The thermodynamic energy density of a mixture of dilute Bose gases.

Analytic and Algebraic Methods in Physics

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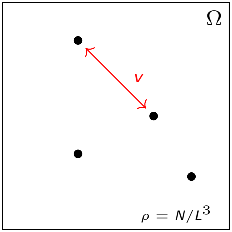
One species of bosons

Math description of Bose gases: interacting particles

- N bosons in a box

$$\Omega = [-L/2, L/2]^3 \subseteq \mathbb{R}^3.$$



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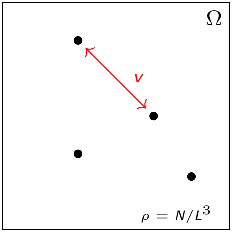

- Hamiltonian:

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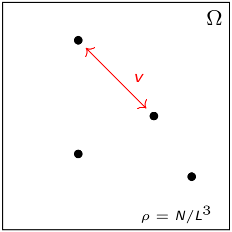

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$$v \geq 0, \quad \text{spherically symmetric (compactly supported).}$$

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- We study an expansion of the energy density in the dilute regime:

$$\rho a^3 \ll 1 \qquad (\Longleftrightarrow \quad a \ll \rho^{-1/3}).$$

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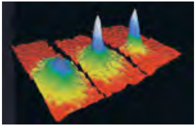

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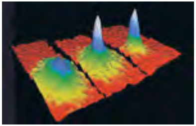

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- Testing Universality: how many terms depend only on a, scattering length of v?

Scattering length

- Pairwise potential $v > 0 \quad \Rightarrow \quad$ Energy is related to the $2-$body problem

$$\inf\left\{\int_{\mathbb{R}^3}\left(|\nabla\phi|^2 + \frac{1}{2}v\,|\phi|^2\right)\mathrm{d}x \,\middle|\, \phi \in \dot{H}^1(\mathbb{R}^3),\ \lim_{|x|\to\infty}\phi = 1\right\} = 4\pi a.$$

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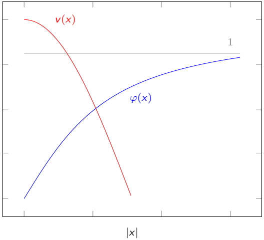
- There exists a unique minimizer φ such that, for $\mathrm{supp}(v) \subseteq B_R(0)$,

$$-\Delta_x\varphi(x) + \frac{1}{2}v(x)\varphi(x) = 0,$$

$$\varphi(x) = 1 - \frac{a}{|x|}, \qquad |x| > R.$$



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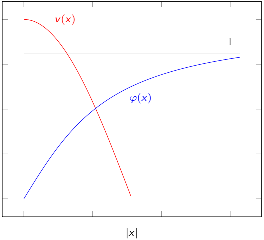

- Important quantities:

$$g(x) := v(x)\varphi(x), \qquad \omega(x) := 1 - \varphi(x) \quad \Rightarrow \quad \widehat{g}(0) = 8\pi a.$$

Historical development for expansions in TD limit

	1st	2nd	3rd	free
UP	[1]	[3,4,5,6]	[8]	[9]
LOW	[2]	[7]	?	[10,11]

$$e(\rho) \simeq 4\pi\rho^2 a, \qquad \text{1st order, TD regime,}$$

[1] Dyson 1957: upper bound by trial state using Jastrow factors

[2] Lieb, Yngvason, 1998: lower bound, obtained by **localization** in small boxes

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$e(\rho) \leq 4\pi\rho^2 a + \mathcal{O}(\rho^2 a\sqrt{\rho a^3}),$ 2nd order, TD regime,

[3] Erdos, Schlein, Yau 2008: upper bound for weak coupling, using quasi-free states,

[4] Basti, Cenatiempo, Giuliani, Olgiati, Pasqualetti, Schlein 2023: hardcore, upper bound, not right constant

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

[5] Yau, Yin 2009: upper bound using the soft pairs contribution in cubic interactions,

[6] Basti, Cenatiempo, Schlein, 2021: upper bound for larger class of potentials and better errors.

[7] Fournais, Solovej, 2020 + 2021 lower bound 2nd order, hardcore included.

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$$e(\rho) \leq 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} + 8\left(\frac{4}{3}\pi - \sqrt{3}\right)\rho a^3 \log(12\pi\rho a^3)\right)$$

[8] Brooks, Oldenburg, Saint Aubin, Schlein 2025: third order correction, upper bound, $v \in L^2$.

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$$f_T(\rho) \simeq 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}\right) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \log\left(1 - e^{-\sqrt{p^4 + 16\frac{\pi}{T}a\rho p^2}}\right) \mathrm{d}p$$

[9] Haberberger, Hainzl, Nam, Seiringer, Triay, 2024: lower bound, $v \in L^1$;

[10] Haberberger, Hainzl, Schlein, Triay, 2024: upper bound, $v \in L^2$.

[11] Fournais, Girardot, Junge, Morin, O., Triay 2024: lower bound, hardcore.

Two species of bosons

Math description of mixture Bose gases: interacting particles

- $N = N_A + N_B$ bosons in a volume $\Omega \subseteq \mathbb{R}^3$.
  - N_A bosons of type A, density $\rho_A = \frac{N_A}{|\Omega|}$,
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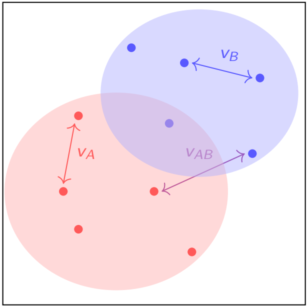

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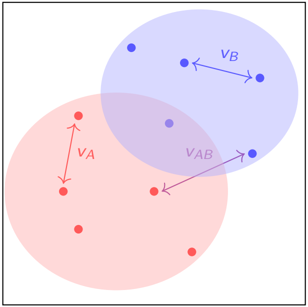

- Hamiltonian:

$$H_{N_A,N_B} = \sum_{j=1}^{N_A} -\Delta_{x_j} + \sum_{k=1}^{N_B} -\Delta_{y_k} + \sum_{i<j}^{N_A} v_A(x_i - x_j) + \sum_{i<j}^{N_B} v_B(y_i - y_j) + \sum_{j=1}^{N_A} \sum_{k=1}^{N_B} v_{AB}(x_j - y_k), \quad \text{acting on } L_s^2(\Omega_{x_j}^{N_A}) \otimes L_s^2(\Omega_{y_k}^{N_B}).$$

Energy density of mixtures in thermodynamic limit

- Potentials:

$$v_A, v_B, v_{AB} \geq 0,$$ non-negative, spherically symmetric (compactly supported), with scattering lengths $a_A, a_B, a_{AB} > 0$.

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- **Energy density** in thermodynamic regime

$$e_{3D}(\rho_A, \rho_B) = \lim_{\substack{N_A, N_B, |\Omega| \to +\infty \\ \rho_A = N_A/|\Omega|, \rho_B = N_B/|\Omega|}} \frac{1}{|\Omega|} E(N_A, N_B, \Omega).$$

Previous results

- **Dynamics**: convergence of Bose mixture dynamics to NLS equations
  - Michelangeli, Olgiati, 2016, 2017
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  - Larsen 1963, Oles, Sacha 2008, Petrov 2015: Physics papers giving the second order expansion of the energy in thermodynamic limit

$$e_{3D}(\rho_A, \rho_B) \simeq 4\pi \Big(\rho_A^2 a_A + 2\rho_A\rho_B a_{AB} + \rho_B^2 a_B + \frac{16\sqrt{2}}{15\sqrt{\pi}} \sum_{\pm} \Big(\rho_A a_A + \rho_B a_B \pm \sqrt{(\rho_A a_A - \rho_B a_B)^2 + 4\rho_A\rho_B a_{AB}^2} \Big)^{5/2} \Big)$$

Assumptions on the potentials

- Assumptions $(*)$ on potentials :

  $v_A, v_B, v_{AB} \in L^1$, positive, spherically symmetric, compactly supported, decreasing, with scattering lengths $a_A, a_B, a_{AB} > 0$.

$$\mathscr{A} := \begin{pmatrix} a_A & a_{AB} \\ a_{AB} & a_B \end{pmatrix}.$$

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- **Born approximation** of the scattering length

$$8\pi a = \widehat{v}(0) - \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{d}k \, \frac{\widehat{v}(k)^2}{2k^2} + \dots$$

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- We say that v is a **soft potential** if there exists $C, \eta > 0$ such that

$$|8\pi a - \widehat{v}(0)| \leq C(\rho a^3)^\eta a$$

Main result

Theorem (O. '25)

There exists $C > 0$ such that, if the potentials v_A, v_B, v_{AB} with scattering lengths $a_A, a_B, a_{AB} > 0$ satisfy the Assumptions $(*)$ and

$$\boxed{a_{AB}^2 \leq a_A a_B} \qquad (\Longleftrightarrow \mathscr{A} \geq 0) \qquad \textit{(miscibility)}$$

then for $\rho \bar{a}^3 \leq C^{-1}$, $\rho = \rho_A + \rho_B$, $\bar{a} = \max\{a_A, a_B, a_{AB}\}$,

$$\boxed{|e_{3D}(\rho_A, \rho_B) - 4\pi(\rho_A^2 a_A + 2\rho_A\rho_B a_{AB} + \rho_B^2 a_B)| \leq C\rho\bar{a}(\rho\bar{a}^3)^{1/2}}$$

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$\binom{N_A}{2}, \binom{N_B}{2}$ pairs, each pair with zero energy $8\pi a_A|\Omega|^{-1}, 8\pi a_B|\Omega|^{-1}$ respectively

$N_A \cdot N_B$ pairs with zero energy $8\pi a_{AB}|\Omega|^{-1}$

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from an effective quadratic Hamiltonian + errors

$$\sum_{k\neq 0} c_k^* \mathcal{A}_k c_k + \frac{1}{2}(c_k^* \mathcal{B}_k c_{-k}^* + c_k \mathcal{B}_k c_{-k})$$

Main result

Corollary (Right constant, soft potentials case)

If, furthermore, I assume there exists $\eta > 0$ such that

$$|\widehat{v}_A(0) - 8\pi a_A| + |\widehat{v}_B(0) - 8\pi a_B| \leq C(\rho\bar{a}^3)^{\eta}\bar{a}, \qquad |\widehat{v}_{AB}(0) - 8\pi a_{AB}| \leq C(\rho\bar{a}^3)^{3\eta}\bar{a},$$

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$$+(\rho_A^2 a_A^2 + 2\rho_A\rho_B a_{AB}^2 + \rho_B^2 a_B^2)^{5/4} J_{AB} + \mathcal{O}\big((\rho\bar{a})^{5/2}(\rho\bar{a}^3)^\eta\big),$$

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where $J_{AB} = \mathcal{O}(1)$,

$$J_{AB} := \frac{1}{2(2\pi)^3}\int_{\mathbb{R}^3} \mathrm{d}k \left(\sqrt{k^4 + 2\mu_+ k^2} + \sqrt{k^4 + 2\mu_- k^2} - \frac{1}{2k^2} - 2k^2 - (\mu_+ + \mu_-)\right),$$

with

$$\mu_\pm := \frac{1}{2}\left(\sqrt{1+\xi_{AB}} \pm \sqrt{1-\xi_{AB}}\right), \qquad \xi_{AB} := \frac{2\rho_A\rho_B(a_A a_B - a_{AB}^2)}{\rho_A^2 a_A^2 + 2\rho_A\rho_B a_{AB} + \rho_B^2 a_B^2}.$$

Remarks

- If w.l.o.g. $\rho_B, a_B \to 0$, $\rho = \rho_A$, $a = a_A$ then

$$e_{3D}(\rho, 0) = 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}\right) + C(\rho\bar{a})^{5/2+\eta},$$

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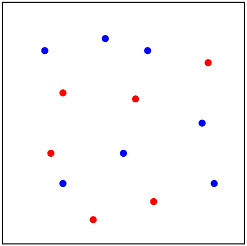

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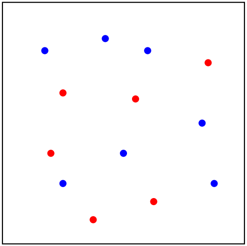

For $a_{AB}^2 > a_A a_B$, other phenomena occur
(dilute liquid-like droplet state
see Petrov 2015)

Sketch of the Proof:
Upper bound

Momenta space

We rewrite the Hamiltonian in momenta space (**second quantization**): $\Omega^* := \frac{2\pi}{L}\mathbb{Z}^3$

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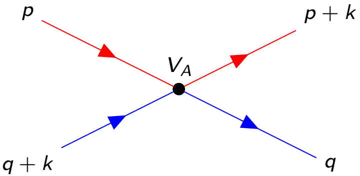
Analogous definition with b_k, b_k^* for bosons of type B.

$$\sum_{1\le i<j\le N_A} v_A(x_i - x_j) = \sum_{k,p,q\in\Omega^*} \widehat{v}_A(k) a^*_{p+k} a^*_q a_{q+k} a_p$$



Upper bound

- Hamiltonian in 2nd quantization on $\mathscr{F} = \mathscr{F}_A \otimes \mathscr{F}_B$

$$\mathcal{H} = \sum_{k \in \Omega^*} k^2 (a_k^* a_k + b_k^* b_k) + \frac{1}{2|\Omega|} \sum_{k,p,q \in \Omega^*} \widehat{v}_A(k) a_{p+k}^* a_q^* a_{q+k} a_p$$
$$+ \frac{1}{2|\Omega|} \sum_{k,p,q \in \Omega^*} \widehat{v}_B(k) b_{p+k}^* b_q^* b_{q+k} b_p + \frac{1}{|\Omega|} \sum_{k,p,q \in \Omega^*} \widehat{v}_{AB}(k) a_{p+k}^* b_q^* b_{q+k} a_p$$

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- **Trial state**: **Quasi-Free state**

$$\boxed{\Psi = W_A \otimes W_B \, T \, \Omega_A \otimes \Omega_B,}$$

  - Ω_A, Ω_B vacuum vectors for $\mathscr{F}_A, \mathscr{F}_B$, respectively;
  - $W_A = e^{\sqrt{N_0^A}(a_o^* - a_0)}$, $W_B = e^{\sqrt{N_0^B}(b_o^* - b_0)}$ depend on parameters

$$N_0^A, N_0^B > 0$$

Weyl and Bogoliubov transformations

- Weyl operator actions

$$W_A^* \otimes W_B^* \, a_0^\# \, W_A \otimes W_B = a_0^\# + \sqrt{N_0^A},$$
$$W_A^* \otimes W_B^* \, b_0^\# \, W_A \otimes W_B = b_0^\# + \sqrt{N_0^B} \quad \Rightarrow \quad \boxed{N_0^A, N_0^B \text{ have to be chosen}}$$

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- Bogoliubov transformation

$$T = e^{\frac{1}{2}\sum_{k\neq 0} c_k^* \cdot S_k c_{-k}^* + h.c.},$$

on $c_k^\# = \begin{pmatrix} a_k^\# \\ b_k^\# \end{pmatrix}$ has the following action

$$T^* c_k T = \tau_k c_k + \sigma_k c_{-k}^*$$

where $\tau_k = \cosh\left(\frac{1}{2} S_k\right)$ and $\sigma_k = \sinh\left(\frac{1}{2} S_k\right) \quad \Rightarrow$

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Number on the state

Introducing

$$\gamma_k := \sigma_k^2 = \langle c_k^* \otimes c_k \rangle_\Psi, \qquad \alpha_k := \tau_k \sigma_k = \langle c_k \otimes c_{-k} \rangle_\Psi,$$

with

$$\gamma_k = \begin{pmatrix} \gamma_k^{AA} & \gamma_k^{AB} \\ \gamma_k^{BA} & \gamma_k^{BB} \end{pmatrix}, \qquad \alpha_k = \begin{pmatrix} \alpha_k^{AA} & \alpha_k^{AB} \\ \alpha_k^{BA} & \alpha_k^{BB} \end{pmatrix}.$$

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We choose the parameters N_0^A, N_0^B such that

$$N_A = N_0^A + \sum_{k \neq 0} \gamma_k^{AA}, \qquad N_B = N_0^B + \sum_{k \neq 0} \gamma_k^{BB},$$

which gives the right **numbers**

$$\langle \Psi, \mathcal{N}_A \Psi \rangle = N_A, \qquad \langle \Psi, \mathcal{N}_B \Psi \rangle = N_B.$$

Calculation of the quadratic form

We have

$$\langle \Psi, \mathcal{H}\Psi \rangle = \frac{1}{2|\Omega|}(N_A^2 \widehat{v}_A(0) + 2N_A N_B \widehat{v}_{AB}(0) + N_B^2 \widehat{v}_B(0)) + \mathscr{F}(\alpha, \gamma)$$

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where

$$\begin{aligned}\mathscr{F}(\alpha, \gamma) := \sum_{k \neq 0} \Big(k^2 + \frac{N_{0,A}}{|\Omega|}\widehat{v}_A(k)\Big)\gamma_k^{AA} + \Big(k^2 + \frac{N_{0,B}}{|\Omega|}\widehat{v}_B(k)\Big)\gamma_k^{BB} \\ + \sum_{k \neq 0} \frac{N_{0,A}}{|\Omega|}\widehat{v}_A(k)\alpha_k^{AA} + \frac{N_{0,A}}{|\Omega|}\widehat{v}_B(k)\alpha_k^{BB} \\ + \sum_{k \neq 0} 2\frac{\sqrt{N_{0,A}N_{0,B}}}{|\Omega|}\widehat{v}_{AB}(k)(\gamma_k^{AB} + \alpha_k^{AB}) + \mathcal{D}(\alpha, \alpha) + \mathcal{D}(\gamma, \gamma)\end{aligned}$$

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Problem to get correct 2nd order constant: change $\widehat{v}(k) \mapsto \widehat{g}(k)$

Solved by soft potentials (needed only same rate) η

.

Renormalized quadratic form

$$\langle \Psi, \mathcal{H}\Psi \rangle \simeq \frac{1}{2|\Omega|}\left(N_A^2 \widehat{g}_A(0) + 2N_A N_B \widehat{g}_{AB}(0) + N_B^2 \widehat{g}_B(0)\right) + \mathcal{K}^{\mathrm{Bog}}$$

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Recall that $\gamma_k = \langle c_k^* \otimes c_k \rangle_\Psi, \quad \alpha_k = \langle c_k \otimes c_{-k} \rangle_\Psi,$

$$\begin{aligned} \mathcal{K}^{\mathrm{Bog}} &= \left\langle \Psi, \sum_{k \neq 0} c_k^* \cdot \mathcal{A}_k c_k + \frac{1}{2}\left(c_k \cdot \mathcal{B}_k c_k + h.c.\right) \Psi \right\rangle \\ &= \left\langle \Psi, \sum_{k \neq 0} d_k^* \cdot \mathcal{D}_k d_k \Psi \right\rangle - \text{(desired 2nd order and constant)} \end{aligned}$$

where $d_k := c_k + \beta_k c_{-k}^*$ and $\mathcal{D}_k \geq 0$.

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$$d_k \Psi = 0 \qquad \Leftrightarrow \qquad S_k = \log((1+\beta_k)^{-1}(1-\beta_k)).$$

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$$S_k \quad \rightsquigarrow \quad \sigma_k, \tau_k \quad \rightsquigarrow \quad \alpha, \gamma \quad \rightsquigarrow \quad \Psi$$

Sketch of the Proof: Lower bound

Strategy for the Lower Bound

- We only need v_{AB} soft for right LHY constant (weak potential satisfies the assumptions).
- v_A, v_B can just be L^1.
- Neumann localization in small boxes: quad $E(\Omega) \to E(\Lambda), \quad \Omega = \bigcup_j \Lambda_j$.

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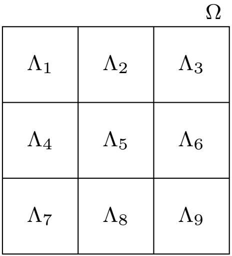

$$\Omega = [-L/2, L/2]^3 = \bigcup_{j=1}^{M} \Lambda_j$$

$$\Lambda = [-\ell/2, \ell/2]^3$$

$$(\rho a)^{-1/2} \ll \ell \ll L$$

$E_{n,m}(\Lambda) =$ GSE for $H_{n,m}$ on Λ with Neumann b.c.

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Ω

Λ_1	Λ_2	Λ_3
Λ_4	Λ_5	Λ_6
Λ_7	Λ_8	Λ_9

$$\Omega = [-L/2, L/2]^3 = \bigcup_{j=1}^{M} \Lambda_j$$

$$\Lambda = [-\ell/2, \ell/2]^3$$

$$\boxed{\frac{1}{L^3} E_{N_A,N_B}(\Omega) \geq \frac{1}{\ell^3} E_{n,m}(\Lambda) + \text{err.}}$$

$E_{n,m}(\Lambda) =$ GSE for $H_{n,m}$ on Λ with Neumann b.c.

- In Λ we can prove **BEC**! $\quad \langle n_+^A + n_+^B \rangle_\Psi \ll n + m$

Renormalization of the potentials

We introduce the projectors

$$P^A = \frac{1}{|\Lambda|}|1_A\rangle\langle 1_A| \otimes 1_B, \qquad Q^A = (1 - P^A) \otimes 1_B,$$
$$P^B = 1_A \otimes \frac{1}{|\Lambda|}|1_B\rangle\langle 1_B|, \qquad Q^B = 1_A \otimes (1 - P^B),$$

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$$\sum_{i<j} v_{i,j} = \sum_{i<j}(P_i + Q_i)(P_j + Q_j)(g_{i,j} - v_{i,j}\omega_{i,j})(P_j + Q_j)(P_i + Q_i)$$
$$= \mathcal{Q}_0^{\text{ren}} + \mathcal{Q}_1^{\text{ren}} + \mathcal{Q}_2^{\text{ren}} + \mathcal{Q}_3^{\text{ren}} + \mathcal{Q}_4^{\text{ren}},$$

$$\widehat{g}(0) = 8\pi a < \widehat{v}(0)$$

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$$Q_0^{\text{ren}} := \frac{1}{2}\sum_{i\neq j} P_i P_j (g + g\omega)(x_i - x_j) P_j P_i,$$

$$Q_1^{\text{ren}} := \sum_{i\neq j} \left(Q_i P_j (g + g\omega)(x_i - x_j) P_j P_i + h.c.\right),$$

$$Q_2^{\text{ren}} := \sum_{i\neq j} P_i Q_j (g + g\omega)(x_i - x_j) P_j Q_i + \sum_{i\neq j} P_i Q_j (g + g\omega)(x_i - x_j) Q_j P_i$$
$$+ \frac{1}{2}\sum_{i\neq j} P_i P_j g(x_i - x_j) Q_j Q_i + h.c.,$$

$$Q_3^{\text{ren}} := \sum_{i\neq j} P_i Q_j g(x_i - x_j) Q_j Q_i + h.c.,$$

$$Q_4^{\text{ren}} := \frac{1}{2}\sum_{i\neq j} \Pi_{ij}^* v(x_i - x_j)\Pi_{ij} \geq 0, \qquad \Pi_{ij} := Q_j Q_i + \omega(x_i - x_j)\left(P_j P_i + P_j Q_i + Q_j P_i\right).$$

Symmetrization of the potentials

$$\frac{1}{2}\sum_{i\neq j} P_i P_j g(x_i - x_j) Q_j Q_i \quad \xrightarrow{(*)} \quad \frac{1}{2}\sum_{i\neq j} P_i P_j g_{\mathsf{sym}}(x_i, x_j) Q_j Q_i$$

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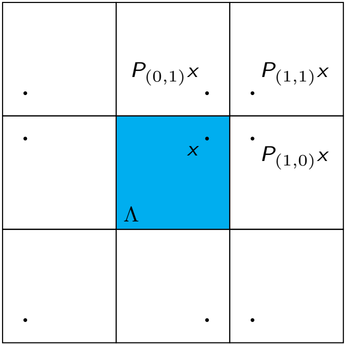

$$g_{\mathrm{sym}}(x, y) = \sum_{z\in\mathbb{Z}^3} g(P_z x - y)$$

We need to control error in $(*)$ via

$$g_v(y) \le v(x), \qquad \text{for } |y| \ge |x|$$

Diagonalization and soft pairs

- Diagonalization of matrix Bogoliubov Hamiltonian

$$\mathcal{Q}_2 \quad \to \quad \mathcal{K}^{\mathsf{Bog}} = \sum_{k\neq 0} c_k^* \cdot \mathcal{A}_k c_k + \frac{1}{2}\big(c_k \cdot \mathcal{B}_k c_k + h.c.\big)$$

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- Bound of the cubic term $\quad\to\quad$ we need softness for the right constant

$$\begin{aligned}\mathcal{Q}_3 + \mathcal{K}^{\mathrm{diag}} \quad \to \quad & \mathcal{O}((\rho a)^{5/2}(\rho \bar{a}^3)^{-2\eta}|\Lambda|(\widehat{v}_{AB}(0) - 8\pi a_{AB})) \\ & = \mathcal{O}((\rho \bar{a})^{5/2}(\rho \bar{a}^3)^{-2\eta}|\Lambda|\delta_{AB}).\end{aligned}$$

More difficult than one species! This term was not there

Point is contraction of indices

Future perspectives

- Derive the result of the Corollary (LHY-type **right constant**) without **smallness assumption** on the potential

$$(\rho_A^2 a_A^2 + 2\rho_A\rho_B a_{AB}^2 + \rho_B^2 a_B^2)^{5/4} J_{AB}$$

$$J_{AB} = \frac{1}{2(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{d}k \left(\sqrt{k^4 + 2\mu_+ k^2} + \sqrt{k^4 + 2\mu_- k^2} - \frac{1}{2k^2} - 2k^2 - (\mu_+ + \mu_-) \right)$$

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- Study what happens without miscibility condition, in the case

$$a_{AB}^2 > a_A a_B.$$

- Check if there are sensible changes for $M > 2$ components of the gas

$$\mathscr{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1,M} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,M} \\ \vdots & \vdots & \ddots & \vdots \\ a_{M,1} & a_{M,2} & \cdots & a_{M,M} \end{pmatrix}$$

Thanks for your attention!