Bose-Einstein Condensation: Bound State of Periodic Microstructure

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Workshop on **Quantum Systems: A Mathematical Journey...**
CSCAMM
University of Maryland, College Park MD
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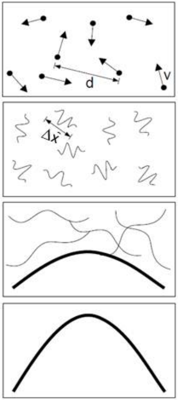
(Simplistic) Schematic of BEC concept in atomic gas

Non-interacting particles in a box (T: temperature) [Ketterle, '99]:



High T:
"billiard balls"

Low T:
Evident wave-like behavior: "wave packets"

$T=T_c$: BEC onset
"Matter wave overlap"
$\Delta x \sim d$

T=0: BE condensate
"Giant matter wave"

Main theme

Evolution of N Boson particles of repulsive interactions, $N \gg 1$:

$$H\breve{\Psi}_N(t,\vec{x}) = i\partial_t \overbrace{\breve{\Psi}_N(t,\vec{x})}^{wave\,fcn}\ ; \quad \breve{\Psi}_N(t,\cdot) \in L^2_s(\mathbb{R}^{3N})$$

$$H = \sum_{j=1}^{N}[-\triangle_j + V_e(x_j)] + \sum_{j<l} \underbrace{\mathcal{V}(x_j,x_l)}_{pos.,symm.} : \text{ Hamiltonian } (\hbar = 2m = 1)$$

Usually: $\mathcal{V}(x_i,x_j) \approx 8\pi a\,\delta(x_i - x_j)\ ;$

a: scattering length; here $a > 0$

1. What macroscopic description, *mean field limit*, **emerges**?
2. What are plausible **corrections** to this limit, $N \gg 1$?

Our focus: (2) **formally***;* **lowest bound state** *with* **microstructure**

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Review: Periodic case [Lee, Huang, Yang, 1957]

N *weakly interacting* particles in periodic box ($N \gg 1$)

- Macroscopic 1-particle state: zero momentum ("condensate")
- Many-bound ground state: Atoms are primarily scattered from 0 momentum to pairs of opposite momenta ("pair excitation")

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Heuristically by Wu, 1961; Gross, 1961; Pitaevskii, 1961; rigorously by Yau *et al.*, 2006-07

Tensor product of 1-particle states (BEC signature)

Approximate N-body wave function for Boson gas (zeroth order):

$$\breve{\Psi}_N(t,\vec{x}) \approx \breve{\Psi}_N^0[\breve{\Phi}](t,\vec{x}) = \prod_{j=1}^{N} \underbrace{\breve{\Phi}(t,x_j)}_{condensate} \ ; \quad \vec{x} = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}$$

- For **constant** sc. length and certain assumptions on interactions:

$$i\partial_t \breve{\Phi}(t,x) = [-\triangle + V_e(x) + 8\pi a|\breve{\Phi}|^2]\breve{\Phi}(t,x) \qquad \text{(Gross-Pitaevskii Eq)}$$

- **Lowest bound (ground) state:**
$\breve{\Psi}_N(t,\vec{x}) = e^{-iE_N t}\Psi_N(\vec{x})$; $\breve{\Phi}(t,x) = e^{-i\mu t}\Phi(x)$ ($\Phi : \mathbb{R}^3 \to \mathbb{R}$)

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Pair Excitation Hypothesis

(Uncontrolled) Ansatz:

$$\breve{\Psi}_N(t,\vec{x}) \propto \underbrace{e^{\mathcal{P}[\breve{K}]}}_{I+\mathcal{P}+\cdots} \breve{\Psi}_N^0[\breve{\Phi}](t,\vec{x})$$

- $\mathcal{P}[\breve{K}] = \mathcal{P}_N$: operator that describes scattering of atoms *in pairs*; $\breve{K} = \breve{K}(t,x,y)$ is **pair collision kernel** ("pair excitation function")
- $\breve{K}(t,x,y)$ is not known a priori; obeys integro-PDE.
- $\mathcal{P}$ induces partial depletion to condensate (Φ)
- $\breve{K}(t,x,y) = \breve{K}(t,y,x)$ (without loss of generality)
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In this talk:

$$H = \sum_{j=1}^{N} [-\Delta_j + V_e(x_j)] + \frac{1}{2}\sum_{i \neq j} \mathcal{V}(x_i, x_j)\ ;\ V_e > 0,\ \text{smooth}\ ;\ V_e(x) \to \infty\ |x| \to \infty$$

- Heuristically introduce spatially varying scattering length:

$$\mathcal{V}(x_i, x_j) = g^\epsilon(x_i)\delta(x_i - x_j)\ ;\ g^\epsilon(x) := 8\pi \overbrace{a^\epsilon(x)}^{sc.\ lgth} = g_0[1 + \overbrace{A(x/\epsilon)}^{\substack{1-\text{periodic};\\ smooth;\langle A\rangle = 0}}\ ] > 0$$

- For **lowest bound state**: derive PDEs for Φ, K.
- Apply: classical homogenization up to two orders in ϵ;
- (singular) perturbations for slowly varying **trap**, $V_e(x) = U(\breve{\epsilon}x)$.
- Describe **depletion** of Φ. Will show:

$$\text{(Fraction at } \Phi)\ \xi \sim 1 - c\int_{\mathfrak{R}_0} dx\, [\underbrace{\mu_0^0}\ - U(x)]^{3/2} + \epsilon^2 f[U]\, \|A\|^2_{H_{av}^{-1}}$$

μ_0^0: lowest chem. pot./particle; $H_{av}^{-1} = \{f \in H^{-1}(\mathbb{T}^3)\ |\ \langle f\rangle = 0\}$

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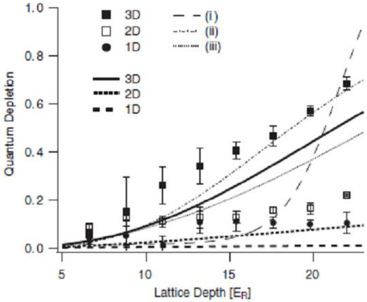
Pair excitation *and* varying scattering length. Why?

- Experimental efforts to study quantum depletion in atomic gases [Cornell, Ensher, Wieman, 1999; Ketterle, Durfee, Stamper-Kurn, 1999; Xu et al., 2006].
- Modification of interactions in atomic gas, e.g., by controlling scattering length via external fields [Claussen et al., 2003; Cornish et al., 2000; Inouye et al., 1998; Stenger et al., 1998; Xu et al., 2006]
- Related theoretical work on bound states for *focusing* (attractive interactions) NLS by Fibich, Sivan and Weinstein [2006] via classical homogenization

Motivation: Condensate depletion

Quantum depletion of ^{23}Na BECondensate [Xu et al, 2006]



Depletion seems to be enhanced by manipulation of ext. potential

Results: I. Consistency of pair excitation hypothesis with many-body dynamics

Proposition 1 [DM, 2012] (Lowest bound state; varying sc. length)

The condensate wave function obeys:

$$\mathcal{L}[\Phi]\Phi(x) := [-\triangle_x + V_e(x) + g(x)\Phi^2 - \underbrace{\mu}_{\text{lowest}}]\Phi(x) = 0\,; \quad N^{-1}\|\Phi\|^2_{L^2(\mathbb{R}^3)} = 1$$

The pair collision kernel $K(x,y)$ satisfies

$$\{\mathcal{L}[\Phi](x) + \mathcal{L}[\Phi](y) + [g(x)\Phi(x)^2 + g(y)\Phi(y)^2]\}K(x,y)$$
$$+ \underbrace{\int_{\mathbb{R}^3} \mathrm{d}z\, g(z)\Phi(z)^2\, K(x,z)\, K(y,z)} = -g(x)\Phi(x)^2\delta(x-y)$$

Addendum: Elements of bosonic Fock space, $\mathbb{F} = \mathbb{C} \oplus \bigoplus_{n\geq 1} \left(L^2(\mathbb{R}^3)\right)^{\otimes_s n}$

- Elements of $\mathbb{F}$: $\upsilon = \{\upsilon^{(n)}\}_{n\geq 0}$ where $\upsilon^{(0)} \in \mathbb{C}$, $\upsilon^{(n)} \in L^2_s(\mathbb{R}^{3n})$ are **symm.** in $x_1, \ldots, x_n$. Hilbert space structure: $\langle \upsilon, \chi\rangle_{\mathbb{F}} = \sum_{n\geq 0} \int_{\mathbb{R}^{3n}} \upsilon^{(n)}(x)\chi^{(n)*}(x)\mathrm{d}x$.

Creation (annihilation) operator a_f^* (a_f): creates (destroys) particle at state f:

$$(a_f^* \upsilon)^{(n)}(\vec{x}_n) = n^{-1/2}\sum_{j=1}^{n} f(x_j)\upsilon^{(n-1)}(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_n)\ ,$$

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$$\Rightarrow [a_f, a_f^*] = a_f a_f^* - a_f^* a_f = 1$$

- Operator-valued distributions, $\psi^*(x)$ and $\psi(x)$, $x \in \mathbb{R}^3$:

$$a_f^* =: \int \mathrm{d}x f(x)\,\psi^*(x)\ , \qquad a_f =: \int \mathrm{d}x f^*(x)\,\psi(x)$$

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$$\Rightarrow [\psi(x), \psi^*(y)] = \delta(x-y)\mathbf{1}\,,\ [\psi^*(x), \psi^*(y)] = [\psi(x), \psi(y)] = 0$$

Sketch of (formal) proof of Proposition 1

- Hamiltonian, $\mathcal{H} : \mathbb{F} \to \mathbb{F}$:

$$\mathcal{H} = \int \mathrm{d}x\, \psi^*(x)[-\Delta_x + V_e(x)]\psi(x) + \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\, \psi^*(x)\psi^*(y) \overbrace{\mathcal{V}(x,y)}^{g(x)\delta(x-y)} \psi(y)\psi(x)$$

- Perturbation scheme: Field operator **splitting**:

$$\psi(x) = N^{-1/2} \underbrace{\Phi(x) a_\Phi}_{\text{condensate}} + \underbrace{\psi_1(x)}_{\langle \Psi_N, \mathcal{N}_1 \Psi_N\rangle_{\mathbb{F}} \ll N} \;;\; (\Phi, \psi_1) = 0,\; \mathcal{N}_1 = \int \psi_1^*(x)\psi_1(x)\,\mathrm{d}x$$

- N-body Schrödinger eq. and pair excitation ansatz [Wu, 1961]:

$$\mathcal{H}\Psi_N = E_N \Psi_N \;;\; \Psi_N \propto e^{\mathcal{P}[K]} \underbrace{\Psi_N^0[\Phi]}_{\text{tensor prod. of } \Phi} \in \mathbb{F};\quad N = \langle \Psi_N, \int \psi^*(x)\psi(x)\Psi_N \rangle$$

- Pair excitation operator:

$$\mathcal{P}[K] = (2N)^{-1} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \mathrm{d}x\,\mathrm{d}y \underbrace{\psi_1^*(x)\psi_1^*(y)}_{\text{creates 2 part.@ states} \perp \Phi} K(x,y) \underbrace{a_\Phi^2}_{\text{annih. 2 part.@ } \Phi}$$

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- **Scheme**: keep up to terms *quadratic* in ψ_1, ψ_1^* in $\mathcal{H}$. Enforce Schr. eq. □

Results: II. Homogenization

Governing (elliptic) PDEs:

$$\mathcal{L}_x[\Phi^\epsilon]\Phi^\epsilon := [-\triangle_x + V_e(x) + g^\epsilon(x)(\Phi^\epsilon)^2 - \mu^\epsilon]\Phi^\epsilon(x) = 0\,, \quad N^{-1}\|\Phi^\epsilon\|_{L^2}^2 = 1\,;$$

$$\{\mathcal{L}_x[\Phi^\epsilon] + \mathcal{L}_y[\Phi^\epsilon] + [g^\epsilon(x)\Phi^\epsilon(x)^2 + g^\epsilon(y)\Phi^\epsilon(y)^2]\}K^\epsilon(x,y)$$
$$+ \int \mathrm{d}z\, g^\epsilon(z)\Phi^\epsilon(z)^2\, K^\epsilon(x,z)\, K^\epsilon(y,z) = -g^\epsilon(x)\Phi^\epsilon(x)^2\delta(x-y)\,.$$

Periodic microstructure:

$$g^\epsilon(x) = g_0[1 + A(x/\epsilon)]\,.$$

Seek (formally) two-scale expansions for $\Phi^\epsilon(x)$, $K^\epsilon(x,y)$:

$$\Phi^\epsilon(x) = \Phi_0(x,\tilde{x}) + \epsilon\Phi_1(x,\tilde{x}) + \epsilon^2\Phi_2(x,\tilde{x}) + \ldots\,, \quad \tilde{x} = x/\epsilon;$$

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Results: II. Homogenization (Continued)

Proposition 2.1 [DM, 2012] (Classical period. homogen. for Φ^ϵ)

The coefficients of two-scale expansion for Φ^ϵ read

$$\Phi_0(x,\tilde{x}) = f_0(x), \quad \Phi_1(x,\tilde{x}) = 0,$$
$$\Phi_2(x,\tilde{x}) = g_0 f_0(x)^3 \, [\triangle_{\tilde{x}}^{-1} A(\tilde{x})] + f_2(x);$$

$$\mathcal{L}_{0,x}[f_0]f_0 := [-\triangle_x + V_e(x) + g_0 f_0(x)^2 - \mu_0] f_0(x) = 0 \,, \; N^{-1}\|f_0\|_{L^2}^2 = 1 \,,$$

$$\mathcal{L}_{2,x} f_2 := [\mathcal{L}_{0,x}[f_0] + 2 g_0 f_0(x)^2] f_2(x) = 3 g_0^2 f_0^5 \|A\|_{H_{av}^{-1}}^2 + \mu_2 f_0 \,, \; \langle f_0, f_2 \rangle = 0;$$

$$\mu_0 = \zeta_0 + \zeta_{\triangle 0} + \zeta_{e0}, \; \mu_1 = 0, \; \mu_2 = -3 g_0^2 \, \|A\|_{H_{av}^{-1}}^2 \, \frac{\langle f_0, \mathcal{L}_2^{-1} f_0^5 \rangle}{\langle f_0, \mathcal{L}_2^{-1} f_0 \rangle};$$

where $\zeta_0 = g_0 N^{-1} \|f_0^2\|_{L^2}^2$, $\zeta_{\triangle 0} = N^{-1} \|\nabla f_0\|_{L^2}^2$, $\zeta_{e0} = N^{-1} \langle f_0, V_e f_0 \rangle$.

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Results: II. Homogenization (Cont.)

Proposition 2.2 [DM, 2012] (Classical periodic homogenization for K^ϵ)

Coefficients in two-scale expansion for K^ϵ:

$$K_0(x,y,\tilde{x},\tilde{y}) = \kappa_0(x,y), \quad K_1(x,y,\tilde{x},\tilde{y}) = 0\ ,$$
$$K_2(x,y,\tilde{x},\tilde{y}) = 2g_0[(\triangle_{\tilde{x}}^{-1}A(\tilde{x}))f_0(x)^2 + (\triangle_{\tilde{y}}^{-1}A(\tilde{y}))f_0(y)^2]\kappa_0 + \kappa_2(x,y);$$

$$\mathcal{L}_{(xy)}\kappa_0 := \{\mathcal{L}_{0,x}[f_0] + \mathcal{L}_{0,y}[f_0] + g_0[f_0(x)^2 + f_0(y)^2]\}\kappa_0(x,y)$$
$$= -\mathcal{C}[f_0^2;\kappa_0]\kappa_0(x,y) + B_0(x,y)\ ; \quad B_0(x,y) = -g_0f_0(x)^2\delta(x-y)\ ;$$
$$\mathcal{L}_{(xy)}\kappa_2 = -2\mathcal{C}[f_0^2;\kappa_0]\kappa_2(x,y) + B_2[f_0,f_2](x,y)\ ;$$

$$\mathcal{C}[f;\kappa]\ell(x,y) := \tfrac{1}{2}g_0\int \mathrm{d}z\, f(z)\,[\kappa(x,z)\ell(y,z) + \ell(x,z)\kappa(y,z)]\ ,$$

$$\begin{aligned}
B_2(x,y) \;=\;& 2g_0\left[3g_0\|A\|^2_{H_{av}^{-1}}f_0(x)^4 - f_0(x)f_2(x)\right]\delta(x-y) + \{2Z_2 \\
&+9g_0^2\|A\|^2_{H_{av}^{-1}}[f_0(x)^4 + f_0(y)^4] - 4g_0[f_0(x)f_2(x) + f_0(y)f_2(y)]\}\kappa_0 \\
&-2\mathcal{C}[f_0f_2,\kappa_0]\kappa_0 + 6g_0\,\|A\|^2_{H_{av}^{-1}}\,\mathcal{C}[f_0^4,\kappa_0]\kappa_0, \\
Z_2 \;=\;& N^{-1}g_0\left[2\langle f_0^3,f_2\rangle - 3g_0\,\|A\|^2_{H_{av}^{-1}}\,\|f_0^3\|^2_{L^2}\right]\ .
\end{aligned}$$

Results: II. Homogenization (Cont.)

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Coefficients in two-scale expansion for K^ϵ:

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$$\mathcal{L}_{(xy)}\kappa_2 = -2\mathcal{C}[f_0^2;\kappa_0]\kappa_2(x,y) + B_2[f_0,f_2](x,y)\,;$$

$$\mathcal{C}[f;\kappa]\ell(x,y) := \tfrac{1}{2}g_0\int \mathrm{d}z\,f(z)\,[\kappa(x,z)\ell(y,z) + \ell(x,z)\kappa(y,z)]\,,$$

$$B_2(x,y) = 2g_0\left[3g_0\|A\|^2_{H_{av}^{-1}}f_0(x)^4 - f_0(x)f_2(x)\right]\delta(x-y) + \{2Z_2$$
$$+9g_0^2\|A\|^2_{H_{av}^{-1}}[f_0(x)^4 + f_0(y)^4] - 4g_0[f_0(x)f_2(x) + f_0(y)f_2(y)]\}\kappa_0$$
$$-2\mathcal{C}[f_0f_2,\kappa_0]\kappa_0 + 6g_0\,\|A\|^2_{H_{av}^{-1}}\,\mathcal{C}[f_0^4,\kappa_0]\kappa_0,$$
$$Z_2 = N^{-1}g_0\left[2\langle f_0^3, f_2\rangle - 3g_0\,\|A\|^2_{H_{av}^{-1}}\,\|f_0^3\|^2_{L^2}\right].$$

Results: II. Homogenization (Cont.)

Proposition 2.2 [DM, 2012] (Classical periodic homogenization for K^ϵ)

Coefficients in two-scale expansion for K^ϵ:

$$K_0(x,y,\tilde{x},\tilde{y}) = \kappa_0(x,y), \quad K_1(x,y,\tilde{x},\tilde{y}) = 0\,,$$
$$K_2(x,y,\tilde{x},\tilde{y}) = 2g_0[(\triangle_{\tilde{x}}^{-1}A(\tilde{x}))f_0(x)^2 + (\triangle_{\tilde{y}}^{-1}A(\tilde{y}))f_0(y)^2]\kappa_0 + \kappa_2(x,y);$$

$$\mathcal{L}_{(xy)}\kappa_0 := \{\mathcal{L}_{0,x}[f_0] + \mathcal{L}_{0,y}[f_0] + g_0[f_0(x)^2 + f_0(y)^2]\}\kappa_0(x,y)$$
$$= -\mathcal{C}[f_0^2;\kappa_0]\kappa_0(x,y) + B_0(x,y)\,; \quad B_0(x,y) = -g_0 f_0(x)^2\delta(x-y)\,;$$
$$\mathcal{L}_{(xy)}\kappa_2 = -2\mathcal{C}[f_0^2;\kappa_0]\kappa_2(x,y) + B_2[f_0,f_2](x,y)\,;$$

$$\mathcal{C}[f;\kappa]\ell(x,y) := \tfrac{1}{2}g_0\int \mathrm{d}z\, f(z)\,[\kappa(x,z)\ell(y,z) + \ell(x,z)\kappa(y,z)]\,,$$

$$\begin{aligned}
B_2(x,y) \;&=\; 2g_0\left[3g_0\|A\|^2_{H_{av}^{-1}}f_0(x)^4 - f_0(x)f_2(x)\right]\delta(x-y) + \{2Z_2\\
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&\quad -2\mathcal{C}[f_0f_2,\kappa_0]\kappa_0 + 6g_0\,\|A\|^2_{H_{av}^{-1}}\,\mathcal{C}[f_0^4,\kappa_0]\kappa_0,\\
Z_2 \;&=\; N^{-1}g_0\left[2\langle f_0^3, f_2\rangle - 3g_0\,\|A\|^2_{H_{av}^{-1}}\,\|f_0^3\|^2_{L^2}\right].
\end{aligned}$$

Remarks on (formal) proof of Proposition 2

- Need "compatibility condition" on terms up to $\mathcal{O}(\epsilon^4)$ (see Lemma 1 below) [Bensoussan, Lions, Papanicolaou, 1978].
- **Difficulty:** Nonlocal term in PDE for K (see Lemmas 2, 3).
- Two-scale convergence is **not** addressed.

(Formal) Proof of Proposition 2: Useful lemmas

By substitution of expansions in PDEs, obtain cascade of equations:

$$-\Delta_{\tilde{x}} u = S(\tilde{x})$$

Lemma 1 (Implication of Fredholm alternative)

The equation $-\Delta_{\tilde{x}} u = S(\tilde{x})$, where $S(\tilde{x})$ is (1-)periodic, admits a (1-)periodic solution $u(\tilde{x})$ only if $\langle S \rangle = 0$ (**compatibility condition**). Then, $u(\tilde{x}) = (-\Delta_{\tilde{x}})^{-1} S(\tilde{x}) + c$.

In nonlocal term for K, some averaging is needed:

Lemma 2 (Asymptotics for nonlocal term. Part I.)

If $P(\tilde{x})$ is 1-periodic with $P \in L^\infty(\mathbb{R}^d)$ and $\langle P \rangle = 0$, and $h \in W^{m,1}(\mathbb{R}^d)$ with vanishing derivatives at ∞, then

$$\int_{\mathbb{R}^d} P\left(\frac{x}{\epsilon}\right) h(x)\, dx = \mathcal{O}(\epsilon^m)\ ;\ m = 1, 2, \ldots\ (\epsilon \downarrow 0)$$

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A few useful lemmas (cont.)

Lemma 3 (Refinement of Lemma 2 via Fourier Transform)

Consider the 1-periodic P where $P \in L^2(\mathbb{T}^d)$ and $\langle P \rangle = 0$, and $h \in L^2(\mathbb{R}^d)$. Suppose $e^{i\lambda\cdot x_0}\widehat{h}(\lambda) = c_1\,\lambda^{-2s} + o(|\lambda|^{-2s})$ as $|\lambda| \to \infty$, $\lambda \in \mathbb{R}^d$, for some $s > d/4$, $x_0 \neq 0$. Then,

$$\int_{\mathbb{R}^d} P\left(\frac{x}{\epsilon}\right) h(x)\,\mathrm{d}x = c_1\,\epsilon^{2s}\,[(-\Delta)^{-s}P](x_0/\epsilon) + o(\epsilon^{2s}) \quad \text{as } \epsilon \downarrow 0\,.$$

In the above, $P(\tilde{x}) \equiv \partial_{\tilde{x}}^{-\alpha} A(\tilde{x})$.

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Slow-varying trap: Classical solution for Φ_n

Assume $V_e(x) = U(\breve{\epsilon}x)$, $\breve{\epsilon} \ll \epsilon$.
Apply heuristics for Φ_n via boundary layer theory

I. Zeroth-order homog. soln., $f_0(x)$. $x \mapsto \breve{x} = \breve{\epsilon}x$, $\phi_0(\breve{x}) := f_0(\breve{x}/\breve{\epsilon})$,

$$[-\breve{\epsilon}^2 \triangle_x^2 + U(x) + g_0\phi_0^2 - \mu_0]\phi_0(x) = 0; \quad \int \phi_0(x)^2\,\mathrm{d}x = \breve{\epsilon}^3 N = 1$$

- Outer solution (for $\breve{\epsilon} = 0$), $\phi_0(x) \sim \phi_0^0(x)$:

$$\phi_0^0(x) = \begin{cases} g_0^{-1/2}\sqrt{\mu_0^0 - U(x)} & x \in \mathfrak{R}_0^\delta \\ 0 & x \in \mathfrak{R}_0^{c,\delta} \end{cases};$$

$$\mathfrak{R}_0^\delta := \mathfrak{R}_0 \setminus \mathfrak{B}(\partial\mathfrak{R}_0, \delta),\ \mathfrak{R}_0^c = \mathbb{R}^3 \setminus \mathfrak{R}_0;\ \mathfrak{R}_0 := \{x \in \mathbb{R}^3 \mid U(x) < \mu_0^0\}$$

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Slowly-varying trap: Classical solutions for Φ_n (cont.)

ϕ_0^0 is not H^1_{loc} near $\partial\mathfrak{R}_0$: Boundary layer

- Inner solution (near $\partial\mathfrak{R}_0$), $\phi_0^{in}(\eta)$:

By $U(x) = U(x_{bd}) + \Upsilon\, \nu \cdot (x - x_{bd}) + o(|x - x_{bd}|)$, fixed $x_{bd} \in \partial\mathfrak{R}_0$:

$$[-\partial_\eta^2 + \eta + (\phi_0^{in})^2]\phi_0^{in} = 0\,;\ \eta := \left(\frac{\Upsilon}{\breve{\epsilon}^2}\right)^{1/3} \nu \cdot (x - x_{bd})\,,\ \phi_0^{in} := \frac{g_0^{1/2}}{(\breve{\epsilon}\Upsilon)^{1/3}}\phi_0$$

Apply matching $\phi_0^{in} \to 0$ as $\eta \to \infty$; $\phi_0^{in} \sim \sqrt{-\eta}$ as $\eta \to -\infty$
$\Rightarrow \phi_0^{in}(\eta) = P_{II}(\eta)$: case of 2nd Painlevé transcendent [DM, '00]

Slowly varying trap: Classical solutions for Φ_n (cont.)

II. Next-order homogenized soln.,

$\Phi_2(x,\tilde{x}) = g_0 f_0(x)^3 \, [\triangle_{\tilde{x}}^{-1} A(\tilde{x})] + f_2(x)$; $\phi_2(x) := f_2(x/\breve{\epsilon})$

- Outer solution, $\phi_2^0(x)$:

$$\phi_2^0(x) = g_0^{-1/2} \{ \tfrac{3}{2} [\mu_0^0 - U(x)]^{3/2} ||A||^2_{H_{av}^{-1}} + \tfrac{1}{2} \mu_2^0 [\mu_0^0 - U(x)]^{-1/2} \}$$

if $x \in \mathfrak{R}_0^\delta$; $\phi_2^0(x) = 0$ if $x \in \mathfrak{R}_0^{c,\delta}$.

$$\mu_2 \sim \mu_2^0 = -3 ||A||^2_{H_{av}^{-1}} |\mathfrak{R}_0|^{-1} \int_{\mathfrak{R}_0} [\mu_0^0 - U(x)]^2 \, \mathrm{d}x$$

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Slowly varying trap: Classical solutions for Φ_n (cont.)

Boundary layer near $\partial\mathfrak{R}_0$

- Inner solution (near $\partial\mathfrak{R}_0$), $\phi_2^{in}(\eta)$

$$[\partial_\eta^2 - \eta - 3P_{II}(\eta)^2]\phi_2^{in}(\eta) = P_{II}(\eta)\,; \quad \phi_2^{in} := -(\mu_2^0)^{-1} g_0^{1/2} (U_o\breve{\epsilon})^{1/3}\phi_2\,,$$

where by **matching** with outer solution:

$$\phi_2^{in}(\eta) \to 0 \quad \text{as } \eta \to \infty\,, \quad \phi_2^{in}(\eta) \sim -\tfrac{1}{2}(-\eta)^{-1/2} \quad \text{as } \eta \to -\infty\,.$$

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Slowly-varying trap: Classical solutions for K_n

Because of $\delta(x-y)$-forcing, K depends on $x-y$ if $V_e \approx$ const.
Transform to center of mass: $(x,y) \mapsto (x_\#, X) = (x-y, \frac{x+y}{2})$
Apply FT in $x_\#$; boundary-layer theory in X.

I. Zeroth-order homg. kernel, $\kappa_0(x,y)$: Let $X \mapsto \check{X} = \check{\epsilon} X$: slow; $x_\# = \mathcal{O}(1)$; define $\mathfrak{K}_0(x_\#, \check{X}) := \kappa_0(\check{X}/\check{\epsilon} + x_\#/2, \check{X}/\check{\epsilon} - x_\#/2)$.
Apply FT in $x_\#$; dual variable is $\lambda \in \mathbb{R}^3$.

Outer solution, $\mathfrak{K}_0^0(x_\#, X)$.

$$\widehat{\mathfrak{K}}_0^0(\lambda, X) = \frac{-\lambda^2 - \lambda_0(X)^2 + \sqrt{[\lambda^2 + \lambda_0(X)^2]^2 - g_0^2 \phi_0^0(X)^4}}{g_0 \phi_0^0(X)^2};$$

$\lambda_0(X)^2 := U(X) + 2g_0\phi_0^0(X)^2 - \mu_0^0$; $X \in \mathbb{R}^3 \setminus \mathfrak{B}(\partial\mathfrak{R}_0, \delta)$, $\delta = \mathcal{O}(\check{\epsilon}^{2/3})$.
Inversion: Lommel's fcns.
Inner solution, $X \in \mathfrak{B}(\partial\mathfrak{R}_0, \delta)$. Obtain ODE near $\partial\mathfrak{R}_0$; λ is parameter [DM, 2012]

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Inner solution, $X \in \mathfrak{B}(\partial\mathfrak{R}_0, \delta)$. Obtain ODE near $\partial\mathfrak{R}_0$; λ is parameter [DM, 2012]

Application: Partial depletion of Φ

Fraction of particles **out** of Φ (depletion fraction) [Wu, 1961; DM, 2011]:

$$\xi^{\epsilon}_{\mathrm{sc}} = \langle \Psi^{\epsilon}_N, (\psi_1^* \psi_1 / N)\Psi^{\epsilon}_N \rangle_{\mathbb{F}} = N^{-1} \mathrm{tr}\mathcal{W}^{\epsilon} \ ; \quad 0 < \xi^{\epsilon}_{\mathrm{sc}} \ll 1;$$

$\mathcal{W}^{\epsilon} := \mathcal{W}^{\epsilon}_1 (1 - \mathcal{W}^{\epsilon}_1)^{-1}$, $\mathcal{W}^{\epsilon}_1 := \mathcal{K}^{\epsilon *}\mathcal{K}^{\epsilon}$, and $\mathcal{K}^{\epsilon}$ has repr. $K^{\epsilon}(x, y)$.

Proposition 3 (Depletion fraction under slowly varying trap) [DM, 2012]

If $g(x) = g_0[1 + A(x/\epsilon)]$ and $V_e(x) = U(\breve{\epsilon}x)$, the depletion fraction is

$$\begin{aligned} \xi_{\mathrm{sc}} \quad \sim \quad & \frac{\sqrt{2}}{12\pi^2} \int_{\mathfrak{R}_0} \mathrm{d}x \, [\mu_0^0 - U(x)]^{3/2} \\ & - \epsilon^2 \frac{3\sqrt{2}}{8\pi^2} \|A\|^2_{H^{-1}_{av}} \int_{\mathfrak{R}_0} \{ g_0^2 \phi_0^0(x)^4 \\ & + |\mathfrak{R}_0|^{-1} \|g_0(\phi_0^0)^2\|^2_{L^2} \} [g_0 \phi_0^0(x)^2]^{1/2} \, \mathrm{d}x \quad \text{as } \epsilon, \ \breve{\epsilon} \downarrow 0, \ \breve{\epsilon}/\epsilon \downarrow 0 \, . \end{aligned}$$

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$$\xi_{\rm sc}^{\epsilon} = \langle \Psi_N^{\epsilon}, (\psi_1^* \psi_1/N)\Psi_N^{\epsilon}\rangle_{\mathbb{F}} = N^{-1}{\rm tr}\mathcal{W}^{\epsilon}\ ; \quad 0 < \xi_{\rm sc}^{\epsilon} \ll 1;$$

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Proposition 3 (Depletion fraction under slowly varying trap) [DM, 2012]

If $g(x) = g_0[1 + A(x/\epsilon)]$ and $V_e(x) = U(\breve{\epsilon}x)$, the depletion fraction is

$$\xi_{\rm sc} \sim \frac{\sqrt{2}}{12\pi^2}\int_{\mathfrak{R}_0} {\rm d}x\,[\mu_0^0 - U(x)]^{3/2} - \epsilon^2 \frac{3\sqrt{2}}{8\pi^2}\|A\|^2_{H_{av}^{-1}} \int_{\mathfrak{R}_0} \{g_0^2\phi_0^0(x)^4 + |\mathfrak{R}_0|^{-1}\|g_0(\phi_0^0)^2\|^2_{L^2}\}[g_0\phi_0^0(x)^2]^{1/2}\,{\rm d}x \quad \text{as } \epsilon,\ \breve{\epsilon}\downarrow 0,\ \breve{\epsilon}/\epsilon \downarrow 0\,.$$

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Remarks on formula for depletion fraction, ξ_{sc}

- Interplay of external potential and spatial variation of scattering length.
- Depletion fraction, ξ_{sc}, can be enhanced via external potential.
- For fixed ϵ: Spatial (periodic) variation of scattering length causes *reduction* of the ξ_{sc} solely due to pair excitation.
- Decreasing oscillations of scattering length (i.e., increasing ϵ) can cause decrease of ξ_{sc}.

Epilogue: Pending issues

- Rigorous analysis/justification for many-body wave function of pair excitation?
  On the basis of recent work [Grillakis, Machedon, DM, 2010] for $V_e = 0$, one may expect (with a trap):
  $$||\Psi_{N,\mathrm{ex}} - \Psi_{N,\mathrm{pair}}||_{L^2(\mathbb{R}^{3N})} \leq C(t) N^{-1/2},$$
  $C(t)$: bounded locally in time.
- In our program, subscale ϵ of scattering length is assumed.
  What may be the physical origin of such ϵ?
  Derivation of spatial variation of a, as an emergent concept when $N \to \infty$?
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  Modified equation of motion for Φ via pair excitation?

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- What is the appropriate macroscopic description for finite but "small" temperatures (below the phase transition point)?

Complication: Particles are distributed over thermally excited states. In addition to Φ and K, one must use $\{\phi_j\}_{j=1}^{\infty}$, 1-particle excitation wave functions.

Coupled PDEs for $\Phi(x)$, $\phi_j(x)$ ($j = 1, 2, \ldots$):

$$\mu\Phi(x) = [-\triangle + V_e(x) + \nu g(x)|\Phi(x)|^2 + 2g(x)\varrho_n(x)]\Phi(x),$$

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