

The free energy of the dilute Bose gas
collaboration with F. Haberberger, C. Hainzl, P.T. Nam

MBQM 2022
Arnaud Triay



N bosons in $[-L/2, L/2]^3$, at density $N/L^3 \rightarrow \rho$, temperature $T > 0$,

$$H_{N,L} = \sum_{i=1}^N -\Delta_i + \sum_{1 \leq i < j \leq N} V(x_i - x_j)$$

$$f(\rho, T) := \lim_{\substack{N \rightarrow \infty \\ N/L^3 \rightarrow \rho}} -\frac{T}{L^3} \log \operatorname{tr}_{L^2_s(\mathbb{R}^{3N})} e^{-\frac{H_{N,L}}{T}}$$

When $T = 0$, **dilute limit** $\rho a^3 \rightarrow 0$ [Dyson 57], [Lieb-Yngvason 99], [Yau-Yin 09], [Basti-Cenatiempo-Schlein 21] [Fournais-Solovej 20,21]

$$e(\rho) = f(\rho, 0) = 4\pi a \rho^2 \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho a^3}) \right)$$

For $0 < T \lesssim \rho^{2/3} \sim T_c(\rho)$, [Seiringer 08], [Yin 10]

$$f(\rho, T) = f_0(\rho, T) + 4\pi a (2\rho^2 - [\rho - \rho_c(T)]_+^2) (1 + o(1))$$

where $f_0(\rho, T)$ is the free energy of the ideal Bose gas.

- Related works in the Gross–Pitaevskii regime: [Deuchert-Seiringer-Yngvason 19], [Deuchert-Seiringer 20]

Second order expansion of the free energy: lower bound

$$f(\rho, T) \simeq f_0(\rho, T) + 4\pi a (2\rho^2 - [\rho - \rho_c(T)]_+^2)$$

We want thermal contribution \lesssim Lee-Huang-Yang $4\pi a \rho^2 \times \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3}$

$$\left\{ \begin{array}{l} \rho_c(T) \sim T^{3/2} \\ f_0(\rho, T) \underset{T \ll T_c(\rho)}{\sim} T^{5/3} \end{array} \right. \implies T \lesssim \rho a = \rho^{2/3} (\rho a^3)^{1/3}$$

LHY correction at positive temperature (conjecture)

Let $0 \leq V \in L^1(\mathbb{R}^3)$, radial, non-increasing, compactly supported, for $T \lesssim \rho a$ and $\rho a^3 \rightarrow 0$, we have

$$f(\rho, T) \geq 4\pi a \rho^2 \left(1 + C_{\text{LHY}} \left(\frac{\rho a}{T} \right) \sqrt{\rho a^3} + o(\sqrt{\rho a^3}) \right)$$

$$\lim_{\alpha \rightarrow 0} C_{\text{LHY}}(\alpha) = \frac{128}{15\sqrt{\pi}}.$$

$$4\pi a(V) := \inf \left\{ \int_{\mathbb{R}^3} |\nabla f|^2 + \frac{1}{2} \int_{\mathbb{R}^3} V |f|^2, f \in H^1(\mathbb{R}^3), f(x) \rightarrow 1 \text{ as } |x| \rightarrow \infty \right\}$$

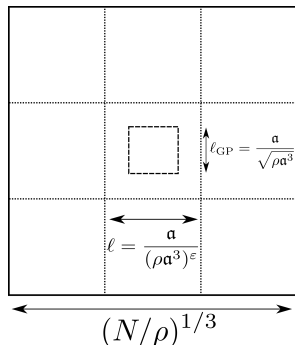
$$e(\rho) = 4\pi a \rho^2 \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho a^3}) \right)$$

- M^3 boxes of size ℓ with Neumann b.c.
($M \simeq L/\ell$)

$$E(N, L) \geq M^3 \inf_{\sum c_k = 1} \sum_k c_k E(k, \ell)$$

- after dilation $\mathcal{U}\Psi = \ell^{3n/2}\Psi(\cdot)$, on $L_s^2([-1/2, -1/2]^{3n})$

$$\mathcal{U}^* H_{n,\ell} \mathcal{U} = \frac{1}{\ell^2} \left(\sum_{i=1}^n -\Delta_i + \sum_{i < j} \ell^2 V(\ell(x_i - x_j)) \right)$$



- **Gross-Pitaevskii length scale ℓ_{GP}** : gap kinetic \sim interaction energy per particle
- 1st order $4\pi a \rho^2$: [Lieb Yngvason 99], [Lieb Seiringer 01] $\ell \ll \ell_{GP} \implies$ interaction = small perturbation (Temple inequality)
- 2nd order LHY: [Fournais Solovej 20,21], [Fournais 20] $\ell \gg \ell_{GP}$ (+ sliding technique) = more work

For $0 \leq \kappa \leq 2/3$, on $L_s^2([-1/2, -1/2]^{3N})$,

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

$\kappa = 0$: Gross–Pitaevskii regime

$\kappa = 2/3$: Thermodynamic limit

- periodic b.c., $\kappa > 0$: [Adhikari Brennecke Schlein 21], [Brennecke Caporaletti Schlein 21] (next order + excitation spectrum)

$$\begin{aligned} E(N, \kappa) &= 4\pi a N^{1+\kappa} + 4\pi \times \frac{125}{15\sqrt{\pi}} a^{5/2} N^{5\kappa/2} + o(N^{5\kappa/2}) \\ 1 - \langle \mathbb{1}, \gamma_{\psi_N} \mathbb{1} \rangle &= o(1) \end{aligned}$$

- Neumann b.c., $\kappa = 0$: optimal rate [Boccato Seiringer 22]

→ following [Lieb-Seiringer 01] or [Lieb Yngvason Seiringer Solovej], BEC for small $\kappa > 0$

Denoting $V_N = N^{2-2\kappa} V(N^{1-\kappa} \cdot)$ and $(V_N)_{p,q,r,s} = \langle u_p \otimes u_q, V_N u_r \otimes u_s \rangle$, $u_0 = \mathbb{1}_{[-1/2, 1/2]^3}$

$$H_N^\kappa = \sum_p p^2 a_p^\dagger a_p + \frac{1}{2} \sum_{p,q,r,s} (V_N)_{p,q,r,s} a_p^\dagger a_q^\dagger a_r a_s$$

$$\underset{\text{c-numb}}{\simeq} \frac{1}{2} N^{1+\kappa} \widehat{V}(0) + \underbrace{\sum_{p \neq 0} (p^2 + N^\kappa \widehat{V}(0)) a_p^\dagger a_p + \sum_{p,q \neq 0} N (V_N)_{p,q,0,0} a_p^\dagger a_q^\dagger + h.c. + Q_3 + Q_4}_{=: Q_2}$$

c-number substitution $a_0 \simeq a_0^\dagger \simeq \sqrt{a_0^\dagger a_0} \simeq \sqrt{N}$ [Lewin-Nam-Serfaty-Solovej 15]

- Vacuum $|\Omega\rangle (\simeq \mathbb{1}^{\otimes N}) \implies$ Hartree energy $\frac{1}{2} N^{1+\kappa} \widehat{V}(0)$
- **Quasi-free states** $e^{\sum_{p,q} (K_1)_{p,q} a_p^\dagger a_q^\dagger - h.c.} |\Omega\rangle \implies$
 $E(N, \kappa) \leq 4\pi a N^{1+\kappa} + \mathcal{O}(N^{5\kappa/2})$ [Erdős-Schlein-Yau 08] in TL
- + **Cubic correlation structure:** $T_2 e^{\sum_{p,q,r} (K_c)_{p,q,r} a_p^\dagger a_q^\dagger a_r - h.c.} T_1 |\Omega\rangle \implies$

$$E(N, \kappa) \leq 4\pi a N^{1+\kappa} + \frac{1}{2} \sum_{p \neq 0} [\sqrt{p^4 + 16\pi a p^2 N^\kappa}] - p^2 - 8\pi a N^\kappa + \frac{(8\pi a N^\kappa)^2}{2p^2} + o(N^{5\kappa/2})$$

[Yau Yin 09], [Boccato-Brennecke-Cenatiempo-Schlein 19], [Basti-Cenatiempo-Schlein 21], ...

First quadratic transform

goal: **renormalize** Q_2

$$T_1 = \exp(B_1), \quad B_1 = \int K_1(x, y) a_x^\dagger a_y^\dagger - h.c.$$

Choose K_1 so that (by the Duhamel formula)

$$\begin{aligned} [d\Gamma(-\Delta) + Q_4, B_1] + Q_2 &\simeq 0 \\ \frac{1}{2} \text{ad}_{B_1}^{(2)}(d\Gamma(-\Delta) + Q_4) - \text{ad}_{B_1}(Q_2) &\simeq \left(4\pi a - \frac{1}{2} \widehat{V}(0)\right) N^{1+\kappa} \end{aligned}$$

→ [Nam T- 21], [Hainzl 21], [Hainzl Schlein T- 22]

- we want to take $K_1(x, y) = -N(1 - f)(N^{1-\kappa}(x - y))$

$$-\Delta f + \frac{1}{2} V f = 0, \quad 4\pi a = \frac{1}{2} \int V f.$$

- cut-off at $\ell > 0$, $K_1(x - y) = -N(1 - f)(N^{1-\kappa}(x - y))\chi(\lambda^{-1}(x - y))$

$$-\Delta K_1 = \frac{1}{2} N V_N (1 - K_1) + 4\pi a N^\kappa \lambda^{-3} W(\lambda^{-1} \cdot), \quad \int_{\mathbb{R}^3} W = 1$$

- Neumann b.c. **symmetrization by reflexion**

$$K_1(x, y) = - \sum_{z \in \mathbb{Z}^3} N(1 - f)(N^{1-\kappa}(P_z x - y)) \chi(\lambda^{-1}(N^{1-\kappa}(P_z x - y)))$$

First quadratic transform

goal: **renormalize** Q_2

$$T_1 = \exp(B_1), \quad B_1 = \int K_1(x, y) a_x^\dagger a_y^\dagger - h.c.$$

Choose K_1 so that (by the Duhamel formula)

$$\begin{aligned} [d\Gamma(-\Delta) + Q_4, B_1] + Q_2 &\simeq \tilde{Q}_2 \\ \frac{1}{2} \text{ad}_{B_1}^{(2)}(d\Gamma(-\Delta) + Q_4) - \text{ad}_{B_1}(Q_2) &\simeq \left(4\pi a - \frac{1}{2} \widehat{V}(0)\right) N^{1+\kappa} + \underbrace{\tilde{C}_{N,\lambda}}_{\simeq \lambda^{-1}} \end{aligned}$$

→ [Nam T- 21], [Hainzl 21], [Hainzl Schlein T- 22]

- we want to take $K_1(x, y) = -N(1 - f)(N^{1-\kappa}(x - y))$

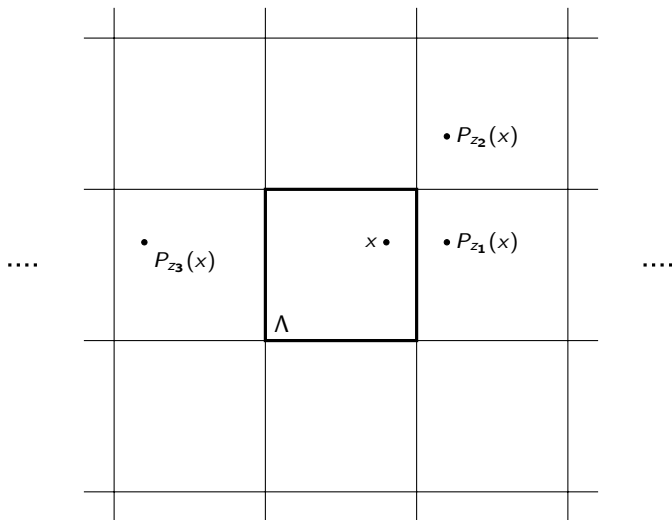
$$-\Delta f + \frac{1}{2} V f = 0, \quad 4\pi a = \frac{1}{2} \int V f.$$

- cut-off at $\ell > 0$, $K_1(x - y) = -N(1 - f)(N^{1-\kappa}(x - y))\chi(\lambda^{-1}(x - y))$

$$-\Delta K_1 = \frac{1}{2} N V_N (1 - K_1) + 4\pi a N^\kappa \lambda^{-3} W(\lambda^{-1} \cdot), \quad \int_{\mathbb{R}^3} W = 1$$

- Neumann b.c. **symmetrization by reflexion**

$$K_1(x, y) = - \sum_{z \in \mathbb{Z}^3} N(1 - f)(N^{1-\kappa}(P_z x - y)) \chi(\lambda^{-1}(N^{1-\kappa}(P_z x - y)))$$



$$K_1(x, y) = - \sum_{z \in \mathbb{Z}^3} N(1 - f)(N^{1-\kappa}(\mathbf{P}_z x - y)) \chi(\lambda^{-1}(N^{1-\kappa}(\mathbf{P}_z x - y)))$$

goal: **renormalize** $Q_3 \lesssim \delta Q_4 + CN^\kappa \mathcal{N}_+$, for (smooth) $\theta \equiv 1$ on $[0, 1]$ and $\theta \equiv 0$ on $[2, \infty]$

$$T_c = \exp(B_c), \quad B_c = N^{-1/2} \theta \left(\frac{\mathcal{N}}{M} \right) \int K_1(x, y) a_x^\dagger a_y^\dagger a_y - h.c. \quad \text{as in [Nam T- 21]}$$

$$\begin{aligned} & [d\Gamma(-\Delta) + Q_4, B_c] + Q_3 \simeq 0 \\ & \frac{1}{2} \text{ad}_{B_c}^{(2)}(d\Gamma(-\Delta) + Q_4) - \text{ad}_{B_c}(Q_3) \simeq \left(4\pi a - \widehat{V}(0)\right) N^\kappa \mathcal{N}_+ \end{aligned}$$

$$\begin{aligned} T_c^* T_1^* H_N^\kappa T_1 T_c & \simeq 4\pi a N^{1+\kappa} + d\Gamma(-\Delta + 8\pi a N^\kappa) + \widetilde{Q}_2 + \widetilde{C}_{N,\lambda} + Q_4 + \mathcal{E}, \\ \pm \mathcal{E} & = o(d\Gamma(-\Delta) + Q_4) + CN^{2\kappa} \log N + C\lambda N^{C\kappa} \mathcal{N}_+ \\ & \quad + C\lambda^{-1/2} \frac{M}{N} \mathcal{N}_+ + CN^{C\kappa} \frac{(\mathcal{N}_+ + 1)^2}{N} + N^\kappa (1 - \theta \left(\frac{\mathcal{N}}{M} \right)) \mathcal{N}_+ + \dots \end{aligned}$$

- We can use BEC for $\kappa > 0$ small $\langle \mathcal{N}_+ \rangle \ll N^{1-\varepsilon(\kappa)}$ from [Lieb-Seiringer 01] + localization in \mathcal{N}_+ from [Lewin-Nam-Serfaty-Solovej]

The system is essentially quadratic

$$T_2^* T_c^* T_1^* H_N^\kappa T_1 T_c T_2 \simeq 4\pi \alpha N^{1+\kappa} + 4\pi \times \frac{128}{15\sqrt{\pi}} \alpha^{5/2} N^{5\kappa/2} + d\Gamma(\sqrt{p^4 + 8\pi \alpha N^\kappa p^2})$$

$$\begin{cases} \ell &= N^{1-\kappa} \\ \rho \ell^3 &= N \end{cases} \implies N^\kappa = \rho \ell^2$$

Using Neumann bracketing and subadditivity of the entropy ([Hainzl-Lewin-Solovej 09]) ,

$$\begin{aligned} -\frac{T}{L^3} \log \operatorname{tr} e^{-\frac{H_N}{T}} &\gtrsim -\frac{T}{\ell^3} \log \operatorname{tr} e^{-\frac{H_{n,\ell}}{T\ell^2}} \\ &\simeq 4\pi \alpha \rho^2 \left\{ 1 + (\rho \alpha^3)^{1/2} \left(\frac{128}{15\sqrt{\pi}} + f_{\text{Bog}}(\rho, T) \right) \right\} \end{aligned}$$

$$f_{\text{Bog}}(\rho, T) = - \left(\frac{T}{\rho \alpha} \right)^{5/2} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \log(1 - e^{-(\sqrt{p^4 + \frac{16\pi \rho \alpha}{T} p^2})}) dp$$

$$= \lim_{\ell \rightarrow \infty} \ell^{-3} \sum_{p \in 2\pi \mathbb{Z}^3} \log(1 - e^{-(\sqrt{(p/\ell)^4 + \frac{16\pi \rho \alpha}{T} (p/\ell)^2})})$$

- **dilute regime** $\rho a^3 \rightarrow 0$ and small temperature $T \lesssim \rho a$

$$f(\rho, T) \geq 4\pi a \rho^2 \left(1 + C_{\text{LHY}} \left(\frac{\rho a}{T} \right) \sqrt{\rho a^3} + o(\sqrt{\rho a^3}) \right)$$

- using **Neumann bracketing** we reduce the problem to analysis on boxes much larger than the GP length scale (**beyond Gross–Pitaevskii**)
- We study H_N^κ with **Neumann boundary** conditions and $\kappa > 0$ (optimal rate for $\kappa = 0$ [Boccato Seiringer 22])

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

- new proof for $T = 0$

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

Thank you for your attention!