $\psi_{\text{Bog}}=(\gamma,\alpha,\rho_0)$ with $\gamma(p):=\langle\psi_{\text{Bog}},a_p^*a_p\psi_{\text{Bog}}\rangle$, $\alpha(p):=\langle\psi_{\text{Bog}},a_pa_{-p}\psi_{\text{Bog}}\rangle$ and $\rho_0=\frac{N_0}{L^d}$; $\varepsilon(p)=p^2$

$$\mathcal{D}=\left\{(\gamma,\alpha,\rho_0)\;\middle|\;\gamma\in L^1((1+p^2)\mathrm{d}p),\gamma(p)\geq 0,\alpha(p)^2\leq\gamma(p)(1+\gamma(p)),0\leq\rho_0\leq\rho\right\}$$

special case ($T=0$) of free energy functional from [3 dimensions: Napiorkowski–Reuvers–Solovej ’17][Critchley–Solomon ’76]

The Bogoliubov variational functional

- minimise Bogoliubov energy functional

$$e(\rho)^{\mathrm{approx}} = \inf_{(\gamma,\alpha,\varrho_0)\in\mathcal{D}} \mathcal{E}(\gamma,\alpha,\varrho_0)$$

- in three dimensions – dilute limit: existence of minimisers, phase transition and critical temperature, free energy expansion [Napiorkowski, Reuvers, Solovej '18 and '17]
- in two dimensions – dilute limit: phase transition and critical temperature , two term asymptotics ground state energy [Napiorkowski–Reuvers–Solovej '18, Fournais–Napiorkowski–Reuvers–Solovej '19]

Testing the Bogoliubov variational principle – the Lieb–Liniger model

Lieb and Liniger 1963

$$H = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{1 \le i < j \le N} \delta(x_i - x_j)\,; \qquad \text{rescaling } x \to \rho x$$

- $c > 0$ coupling constant; one parameter $\xi = \frac{c}{\varrho}$, $\varrho = \frac{N}{L}$ particle density
- exactly solvable: all eigenfunctions and eigenvalues determined (implicitly)
- well suited for testing approximation methods

Testing the Bogoliubov variational principle - the Lieb-Liniger model

Lieb and Liniger 1963

$$H\rho^{-2} = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2\xi \sum_{1\leq i<j\leq N} \delta(x_i - x_j)$$

- $c > 0$ coupling constant; one parameter $\xi = \frac{c}{\varrho}$, $\rho = \frac{N}{L}$ particle density
- exactly solvable: all eigenfunctions and eigenvalues determined (implicitly)
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Results – large ξ – strong coupling/low density

In the limit of strong coupling or low density when $\xi \to \infty$, we have

$$e(\xi)^{\mathsf{approx}} \rho^{-3} = 4\xi^{1/2} + \mathcal{O}(1) \ .$$

- diverging – true ground state energy (e.g. Agerskov–Reuvers–Solovej '22):

$$e(\xi)\rho^{-3} = \frac{\pi^2}{3}\left(1 + 2\xi^{-1}\right)^{-2} + \mathcal{O}(\xi^{-3})$$

- better than Bogoliubov: predicts a negative energy
- limit of the Tonks-Girardeau gas: leading term = free Fermi gas, ground state = fermionic state

Results - small ξ – weak coupling/high density

In the limit of weak coupling or high density when $\xi \to 0$, we have

$$e(\xi)\rho^{-3} = \xi - \frac{4}{3\pi}\xi^{3/2} + \frac{1}{32\pi^2}\xi^2(\ln\xi)^2 + \mathcal{O}(\xi^2 \ln\xi \ln(-\ln\xi))\,.$$

- original Bogoliubov approximation (LL '63): $\frac{E_0}{N\varrho^2} = \xi - \frac{4}{3\pi}\xi^{3/2}$
- (believed to be true) expansion (Tracy–Widom 2016)

$$e(\xi)\rho^{-3} = \xi - \frac{4}{3\pi}\xi^{3/2} + \left[\frac{1}{6} - \frac{1}{\pi^2}\right]\xi^2 + o(\xi^2)\,.$$

Lieb and Liniger's solution

1. $$e(\xi) = \frac{\xi^3}{\lambda^3} \int_{-1}^{1} g(x) x^2 \mathrm{d}x$$

2. $$1 + 2\lambda \int_{-1}^{1} \frac{g(x) x^2}{\lambda^2 + (x-y)^2} \mathrm{d}x = 2\pi g(y)$$

3. $$\xi \int_{-1}^{1} g(x) \mathrm{d}x = \lambda$$