GP Upper Bound General

ISTA 13. Feb. 2024

Upper bound for the grand canonical free energy of the Bose gas in the Gross-Pitaevskii limit

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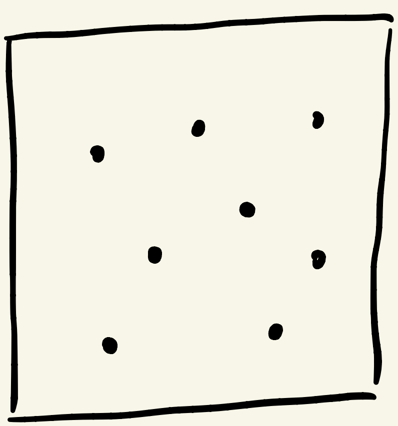
1) Set-up

Λ



← Torus with side length L.

$$\mathcal{H}_N = \int_\Lambda a_x^* (-\Delta_x) a_x \, dx + \frac{1}{2} \int_{\Lambda \times \Lambda} a_x^* a_y^* \, V_N(x-y) \, a_y a_x \, d(x,y)$$

with $V_N(x) = N^2 v(Nx)$ and $v \geq 0$ — measurable, radial, compact support

$$a_N = \frac{a}{N} > 0$$

a — scattering length of v.

Set of probability distributions over rank 1 projections.

- **States:** $S_N = \{ \Gamma \in \mathcal{B}(\mathcal{F}) \mid \Gamma \geq 0,\ \operatorname{tr}\Gamma = 1,\ \operatorname{tr} \mathcal{N}\Gamma = N \}$

Same N as in definition of Hamiltonian

bosonic Fock space

number op.

von-Neumann entropy

- **Gibbs free energy functional:** $\mathcal{F}(\Gamma) = \operatorname{tr}[H_N \Gamma] - \frac{1}{\beta} S(\Gamma)$ with

$$S(\Gamma) = -\operatorname{tr}\Gamma \ln(\Gamma)$$

inverse temperature

(grand canonical)

- **Free energy:** $F(\beta, N, L) = \inf_{\Gamma \in S_N} \mathcal{F}(\Gamma)$ ← grand canonical Gibbs state is unique minimizer

$$= \phi(\beta, \mu(\beta, N, L), L) + \mu(\beta, N, L) N$$

grand canonical potential

Parameters:

→ easier because N also in def. of $\mathcal{H}_N$

- expected part. numb. N (instead of chem. pot. μ)
- side length $L = O(1)$ in N
- inverse temp. $\beta \gtrsim \beta_c = \text{const.}\ \varrho^{-2/3} \sim L^2 N^{-2/3}$

inverse crit. temp. for BEC in ideal gas and interacting system

$\hookrightarrow \varrho = \frac{N}{L^3}$

D., Seiringer '20 (canonical ensemble)

2.) The main result (for the sake of simplicity: $\beta > \beta_c$)

density $\quad$ density of BEC

Thm.:

$$F(\beta,N,L) \le F_0^+(\beta,N,L) + 8\pi a_N L^3 \left(\varrho^2 - \varrho_0^2\right) + F^{BEC}(\beta,N,L,a_N)$$

free energy of thermal cloud $\quad$ free energy of BEC

$$- \frac{1}{2\beta} \sum_{p \neq 0} \left[\frac{16\pi a_N \varrho_0}{p^2} - \ln\left(1 + \frac{16\pi a_N \varrho_0}{p^2}\right)\right] + o\left(L^{-2} N^{2/3}\right)$$

Correction to free energy of thermal cloud from Bogoliubov theory

:] $F_0^+(\beta,N,L) = \frac{1}{\beta}\sum_{p\neq 0} \ln\left(1-\exp\left(-\beta\left(p^2-\mu_0\right)\right)\right) + \mu_0 N$

$\mu_0(\beta,N,L)$ = chem. pot. in ideal gas with N particles

We find this by minimizing the free energy of the condensate

:] $F^{BEC}(\beta,N_0,L,a_N) = -\frac{1}{\beta}\ln\left(\int_{\mathbb{C}} \exp\left(-\beta\left(4\pi a_N L^{-3}|z|^4 - \mu|z|^2\right)\right)dz\right)$

$z = x+iy$

$dz = \frac{dx\,dy}{\pi}$

$+\mu N_0$, where μ is chosen s.t.

exp. # of cond. particles

$$\int_{\mathbb{C}} |z|^2 \rho(z)\, dz = N_0 \quad \text{with} \quad \rho(z) = \frac{\exp\left(-\beta\left(4\pi a_N L^{-3}|z|^4 - \mu|z|^2\right)\right)}{\int_{\mathbb{C}} \exp(\dots)\, dz}.$$

$\boxed{\text{Van der Wurff et al.}}$

← discrete version for trapped gas

Prop.: Assume that $N_0 \gtrsim N^{5/6+\varepsilon}$, then

$$F^{BEC}(\beta, N_0, L, a_N) = 4\pi a_N L^3 \rho_0^2 + \frac{1}{2\beta}\ln\left(4\pi a_N \beta L^{-3}\right) + O\left(L^{-2}\exp(-cN^{\varepsilon})\right).$$

Cor.: Assume that $N_0 \gtrsim N^{5/6+\varepsilon}$, then

$$F(\beta,N,L) \le \underbrace{F_0^+(\beta,N,L)}_{\sim L^{-2}N^{5/3}} \overbrace{+\, 4\pi a_N \left(2\rho^2-\rho_0^2\right)}^{(*),\ \sim L^{-2}N} + \overbrace{\underbrace{\frac{1}{2\beta}\ln\left(4\pi a_N \beta L^{-3}\right)}_{\text{BEC}}}^{L^{-2}N^{2/3}(1+\ln(N))}$$

$$\underbrace{-\frac{1}{2\beta}\sum_{p\neq 0}\left[\frac{16\pi a_N \rho_0}{p^2} - \ln\left(1+\frac{16\pi a_N\rho_0}{p^2}\right)\right]}_{L^{-2}N^{2/3},\ \text{Bog}} + o\left(L^{-2}N^{2/3}\right)$$

(*): Thermodyn. limit: Seiringer '08, Yin '10

GP limit (Proof of cond., can. ensemble): D., Seiringer '20

Remarks:

only logarithmic growth with volume

- The term BEC vanishes in the thermodynamic limit.
- The term Bog converges in the thermodynamic limit to

$$-\frac{16\sqrt{\pi}}{3\beta}(a\varrho_0)^{3/2}$$

← compare to: Napiórkowski, Reuvers, Solovej '17

corrections from dispersion relation $\varepsilon(p)$ <u>not</u> E_0

- We have $\int_{\mathbb{C}} |z|^4 \varrho(z)\, dz - \left(\int_{\mathbb{C}} |z|^2 \varrho(z)\, dz\right)^2 \sim N^{5/3}$.

ideal gas: N^2

compare to: Buffet, Pulé '83 (Imperfect Bose gas); E.B. Davies '72

3) Heuristics and some ideas of the proof

• uncorrelated trial state : $\Gamma_0 = \int_{\mathbb{C}} |z\rangle\langle z| \otimes G(z)\, \rho(z)\, dz$

prob. density from BEC effective theory

$|z\rangle = \exp(z a_0^* - \bar{z} a_0)|\mathrm{vac}\rangle$

$G(z)$: Gibbs state related to $H^B(z)$ with

$$H^B(z) = \sum_{p \neq 0} (p^2 - \mu_0) a_p^* a_p + 4\pi a_N \rho_0(\beta, N, L) \sum_{p \neq 0} \left[2 a_p^* a_p + \frac{z^2}{|z|^2} a_p^* a_{-p}^* + \frac{\bar{z}^2}{|z|^2} a_p a_{-p} \right]$$

temperature-dependent Bogoliubov Hamiltonian, compare with Lee, Yang '58

Spectral thm.: $\Gamma_0 = \int_{\mathbb{C}} \sum_\alpha \lambda_\alpha(z)\, |\Psi_\alpha(z)\rangle\langle\Psi_\alpha(z)|\, \wp(z)\, dz$

$\boxed{\cdot}$ Trial state with correlations:

$$\Gamma = \int_{\mathbb{C}} \sum_\alpha \lambda_\alpha(z)\, |\Phi_\alpha(z)\rangle\langle\Phi_\alpha(z)|\, \wp(z)\, dz, \quad \text{where}$$

$$\Phi_\alpha(z) = \frac{F\Psi_\alpha(z)}{\|F\Psi_\alpha(z)\|} \quad \text{and} \quad F\Psi_\alpha(z)\Big|_n = \prod_{1\le i<j\le n} f(x_i - x_j)\, \Psi_\alpha^{(n)}(z).$$

$$\Delta f(x) = \frac{V_N(x)}{2} f(x)$$

See e.g. Dyson; Lieb, Yngvason, Seiringer; ...

Comment on correlations inside the integral.

Bogoliubov correction to free energy of thermal cloud

$$\varepsilon(p) = \sqrt{p^2-\mu_0}\sqrt{p^2-\mu_0+16\pi a_N \rho_0}$$

$$\phi_\varepsilon(\beta,\mu_0,L) = \frac{1}{\beta}\sum_{p\neq 0} \ln\left(1-\exp\left(-\beta\varepsilon(p)\right)\right)$$

density-density interaction

$$= \frac{1}{\beta}\sum_{p\neq 0} \ln\left(1-\exp\left(-\beta(p^2-\mu_0)\right)\right) + 8\pi a_N L^3(\rho-\rho_0)\rho_0$$

Contributes to F_0^+

$$-\frac{1}{2\beta}\sum_{p\neq 0}\left[\frac{16\pi a_N\rho_0}{p^2} - \ln\left(1+\frac{16\pi a_N \rho_0}{p^2}\right)\right] + o\left(L^{-2}N^{2/3}\right)$$

new term

⊡ Heuristics for condensate effective theory

This is forced upon us by the result for BEC!

Ansatz: $\Gamma_0 = \int_{\mathbb{C}} |z\rangle\langle z| \, p(z) \, dz$ with $\int_{\mathbb{C}} |z|^2 p(z) \, dz = N_0$

Correlations implemented before

Hamiltonian: $4\pi a_N L^{-3} a_0^* a_0^* a_0 a_0$ (condensate has no kinetic energy)

free energy: $4\pi a_N L^{-3} \int_{\mathbb{C}} |z|^4 p(z) \, dz - \frac{1}{\beta} \underbrace{S(\Gamma_0)}$

$$\geq - \int_{\mathbb{C}} p(z) \ln(p(z)) \, dz$$

Berezin, Lieb

$$\geq \inf_{\substack{p \geq 0 \\ \int p(z) dz = 1 \\ \int |z|^2 p(z) = N_0}} \ldots = F^{BEC}(\beta, N_0, L, a_N)$$

c-number substitution for one mode gives $O(L^{-2})$ remainder, Lieb, Seiringer, Yngvason '05

4) Outlook

- Lower bound in mean-field coming (Marcin, Nam)

  ↪ next step : thermodynamic limit

  ↪ lower bound in GP

$$\frac{1}{2}\int_{\mathbb{C}}\sum_{\alpha}\lambda_\alpha(z)\int_{\Lambda^2}\rho^{(2)}_{\Psi_\alpha(z)}(x_1,x_2)\,(1-f)(x_1-x_2)\,d(x_1,x_2)$$

$$\int_{\Lambda^2}\rho^{(2)}_{\Psi_\alpha(z)}(x_1,x_2)\,\xi_N(x_1-x_2)\,d(x_1,x_2)\;\rho(z)\,dz$$

$$-\frac{1}{2}\int_{\mathbb{C}}\sum_{\alpha}\lambda_\alpha(z)\int_{\Lambda^4}\rho^{(4)}_{\Psi_\alpha(z)}(x_1,x_2,x_3,x_4)\,\xi_N(x_1-x_2)\,(1-f)(x_3-x_4)\,d(x_1\ldots x_4)$$

$$\rho(z)\,dz$$