

A minimisation approach for computing the ground state of Gross–Pitaevskii systems

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Abstract We present a minimisation method for computing the ground state of systems of coupled Gross–Pitaevskii equations. We employ a spectral decomposition of the solution into Hermite basis functions. Inserting the spectral representation into the energy functional yields a constrained nonlinear minimisation problem. For its numerical solution, we use a Newton-like method with an approximate line-search strategy. We analyse this method and prove global convergence. Appropriate starting values for the minimisation process are determined by a continuation strategy. Numerical examples with three-component two-dimensional condensates are included. These experiments demonstrate the reliability of our method and nicely illustrate the effect of phase segregation.

1 A system of Gross–Pitaevskii equations

$$\begin{cases} i\hbar\partial_t\psi^{(l)} = \left(-\frac{\hbar^2}{2m_l}\Delta + V_l + \hbar^2 g_{ll} |\psi^{(l)}|^2 + \hbar^2 \sum_{\substack{k=1 \\ k \neq l}}^{\ell} g_{lk} |\psi^{(k)}|^2 \right) \psi^{(l)}, \\ \|\psi^{(l)}\|_{L^2}^2 = N_l, \quad l = 1, \dots, \ell \end{cases}$$

It describes the wave functions $\psi^{(l)}: \mathbb{R}^d \times \mathbb{R}_{\geq 0} \rightarrow \mathbb{C}$ of atomic species with masses m_l in a BECs. We call g_{ll} **intra-species** and $g_{lk} = g_{kl}$, $l \neq k$ **inter-species** coupling constants (**defocusing**, $g_{lk} \geq 0$). V_l are real potentials. By a linear transformation, we obtain

$$\begin{cases} i\partial_t\psi^{(l)} = \left(-\frac{\hbar c}{2m_l}\Delta + U_l + \sum_{k=1}^{\ell} \vartheta_{lk} |\psi^{(k)}|^2 \right) \psi^{(l)}, \\ \|\psi^{(l)}\|_{L^2}^2 = N_l, \quad l = 1, \dots, \ell \end{cases} \quad (1)$$

with

$$\hbar c = \sqrt{m_1 \cdots m_\ell} \quad \text{and} \quad \vartheta_{lk} = \hbar g_{lk} C^2, \quad C = \sqrt{c^d}.$$

The **ground state** ψ of the system of GPEs (1) is a special solution

$$\psi^{(l)}(\xi, t) = e^{-i\mu_l t} \varphi^{(l)}(\xi), \quad l = 1, \dots, \ell$$

that minimises the energy functional

$$E(\varphi) = \sum_{l=1}^{\ell} \left(\left(-\frac{\hbar c}{2m_l}\Delta + U_l + \frac{1}{2} \sum_{k=1}^{\ell} \vartheta_{lk} |\varphi^{(k)}|^2 \right) \varphi^{(l)} | \varphi^{(l)} \right)_{L^2}.$$

We thus consider the **constrained minimisation problem**

$$E(\varphi) \rightarrow \min, \quad G_l(\varphi) = \|\varphi^{(l)}\|_{L^2}^2 - N_l = 0, \quad 1 \leq l \leq \ell.$$

2 Hermite spectral decomposition

We denote by $H_j^\gamma(\xi)$ the Hermite polynomial of degree j , normalised with respect to the weight $w(\xi) = e^{-\gamma^2 \xi^2}$. They satisfy the recurrence relation

$$\begin{aligned} H_0^\gamma(\xi) &= \sqrt{\frac{\gamma^2}{\pi}}, & H_1^\gamma(\xi) &= \sqrt{\frac{4\gamma^6}{\pi}} \xi, \\ \sqrt{j} H_j^\gamma(\xi) &= \sqrt{2\gamma} \xi H_{j-1}^\gamma(\xi) - \sqrt{j-1} H_{j-2}^\gamma(\xi), & j &\geq 2. \end{aligned}$$

The corresponding **Hermite function** $\mathcal{H}_j^\gamma(\xi)$ is

$$\mathcal{H}_j^\gamma(\xi) = H_j^\gamma(\xi) e^{-\frac{1}{2}\gamma^2 \xi^2}.$$

Hence, the Hermite functions (\mathcal{H}_j^γ) form an **orthonormal basis** of the function space $L^2(\mathbb{R})$: for every function $\varphi \in L^2(\mathbb{R})$, the representation

$$\varphi = \sum_j \varphi_j \mathcal{H}_j^\gamma, \quad \varphi_j = (\varphi | \mathcal{H}_j^\gamma)_{L^2(\mathbb{R})}$$

is valid. Moreover

$$(-\partial_\xi^2 + \gamma^4 \xi^2) \mathcal{H}_j^\gamma(\xi) = 2\lambda_j \mathcal{H}_j^\gamma(\xi), \quad 2\lambda_j = \gamma^2(1 + 2j); \quad (2)$$

that is, the Hermite functions (\mathcal{H}_j^γ) are **eigenfunctions** of the differential operator $-\partial_\xi^2 + \gamma^4 \xi^2$, with corresponding eigenvalues $2\lambda_j$. Using the tensor basis of the Hermite functions, the extension to the d -variate case is straightforward. We only notice that (2) rewrites

$$(-\Delta + U^\gamma(\xi)) \mathcal{H}_j^\gamma(\xi) = 2\lambda_j \mathcal{H}_j^\gamma(\xi), \quad 2\lambda_j = \sum_{k=1}^d \gamma_k^2 (1 + 2j_k),$$

with the standard harmonic potential $U^\gamma(\xi) = \sum_{k=1}^d \gamma_k^2 \xi_k^2$.

3 Minimisation problem

We employ a spectral decomposition of $\varphi^{(l)}$ into a common basis of Hermite functions; truncating the infinite sums we finally get

$$\begin{aligned} E_\rho(\varphi) &= \sum_{l=1}^{\ell} \left[\frac{\hbar c}{m_l} \sum_{|j|=0}^{J-1} \lambda_j (\varphi_j^{(l)})^2 \right. \\ &\quad \left. + \rho_l \int_{\mathbb{R}^d} \left(U_l(\xi) - \frac{\hbar c}{2m_l} U^\gamma(\xi) \right) \left(\sum_{|j|=0}^{J-1} \varphi_j^{(l)} \mathcal{H}_j^\gamma(\xi) \right)^2 d\xi \right. \\ &\quad \left. + \frac{1}{2} \sum_{k=1}^{\ell} \vartheta_{lk} \int_{\mathbb{R}^d} \left(\sum_{|j|=0}^{J-1} \varphi_j^{(k)} \mathcal{H}_j^\gamma(\xi) \right)^4 d\xi \right] \rightarrow \min, \\ G_l(\varphi) &= \sum_{|j|=0}^{J-1} (\varphi_j^{(l)})^2 - N_l = 0, \quad 1 \leq l \leq \ell. \end{aligned}$$

Henceforth, we write the **minimisation problem in the abstract form**

$$F(x) \rightarrow \min, \quad G_l(x) = 0, \quad 1 \leq l \leq \ell. \quad (3)$$

4 Newton-like method with line-search

In order to find a (local) minimiser x^* of (3), we consider (see Han [10]) the **exact penalty function**

$$P(x) = F(x) + r \sum_{i=1}^{\ell} |G_i(x)| \quad (4)$$

with an appropriate penalty parameter $r > 0$. A solution x^* satisfies

$$\nabla F(x^*)^T + y^*{}^T \nabla G(x^*)^T = 0, \quad G(x^*) = 0$$

with a corresponding Lagrange multiplier y^* .

Starting from $x^{(k)} \approx x^*$, we consider the quadratic minimisation problem

$$Q(x^{(k)}, H^{(k)}) : \begin{cases} \nabla F(x^{(k)})^T s + \frac{1}{2} s^T H^{(k)} s \rightarrow \min \\ G_i(x^{(k)}) + \nabla G_i(x^{(k)})^T s = 0, \quad i = 1, \dots, \ell. \end{cases} \quad (5)$$

Here, $H^{(k)}$ is a symmetric matrix that approximates the Hessian of F (essentially, its **diagonal part**). Han shows that a solution $s^{(k)}$ of (5) is a descent direction of (4) if $H^{(k)}$ is positive definite and y^* is bounded by r . For an appropriate step length λ_k satisfying

$$P(x^{(k)} + \lambda_k s^{(k)}) < P(x^{(k)}),$$

the new approximation $x^{(k+1)}$ is defined by

$$x^{(k+1)} = x^{(k)} + \lambda_k s^{(k)}.$$

In order to get a globally convergent method, we enforce λ_k to satisfy the first **Armijo–Goldstein condition**

$$P(x^{(k)} + \lambda_k s^{(k)}) \leq P(x^{(k)}) + \alpha \lambda_k \nabla P(x^{(k)})^T s^{(k)} \quad (6)$$

for some fixed $0 < \alpha < 1$, independently of k .

We employ a **backtracking line-search** strategy. Starting with an initial guess $\lambda = 1$ for the step length, we reduce λ step by step by a factor $\beta \in [0.1, 0.5]$ until (6) holds (see [6, Algorithm A6.3.1], for details).

Theorem 1 Let F and $G = (G_1, \dots, G_\ell)^T$ be continuously differentiable and:

- The function F is bounded from below and ∇G has full rank.
- The matrices $H^{(k)} = H(x^{(k)})$ are positive definite, and for all critical points x^* of (3) there exists a neighborhood where H is continuous.
- The solution of each quadratic minimisation problem $Q(x^{(k)}, H^{(k)})$ has a Lagrange multiplier that is bounded by r in the maximum norm.

Then, the sequence $\{x^{(k)}\}$ converges to a critical point x^* of (3), or any of its accumulation points is a critical point.

Appropriate starting values for ρ_l and ϑ_{lk} in the local optimisation procedure are determined with the help of a **continuation method**.

5.1 Strongly anisotropic potentials

We consider a three-component condensate in \mathbb{R}^2 , with the same atomic species ^{87}Rb , mass $m_l = m = 1.44 \cdot 10^{-25}$ and number of particles $N_l = N = 10^7$. The coupling constants are $\vartheta_{ll} = 1.3 \cdot 10^{-5}$ and $\vartheta_{lk} = 1.3 \cdot 10^{-4}$, $l \neq k$. The potentials are **strongly anisotropic harmonic**, namely

$$U_l(\xi_1, \xi_2) = \frac{1}{2} \left[(\omega_{1l} \xi_1)^2 + (\omega_{2l} \xi_2)^2 \right]$$

with

$$\omega_{11} = \pi, \quad \omega_{22} = \pi, \quad \omega_{13} = \pi, \quad \omega_{23} = \pi.$$

We take $\omega_{21} = \omega_{12}$ ranging from π to 10π .

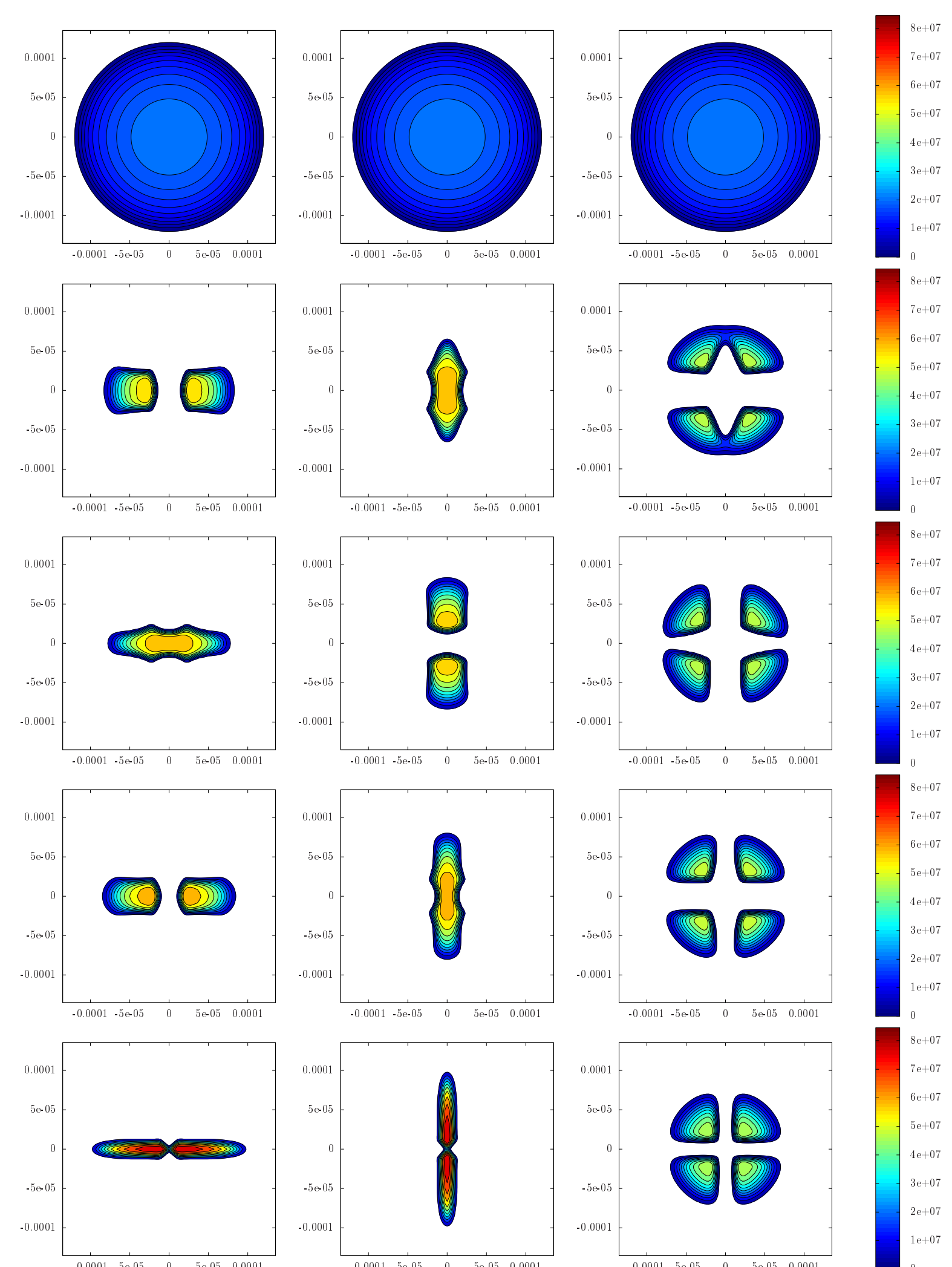


FIGURE 1. Contour plots of the ground state $(\varphi^{(1)}, \varphi^{(2)}, \varphi^{(3)})$ (left–right), for increasing anisotropy of the potentials (top–bottom).

5.2 Phase segregation

We consider the case of a three-component condensate in \mathbb{R}^2 , with the same atomic species ^{87}Rb , mass $m_l = m = 1.44 \cdot 10^{-25}$ and number of particles $N_l = N = 10^7$. The intra-species coupling constants are $\vartheta_{11} = \vartheta_{33} = 1.3 \cdot 10^{-5}$ and $\vartheta_{22} = 6.3 \cdot 10^{-8}$. The potentials are **off-centered and rotated harmonic**, namely

$$U_l(\xi_1, \xi_2) = \frac{1}{2} \left[(\omega_{1l}((\xi_1 - \xi_{1l}) \cos \Omega_l + (\xi_2 - \xi_{2l}) \sin \Omega_l))^2 + (\omega_{2l}((\xi_1 - \xi_{1l}) \sin \Omega_l - (\xi_2 - \xi_{2l}) \cos \Omega_l))^2 \right]$$

with

$$\begin{aligned} \omega_{11} &= \frac{3}{2}\pi, & \omega_{21} &= \pi, & \Omega_1 &= 0, & \xi_{11} &= 10^{-5}, & \xi_{21} &= 0, \\ \omega_{12} &= \frac{3}{2}\pi, & \omega_{22} &= \pi, & \Omega_2 &= 0, & \xi_{12} &= -10^{-5}, & \xi_{22} &= 0, \\ \omega_{13} &= \pi, & \omega_{23} &= 2\pi, & \Omega_3 &= \frac{\pi}{4}, & \xi_{13} &= 0, & \xi_{23} &= 0. \end{aligned}$$

We take identical ϑ_{lk} , $l \neq k$, ranging from 0 to 10^{-5} .

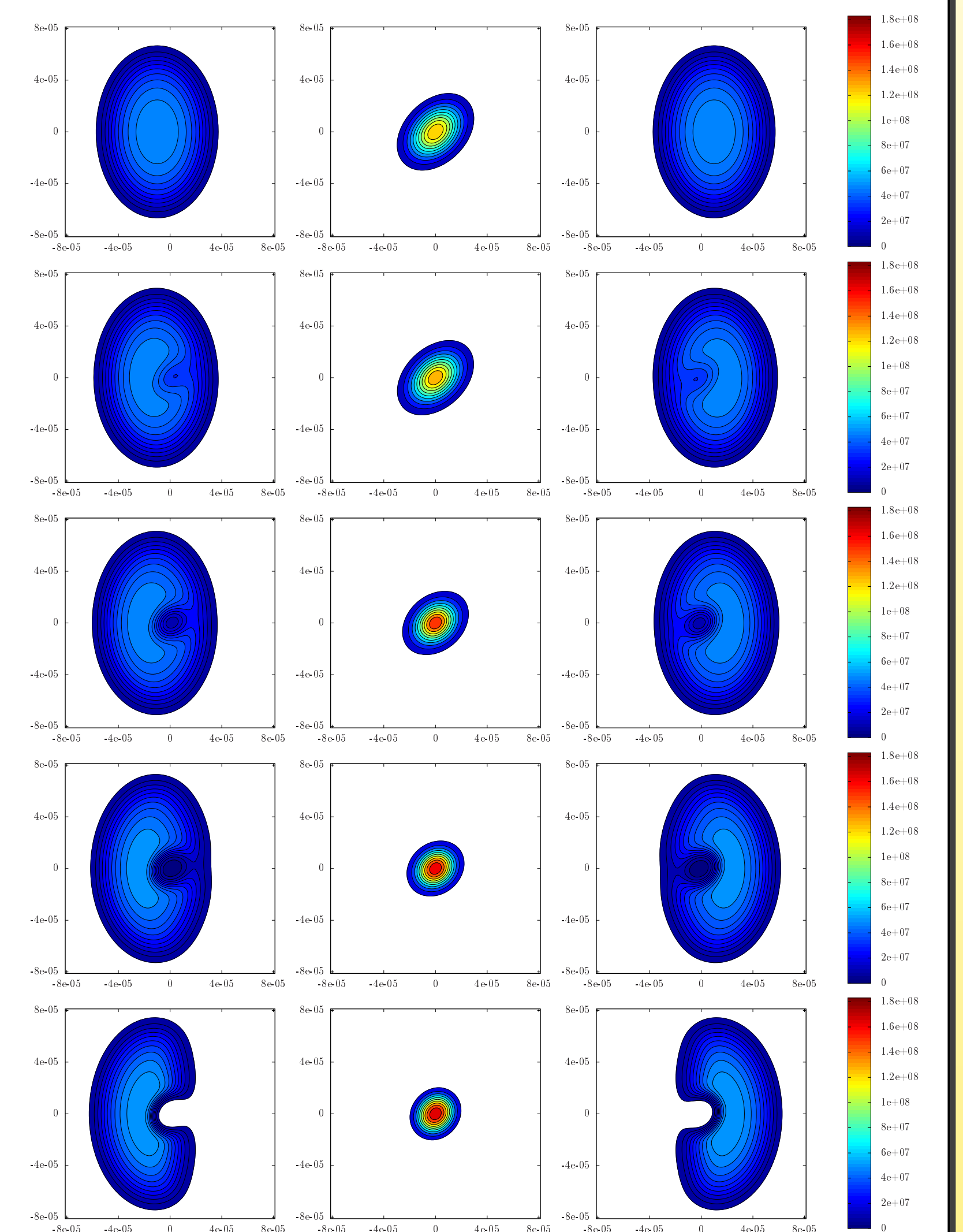


FIGURE 2. Contour plots of the ground state $(\varphi^{(1)}, \varphi^{(2)}, \varphi^{(3)})$ (left–right), for increasing values of the inter-species coupling constants (top–bottom).

Conclusions We provided an efficient and reliable method for computing the ground state of systems of coupled Gross–Pitaevskii equations (code, in MATLAB, available on request). Moreover, we numerically showed that the increasing of the inter-species coupling constant ϑ_{lk} clearly shows the phase segregation phenomenon (see [13, 15]) already discussed and analytically proved in [4] and [5] for the two-component and the three-component condensate, respectively.

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