Ground states of Bose-Einstein condensate with higher order interaction

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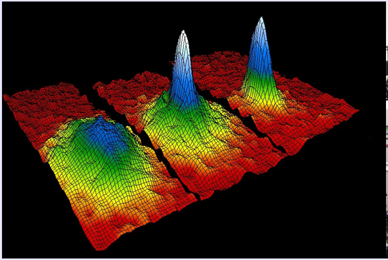
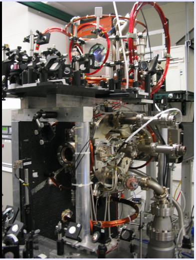
Bose-Einstein Condensation

- Bose-Einstein condensation (BEC) is a state where the bosons collapse into the lowest quantum state near temperature absolute zero.
- Predicted by Satyendra Nath Bose and Albert Einstein in 1924-1925
- First experiments in 1995, *Science 269 (E. Cornell and C. Wieman et al., ^{87}Rb JILA), PRL 75 (Ketterle et al., ^{23}Na MIT) and PRL 75 (Hulet et al., ^{7}Li Rice).*





Mathematical model for BEC at extremely low temperature

- Quantum N-body problem
  - $3N+1$ dim linear Schrödinger equation
- Mean-field theory: weakly interacting dilute ultra cold gases
  - Gross-Pitaevskii equation (GPE): $T \ll T_c$
  - $3+1$ dim NLSE with cubic nonlinearity and external potential

Mathematical model for BEC with N identical bosons

- N-body problem: $3N+1$ dim linear Schrödinger equation

$$i\hbar\partial_t\Psi_N(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,t) = H_N\Psi_N(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,t) \text{ with}$$

$$H_N = \sum_{j=1}^{N}\left(-\frac{\hbar^2}{2m}\Delta_j + V(\mathbf{x}_j)\right) + \sum_{1\le j<k\le N} V_{\rm int}(\mathbf{x}_j-\mathbf{x}_k)$$

- Hatree anstaz: $\Psi_N(\mathbf{x}_1,\ldots,\mathbf{x}_N,t) = \prod_{j=1}^{N}\psi(\mathbf{x}_j,t), \quad \mathbf{x}_j\in\mathbb{R}^3$
- Ultracold dilute regime: $V_{\rm int}(\mathbf{x}_j-\mathbf{x}_k)\approx g\,\delta(\mathbf{x}_j-\mathbf{x}_k)$, with $g=\frac{4\pi\hbar^2 a_s}{m}$
- Ultracold dilute quantum gas: two-body interactions

$$E_N(\Psi_N) = \int_{\mathbb{R}^{3N}} \overline{\Psi}_N H_N\Psi_N\, d\mathbf{x}_1\cdots d\mathbf{x}_N \approx NE(\psi) - - - \text{Energy per particle}$$

Mathematical model for BEC

- Energy per particle: mean-field theory (Lieb et al. 00'),

$$E(\psi) = \int_{\mathbb{R}^3} \left[\frac{\hbar^2}{2m}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{Ng}{2}|\psi|^4\right] d\mathbf{x}$$

- Dynamics: (Gross, 61'; Pitaevskii, 61'; Erdös, Schlein&Yau, 10')

$$i\hbar\partial_t\psi(\mathbf{x},t) = \frac{\delta E(\psi)}{\delta\overline{\psi}} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + Ng|\psi|^2\right]\psi$$

- Proper nondimensionalization&dimension reduction GPE/NLSE

$$i\partial_t\psi = -\frac{1}{2}\nabla^2\psi + V(\mathbf{x})\psi + \beta|\psi|^2\psi,\ \mathbf{x}\in\mathbb{R}^d,\ \beta = \frac{4\pi N a_s}{x_s}.$$

Mathematical model for BEC

- Gross-Pitaevskii equation-(GPE/NLSE) by Gross 1961, Pitaevskii 1961

$$i\partial_t\psi = -\frac{1}{2}\nabla^2\psi + V(\mathbf{x})\psi + \beta|\psi|^2\psi, \quad \mathbf{x}\in\mathbb{R}^d,\ t>0$$

  - t time; $\mathbf{x}\in\mathbb{R}^d$ spatial coordinates in $d=1,2,3$ dimensions
  - $\psi(\mathbf{x},t)$: complex valued wave-function
  - $V(\mathbf{x})$: real valued external potential
  - β: dimensionless interaction constant

    $\beta>0$ repulsive; $\beta<0$ attractive

Two conservation laws

- Mass conservation

$$\|\psi(\cdot,t)\|_{L^2}^2 = \int_{\mathbb{R}^3} |\psi(x,t)|^2\, dx = \int_{\mathbb{R}^3} |\psi(x,0)|^2\, dx = \|\psi(\cdot,0)\|_{L^2}$$

- Energy conservation

$$E(\psi(\cdot,t)) := \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta|\psi|^4}{2}\right] dx = E(\psi(\cdot,0))$$

Finite size effect/shape dependence

- δ function approximation of atomic interaction potential is good for low momentum

$$V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k) = V_{\text{mf}}(\mathbf{x}_j - \mathbf{x}_k) := g_0\delta(\mathbf{x}_j - \mathbf{x}_k), \quad g_0 = \frac{4\pi\hbar^2 a_s}{m}$$

- For higher momentum (high density)–improved pseudopotential[1]

$$V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k) = V_{\text{mf}}(\mathbf{x}_j - \mathbf{x}_k) + V_{\text{hoi}}(\mathbf{x}_j - \mathbf{x}_k), \quad V_{\text{hoi}}(\mathbf{x}) = \frac{g_0 g_1}{2}\left[\delta(\mathbf{x})\nabla^2 + \nabla^2\delta(\mathbf{x})\right]$$

- $g_1 = \frac{a_s^2}{3} - \frac{a_s r_e}{2}$;
- r_e: the effective range of the two-body interactions

$$k^2 = -\nabla^2 + 4\pi a\delta(\mathbf{r})\frac{\partial}{\partial r}r - \frac{4\pi}{3}a^3\delta(\mathbf{r})\nabla^2\frac{\partial}{\partial r}r + \cdots. \quad (16)$$

Equations (12), (15), and (16) define the pseudopotential for the two-body system under consideration. It yields the exact energy and the exact wave function for $r \geq a$.

It should be pointed out that the pseudopotential derived here is not a Hermitian operator. This should not cause any misgivings since the extended wave function is not supposed to represent a wave function for any physical system. It coincides, however, with the actual wave function except for a limited region of space which is of no physical interest. The non-Hermiticity of

For spherically symmetric solutions the S-wave pseudopotential exactly replaces the boundary condition at $r=a$, so that from (12), (13), and (16) the equation

$$(\nabla^2 + k^2)\psi = \frac{4\pi}{-k\cot ka}\delta(\mathbf{r})\frac{\partial}{\partial r}(r\psi)$$

$$= 4\pi a\delta(\mathbf{r})[1 + \tfrac{1}{3}a^2\nabla^2 + \cdots]\frac{\partial}{\partial r}(r\psi) \quad (22)$$

is exactly equivalent to (17) and (18). We can be certain that a perturbation calculation based on (22) with a as

[1] Esry-Greene 99'; Collin-Massignan-Pethick, 07'; Fu-Wang-Gao, 02'; K.Huang-C.N.Yang, T.D Lee 57'

Modified GPE

- Modified Gross-Pitaevskii equation:

$$i\partial_t\psi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\psi|^2 - \delta\nabla^2|\psi|^2\right]\psi,$$

- $V(\mathbf{x})$: confinement
- β: contact interaction/ proportional to N
- δ: higher order interaction/ proportional to N
- other applications
    - ultrashort laser pulses in plasmas
    - description of the thin-film super fluid condensates
    - study of the Heisenberg ferromagnets

Normalization and energy

- Normalization (mass) conservation

$$\|\psi(\cdot,t)\|_{L^2}^2 = \int_{\mathbb{R}^3} |\psi(x,t)|^2\, dx = \int_{\mathbb{R}^3} |\psi(x,0)|^2\, dx = \|\psi(\cdot,0)\|_{L^2} = 1$$

- Energy

$$E(\psi(\cdot,t)) := \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta|\psi|^4}{2} + \frac{\delta}{2}|\nabla|\psi|^2|^2\right] dx = E(\psi(\cdot,0))$$

Mathematical studies

- Cauchy problem for Time dependent MGPE
  - global well-posedness in H^∞ (M. Poppenberg 01')
  - local well-posedness in H^s ($s \geq 2[N/2] + 2$)(M. Colin 02')
  - local well-posedness in H^s $s \geq (d+5)/2$(J. Marzuola, J. Metcalfe, D. Tataru, 12' 14')
  - numerical studies (J. Lu, J. L. Marzuola, 15')
- Time-independent MGPE
  - Standing waves/stability (M. Colin, L. Jeanjean, M. Squassina 03' 04'...)
  - existence.. (J. Liu, Y. Wang, Z. Wang 02',03'...)

Ground States in the context of BEC

- Nonconvex minimization problem

$$E(\phi_g) = \min_{\phi \in S} E(\phi), \quad S = \left\{\phi \middle| \|\phi\| = 1,\ E(\phi) < \infty \right\}$$

- Nonlinear Eigenvalue problem (Euler-Lagrange eq.)

$$\mu\phi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\phi|^2 - \delta\nabla^2|\phi|^2\right]\phi, \quad \|\phi\|_2 = 1$$

- Chemical potential μ:

$$\mu = E(\phi) + \int_{\mathbb{R}^d} \left(\frac{\beta}{2}|\phi|^4 + \frac{\delta}{2}\left|\nabla|\phi|^2\right|^2\right) d\mathbf{x}$$

Ground state, existence and uniqueness

Theorem

(i)Suppose $\delta \neq 0$ *and* $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$, *then there exists a minimizer* $\phi_g \in S$ *of if and only if* $\delta > 0$.
(2) $e^{i\theta}\phi_g$ *is also a ground state. The ground state* ϕ_g *can be chosen as non-negative* $|\phi_g|$ *and the non-negative ground state is unique if* $\delta \geq 0$ *and* $\beta \geq 0$.

Properties of ground state

Theorem

Let $\delta > 0$ and $\phi_g \in S$ be the nonnegative ground state, we have:
(i) There exists $\alpha > 0$ and $C > 0$ such that $|\phi_g(\mathbf{x})| \le Ce^{-\alpha|\mathbf{x}|}$
(ii) If $V(\mathbf{x}) \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$, we have ϕ_g is once continuously differentiable and $\nabla\phi_g$ is Hölder continuous with order 1. In particular, if $V(\mathbf{x}) \in C^\infty$, ϕ_g is smooth.

Proof by De Giorgi iteration

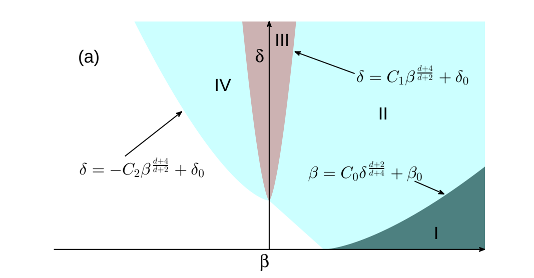
limit as $|\beta| \to +\infty$, $\delta \to +\infty$

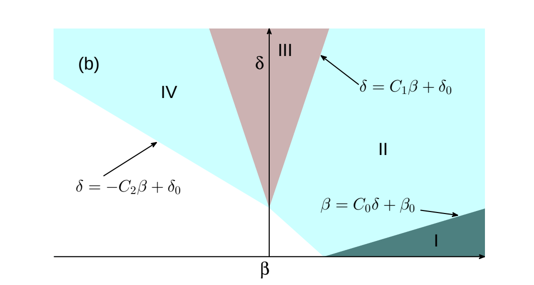
- $V(s\mathbf{x}) = |s|^2 V(\mathbf{x})$ (Harmonic potential/ whole space case)
- Introduce

$$\phi(\mathbf{x}) = \varepsilon^{d/2}\phi^{\varepsilon}(\mathbf{x}\varepsilon),$$

$$E(\phi) = \frac{1}{\varepsilon^2}\int_{\mathbb{R}^d}\left[\frac{\varepsilon^4}{2}|\nabla\phi^{\varepsilon}|^2 + V(\mathbf{x})|\phi^{\varepsilon}|^2 + \frac{\beta\varepsilon^{d+2}}{2}|\phi^{\varepsilon}|^4 + \frac{\delta\varepsilon^{4+d}}{2}\left|\nabla|\phi^{\varepsilon}|^2\right|^2\right] d\mathbf{x},$$

- critical when $\delta\varepsilon^{4+d} \sim \beta\varepsilon^{d+2}$


(a)
δ
β
III
IV
II
I
$\delta = C_1\beta^{\frac{d+4}{d+2}} + \delta_0$
$\delta = -C_2\beta^{\frac{d+4}{d+2}} + \delta_0$
$\beta = C_0\delta^{\frac{d+2}{d+4}} + \beta_0$


(b)
δ
β
III
IV
II
I
$\delta = C_1\beta + \delta_0$
$\delta = -C_2\beta + \delta_0$
$\beta = C_0\delta + \beta_0$

Whole space case

- Case 1: $\beta \to +\infty$ and $\delta/\beta^{\frac{4+d}{2+d}} \ll 1$, i.e. $\delta = o(\beta^{\frac{4+d}{2+d}})$;
- Case 2: $\beta \to +\infty$ and $\lim_{\beta\to+\infty} \delta/\beta^{\frac{4+d}{2+d}} = \delta_\infty > 0$;
- Case 3: $\beta \to +\infty$ and $\delta/\beta^{\frac{4+d}{2+d}} \gg 1$, i.e. $\beta = o(\delta^{\frac{2+d}{4+d}})$ as $\delta \to +\infty$;
- Case 1′: $\beta \to -\infty$ and $\delta/|\beta|^{\frac{4+d}{2+d}} \ll 1$, i.e. $\delta = o(|\beta|^{\frac{4+d}{2+d}})$;
- Case 2′: $\beta \to -\infty$ and $\lim_{\beta\to-\infty} \delta/|\beta|^{\frac{4+d}{2+d}} = \delta_\infty > 0$;
- Case 3′: $\beta \to -\infty$ and $\delta/|\beta|^{\frac{4+d}{2+d}} \gg 1$, i.e. $|\beta| = o(\delta^{\frac{2+d}{4+d}})$ as $\delta \to +\infty$.

Whole space case

$$E_1(\phi) = \int_{\mathbb{R}^d} \left(V(\mathbf{x})|\phi|^2 + \frac{1}{2}|\phi|^4 \right) d\mathbf{x}, \quad \text{for case 1,}$$

$$E_2(\phi) = \int_{\mathbb{R}^d} \left(V(\mathbf{x})|\phi|^2 + \frac{|\phi|^4}{2} + \frac{\delta_\infty}{2}|\nabla|\phi|^2|^2 \right) d\mathbf{x}, \quad \text{for case 2,}$$

$$E_3(\phi) = \int_{\mathbb{R}^d} \left(V(\mathbf{x})|\phi|^2 + \frac{1}{2}|\nabla|\phi|^2|^2 \right) d\mathbf{x}, \quad \text{for case 3 and } 3',$$

$$E_{2'}(\phi) = \int_{\mathbb{R}^d} \left(V(\mathbf{x})|\phi|^2 - \frac{1}{2}|\phi|^4 + \frac{\delta_\infty}{2} \left|\nabla|\phi|^2\right|^2 \right) d\mathbf{x}, \quad \text{for case } 2',$$

$$E_{1'}(\phi) = \int_{\mathbb{R}^d} \left(\frac{1}{2} \left|\nabla|\phi|^2\right|^2 - \frac{1}{2}|\phi|^4 \right) d\mathbf{x}, \quad \text{for case } 1',$$

properties of limiting state

$\rho_g = |\phi_g|^2$

- For E_1, the density ρ_g is given by $\rho_g = \max\{\mu - V(\mathbf{x}), 0\}$ with $\mu = E_1(\sqrt{\rho_g}) + \frac{1}{2}\|\rho_g\|_{L^2}^2$ and $\|\rho_g\|_{L^1} = 1$.
- For E_2, $\rho_g \in C^{1,\alpha}_{\mathrm{loc}} \subset W^{2,p}_{\mathrm{loc}}$ $(1 < p < \infty$ and $\alpha < 1)$ solves the free boundary value problems

$$-\delta_\infty \Delta \rho_g + \rho_g = (\mu - V(\mathbf{x}))\,\chi_{\{\rho_g > 0\}},$$

  The conditions at the free boundaries are

$$\rho_g|_{\partial\{\rho_g>0\}} = 0, \quad |\nabla \rho_g||_{\partial\{\rho_g>0\}} = 0.$$

  If $V(\mathbf{x})$ is radially increasing, we have that $\rho_g(\mathbf{x})$ is radially decreasing and compactly supported.
- For E_3, $\rho_g \in C^{1,\alpha}_{\mathrm{loc}} \subset W^{2,p}_{\mathrm{loc}}$ $(1 < p < \infty$ and $\alpha < 1)$ solves a free boundary value problems

$$-\delta_\infty \Delta \rho_g = (\mu - V(\mathbf{x}))\,\chi_{\{\rho_g > 0\}},$$

- For $E_{1'}$, there exists a non-increasing radially symmetric minimizer ϕ_g which is unique and compactly supported. In fact, ρ_∞ solves the equation

$$-\Delta \rho_g - \rho_g = \mu \chi_{\{\rho_g > 0\}}, \quad \mu = 2E_{1'}(\sqrt{\rho_g}).$$

Scaling of the limiting profiles

- case 1 $\delta/\beta^{\frac{4+d}{2+d}} \ll 1$, set $\varepsilon = \beta^{-\frac{1}{2+d}}$
- case 2 $\lim_{\beta\to+\infty} \delta/\beta^{\frac{4+d}{2+d}} = \delta_\infty$, $\varepsilon = \beta^{-\frac{1}{2+d}}$
- case 3 $\delta/\beta^{\frac{4+d}{2+d}} \gg 1$, $\varepsilon = \delta^{-\frac{1}{4+d}}$
- case 1′ $\delta = o(|\beta|^{\frac{4+d}{2+d}})$, $\varepsilon = |\beta|^{1/2}/\delta^{1/2}$
- case 2′, $\lim_{\beta\to-\infty} \delta/|\beta|^{\frac{4+d}{2+d}} = \delta_\infty > 0$, $\varepsilon = |\beta|^{-\frac{1}{2+d}}$.
- case 3′, $\delta/|\beta|^{\frac{4+d}{2+d}} \gg 1$, $\varepsilon = \delta^{-\frac{1}{4+d}}$

Bounded domain

$$E_\Omega(\phi) = \int_\Omega \left[\frac{1}{2}|\nabla\phi|^2 + \frac{\beta}{2}|\phi|^4 + \frac{\delta}{2}\left|\nabla|\phi|^2\right|^2 \right] d\mathbf{x}$$

- Case B1: $\beta \to +\infty$ and $\delta = o(\beta)$;
- Case B2: $\beta \to +\infty$ and $\lim_{\beta\to+\infty} \delta/\beta = \delta_\infty > 0$;
- Case B3: $\beta \to +\infty$ and $\delta/\beta \gg 1$, i.e. $\beta = o(\delta)$ as $\delta \to +\infty$;
- Case B1′: $\beta \to -\infty$ and $\delta = o(\beta)$;
- Case B2′: $\beta \to -\infty$ and $\lim_{\beta\to-\infty} \delta/|\beta| = \delta_\infty > 0$;
- Case B3′: $\beta \to -\infty$ and $\delta/|\beta| \gg 1$, i.e. $|\beta| = o(\delta)$ as $\delta \to +\infty$.

Bounded domain

- Case B1: $E_b(\phi) = \int_\Omega \frac{1}{2}|\phi|^4 \, d\mathbf{x}$;
- Case B2: $E_{bd}^{+}(\sqrt{\rho}) = \int_\Omega \left[\frac{1}{2}|\rho|^2 + \frac{\delta_\infty}{2}|\nabla\rho|^2\right] \, d\mathbf{x}$;
- Case B3 and B3′: $E_d(\sqrt{\rho}) = \int_\Omega \frac{1}{2}|\nabla\rho|^2 \, d\mathbf{x}$;
- Case B1′: $\varepsilon = |\beta|^{1/2}/\delta^{1/2}$ with $E_{1'}(\phi) = \int_{\mathbb{R}^d} \left(\frac{1}{2}\left|\nabla|\phi|^2\right|^2 - \frac{1}{2}|\phi|^4\right) \, d\mathbf{x}$
- Case B2′: $E_{bd}^{-}(\sqrt{\rho}) = \int_\Omega \left[-\frac{1}{2}|\rho|^2 + \frac{\delta_\infty}{2}|\nabla\rho|^2\right] \, d\mathbf{x}$

Numerical methods

- Gradient flow with discrete normalization (imaginary time Bao&Du 04'):

$$\partial_t \phi = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \beta|\phi(\mathbf{x},t)|^2 + \delta\nabla^2|\phi|^2\right]\phi(\mathbf{x},t),$$

$$\phi(\mathbf{x},t_{n+1}) := \phi(\mathbf{x},t_{n+1}^+) = \frac{\phi(\mathbf{x},t_{n+1}^-)}{\|\phi(\cdot,t_{n+1}^-)\|_2}, \qquad \mathbf{x}\in\Omega, \quad n\geq 0,$$

$$\phi(\mathbf{x},t)|_{\mathbf{x}\in\partial\Omega} = \varphi(\mathbf{x},t)|_{\mathbf{x}\in\partial\Omega} = 0,\ t\geq 0; \phi(\mathbf{x},0) = \phi_0(\mathbf{x}), \text{with } \|\phi_0\|_2 = 1$$

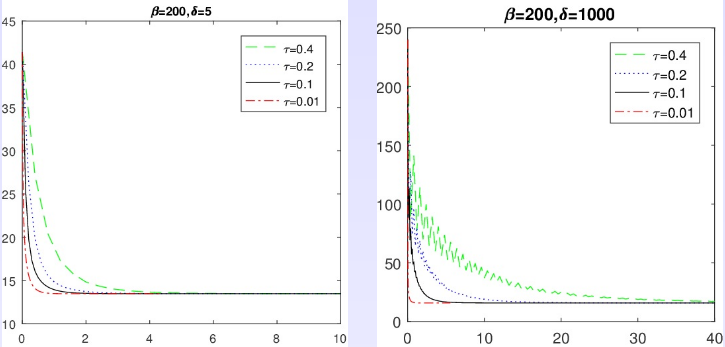
- Full discretization
  - Backward Euler?—$\nabla^2|\phi|^2$? explicit treatment of $\nabla^2|\phi|^2$

IEQ

- Invariant energy quadratization (X. Yang, J. Shen, Q. Wang, L. Ju, H. Zhang, ... 16' 17'):

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \frac{1}{2}\nabla^2\phi^{n+1} - V(\mathbf{x})\phi^{n+1} - \beta(\phi^n\phi^{n+1})\phi^n + \delta\Delta(\phi^n\phi^{n+1})\phi^n,$$

$$\phi(\mathbf{x},t_{n+1}) := \phi(\mathbf{x},t_{n+1}^+) = \frac{\phi(\mathbf{x},t_{n+1}^-)}{\|\phi(\cdot,t_{n+1}^-)\|_2}, \qquad \mathbf{x}\in\Omega, \quad n\geq 0$$



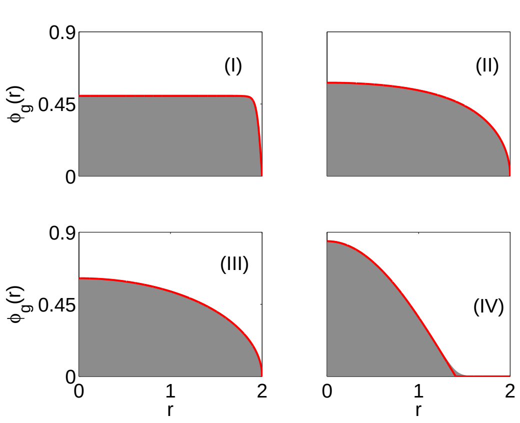


FIG. 6. Comparisons of 1D numerical ground states with TF densities, the box potential case in region I, II, III and IV, which are defined in Fig. 3(b). Red line: analytical TF approximation, and shaded area: numerical solution obtained from (22). Domain is $\{r|0 \leq r < 2\}$ and the corresponding β's and δ's are (I) $\beta = 1280$, $\delta = 1$; (II) $\beta = 320$, $\delta = 160$; (III) $\beta = 1$, $\delta = 160$; (IV) $\beta = -400$, $\delta = 80$.

conclusion

- modified GPE for BEC with higher order interactions
- ground states: existence/uniqueness/ regularity
- large interaction limit whole space v.s. bounded domain
- time-dependent problem, well-posedness, numerics, etc?

THANK YOU!