SPATIAL PATTERNS FOR THE THREE SPECIES GROSS–PITAEVSKII SYSTEM IN THE PLANE

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ABSTRACT. In this paper we highlight some particular spatial patterns of ground state solutions for the three species Gross–Pitaevskii system in the plane having physical coefficients with particular attention to the cases where the inter-species coefficients become large. The solutions models least energy stationary states of a mixture of three Bose–Einstein repulsive condensates.

1. INTRODUCTION

Although Bose–Einstein condensates were predicted by Einstein [9] around 1925, their successful experimental realization for atomic gases was firstly achieved in 1995, see [1]. Next, in 1997, the condensation for a mixture of two interacting species with the same mass was realized, see [14]. Finally, around 2003, triplet species states were observed in [17]. In two recent papers [5, 6] we investigated the numerical approximation (via spectral methods) and the large interaction patterns (via variational arguments) of ground state solutions for a class of vector Gross–Pitaevskii equations in $\mathbb{R}^2$ modelling a binary mixture of Bose–Einstein condensates [8, 15]. As known, depending upon the anisotropy of the trapping potentials, there are various situations where the full physical model in $\mathbb{R}^3$ can be reduced, with a good approximation, to the planar case (see [2, Section 2.2]), which, therefore, is physically meaningful. In this paper we consider some spatial pattern for ground state solutions of the three species repulsive Gross–Pitaevskii system in $\mathbb{R}^2$

$$\begin{cases} \hbar i\partial_t\psi_1 = -\frac{\hbar^2}{2m_1}\Delta\psi_1 + V_1(x_1,x_2)\psi_1 + \theta_{11}\hbar^2|\psi_1|^2\psi_1 + \sum_{j\neq 1}^{3}\theta_{1j}\hbar^2|\psi_j|^2\psi_1, \\ \hbar i\partial_t\psi_2 = -\frac{\hbar^2}{2m_2}\Delta\psi_2 + V_2(x_1,x_2)\psi_2 + \theta_{22}\hbar^2|\psi_2|^2\psi_2 + \sum_{j\neq 2}^{3}\theta_{2j}\hbar^2|\psi_j|^2\psi_2, \\ \hbar i\partial_t\psi_3 = -\frac{\hbar^2}{2m_3}\Delta\psi_3 + V_3(x_1,x_2)\psi_3 + \theta_{33}\hbar^2|\psi_3|^2\psi_3 + \sum_{j\neq 3}^{3}\theta_{3j}\hbar^2|\psi_j|^2\psi_3, \end{cases}$$

for the unknown $\psi_i : \mathbb{R}^2 \to \mathbb{C}$, where $\hbar$ denotes the reduced Planck constant and m_i are the masses of the atomic species composing the Bose–Einstein triple mixture. The coefficients of the coupling matrix (θ_{ij}), which is symmetric so as to give the system a variational structure, are positive and play the role of intra-species (θ_{ii}) and inter-species $(\theta_{i\neq j})$ coefficients respectively and can be represented as

$$\theta_{ij} = 2\pi\frac{\sigma_{ij}}{m_{ij}}, \qquad \frac{1}{m_{ij}} = \frac{1}{m_i} + \frac{1}{m_j}, \quad \sigma_{ij} = \sigma_{ji}, \quad i,j = 1,2,3,$$

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where the constants σ_{ij} are related to the scattering lengths for the i-j species, depending on the interaction potential between atoms. We point out that, due to Feshbach resonance, the interspecies scattering lengths can be made positive and large, by applying a suitable external magnetic field [12]. Concerning the potentials, we consider the general harmonic off-centered case, that is there exist three centers (x_1^i, x_2^i) and six positive constants ω_{ix}, ω_{iy}, $i = 1,2,3$, such that

$$V_i(x_1, x_2) = \tfrac{m_i}{2}\big(\omega_{ix}^2 (x_1 - x_1^i)^2 + \omega_{iy}^2 (x_2 - x_2^i)^2\big).$$

The potential V_is are often taken with the same centers, typically, without loss of generality, the origin. On the other hand, there are some relevant physical situations which lead to consider the off-centered case (see e.g. [16]).

As we will prove, when a inter-species coefficient, say $\theta_{i_0 j_0}$, becomes very large, then phase separation behaviour between the wave densities ψ_{i_0} and ψ_{j_0} tends to appear. We shall highlight analytically and numerically (see Figures 1, 2, 3, 4, 5 within Section 5) the spatial segregation of components of the ground state solutions. In general, this phenomenon can appear by two possibly coexisting causes, that is the separation of the trapping potential centers (see Section 4 and Figure 2) and the large interaction regime (see Section 3 and Figure 3), the second one persisting also in absence of external potentials.

2. FUNCTIONAL SETTING

Let $\mathscr{H}$ be the Hilbert subspace of $H^1(\mathbb{R}^2, \mathbb{C}^3)$ defined by

$$\mathscr{H} = \Big\{(\psi_1, \psi_2, \psi_3) \in H^1(\mathbb{R}^2, \mathbb{C}^3) : \int_{\mathbb{R}^2} V_i(x_1, x_2)|\psi_i|^2 < \infty,\ i = 1,2,3\Big\},$$

which is the natural framework for bound state solutions, endowed with the norm

$$\|(\psi_1, \psi_2, \psi_3)\|_{\mathscr{H}}^2 = \sum_{i=1}^{3} \int_{\mathbb{R}^2} \frac{\hbar^2}{2m_i}|\nabla\psi_i|^2 + V_i(x_1, x_2)|\psi_i|^2,$$

and consider the total energy associated with the system, given by the Hamiltonian E, with $E = E_\infty + J$, $E_\infty, J : \mathscr{H} \to \mathbb{R}$, where we have set

$$E_\infty(\psi_1, \psi_2, \psi_3) = \sum_{i=1}^{3} E_\infty^i(\psi_i),$$

$$J(\psi_1, \psi_2, \psi_3) = \sum_{i\neq j}^{3} J^{ij}(\psi_i, \psi_j),$$

being, for any $i, j = 1,2,3$,

$$E_\infty^i(\psi_i) = \int_{\mathbb{R}^2} \frac{\hbar^2}{2m_i}|\nabla\psi_i|^2 + V_i(x_1, x_2)|\psi_i|^2 + \frac{\theta_{ii}\hbar^2}{2}|\psi_i|^4,$$

$$J^{ij}(\psi_i, \psi_j) = \theta_{ij}\hbar^2 \int_{\mathbb{R}^2} |\psi_i|^2|\psi_j|^2.$$

By standard arguments, it follows that, along a solution, the energy map

$$\{t \mapsto E(\psi_1(\cdot, t), \psi_2(\cdot, t), \psi_3(\cdot, t))\}, \qquad t \geq 0$$

is a constant and that the total particle numbers are time independent,

$$\int_{\mathbb{R}^2} |\psi_i(\cdot, t)|^2 = N_i, \qquad t \geq 0,\ i = 1,2,3. \tag{2.1}$$

The *ground state* solution (also, often, known as *least energy* solution) of the Gross–Pitaevskii system is a solution $(\psi_1,\psi_2,\psi_3)\in\mathcal{H}$ with ansatz

$$\psi_i(x_1,x_2,t)=e^{-\mathrm{i}\frac{\mu_i t}{\hbar}}\phi_i(x_1,x_2),\quad (x_1,x_2)\in\mathbb{R}^2,\ t\geq 0,\ i=1,2,3 \tag{2.2}$$

where $(\phi_1,\phi_2,\phi_3)\in\mathcal{H}$ is real valued and minimizes the functional E constrained to the normalization conditions (2.1) (with ϕ_i in place of ψ_i). Consequently, the functions ϕ_is solve the nonlinear eigenvalue problem

$$\begin{cases} -\frac{\hbar^2}{2m_1}\Delta\phi_1+V_1(x_1,x_2)\phi_1+\theta_{11}\hbar^2|\phi_1|^2\phi_1+\sum\limits_{j\neq 1}^{3}\theta_{1j}\hbar^2|\phi_j|^2\phi_1=\mu_1\phi_1,\\ -\frac{\hbar^2}{2m_2}\Delta\phi_2+V_2(x_1,x_2)\phi_2+\theta_{22}\hbar^2|\phi_2|^2\phi_2+\sum\limits_{j\neq 2}^{3}\theta_{2j}\hbar^2|\phi_j|^2\phi_2=\mu_2\phi_2,\\ -\frac{\hbar^2}{2m_3}\Delta\phi_3+V_3(x_1,x_2)\phi_3+\theta_{33}\hbar^2|\phi_3|^2\phi_3+\sum\limits_{j\neq 3}^{3}\theta_{3j}\hbar^2|\phi_j|^2\phi_3=\mu_3\phi_3,\\ \int_{\mathbb{R}^2}\phi_i^2=N_i,\quad i=1,2,3. \end{cases} \tag{2.3}$$

A direct computation yields the representation formula for the eigenvalues

$$N_i\mu_i=E^i_\infty(\phi_i)+\frac{\theta_{ii}\hbar^2}{2}\int_{\mathbb{R}^2}|\phi_i|^4+\sum_{j\neq i}^{3}J^{ij}(\phi_i,\phi_j), \tag{2.4}$$

for any i. The existence of nontrivial solutions of the nonlinear eigenvalue system (2.3) is straightforward as we limit ourself to the case where all of the coupling constants are positive, which makes the Hamiltonian E coercive and weakly lower semicontinuous on the $L^2\times L^2$ sphere (2.1) in $\mathcal{H}$. In addition, by the standard gradient inequality $\int_{\mathbb{R}^2}|\nabla|u||^2\leq\int_{\mathbb{R}^2}|\nabla u|^2$, it follows that the ground state solutions can be sought among nonnegative functions.

3. LARGE INTER-SPECIES PARAMETERS

Let $\mathcal{H}\subset H^1(\mathbb{R}^2)\times H^1(\mathbb{R}^2)$ be the realization of the Hilbert subspace given in the introduction. For any index pair $i\neq j$, we set

$$\mathcal{S}=\Big\{(\phi_1,\phi_2,\phi_3)\in\mathcal{H}:\int_{\mathbb{R}^2}\phi_i^2=N_i,\ \forall i=1,2,3\Big\},$$
$$\mathcal{S}^\infty_{ij}=\Big\{(\phi_1,\phi_2,\phi_3)\in\mathcal{S}:\int_{\mathbb{R}^2}\phi_i^2\phi_j^2=0\Big\},$$
$$\mathcal{S}^\infty=\bigcap_{\substack{i,j=1\\ i\neq j}}^{3}\mathcal{S}^\infty_{ij}.$$

Assume now that one of the inter-species parameter, say $\theta_{i_0j_0}$ with $i_0\neq j_0$, gets very large, say $\theta_{i_0j_0}=\kappa\to\infty$ while the other remain bounded, say $\theta_{lm}\in(0,1]$ for any $l,m=1,2,3$ with $l\neq m$. The least energy level of the ground state solutions is then defined and denoted as follows

$$c^{i_0j_0}_\kappa=\inf_{(\phi_1,\phi_2,\phi_3)\in\mathcal{S}}\big[E_\infty(\phi_1,\phi_2,\phi_3)+J_\kappa(\phi_1,\phi_2,\phi_3)\big],$$

where the Hamiltonian is $E_\infty+J_\kappa=E_\kappa=E:\mathcal{H}\to\mathbb{R}$, with

$$J_\kappa(\phi_1,\phi_2,\phi_3)=\kappa\hbar^2\int_{\mathbb{R}^2}|\phi_{i_0}|^2|\phi_{j_0}|^2+\sum^{3}_{n\neq m,\,n\neq i_0,\,m\neq j_0}J^{nm}(\phi_n,\phi_m).$$

We also define the candidate for the limiting (as $\kappa \to \infty$) segregated energy $c_\infty^{i_0 j_0}$,

$$c_\infty^{i_0 j_0} = \inf_{(\phi_1,\phi_2,\phi_3)\in\mathscr{S}^\infty_{i_0 j_0}} \Big[E_\infty(\phi_1,\phi_2,\phi_3) + \sum_{n\neq m,\, n\neq i_0,\, m\neq j_0}^{3} J^{nm}(\phi_n,\phi_m)\Big]. \tag{3.1}$$

With obvious modifications one can define the energy levels corresponding to the case where more than one parameter diverges. In the case where $\theta_{ij} \to \infty$ for *all* $i \neq j$ then the limiting energy is c_∞,

$$c_\infty = \inf_{(\phi_1,\phi_2,\phi_3)\in\mathscr{S}^\infty} E_\infty(\phi_1,\phi_2,\phi_3). \tag{3.2}$$

As $\mathscr{S}^\infty \subset \mathscr{S}^\infty_{i_0 j_0} \subset \mathscr{S}$, taking into account the definition of $c_\kappa^{i_0 j_0}$, $c_\infty^{i_0 j_0}$ and c_∞ it holds

$$c_\kappa^{i_0 j_0} \leq c_\infty^{i_0 j_0} \leq c_\infty, \tag{3.3}$$

for any $\kappa > 0$. In this setting the following result holds.

Proposition 3.1. *As κ goes to infinity, the sequence of ground state solutions $(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa) \subset \mathscr{S}$ converges in $\mathscr{H}$ to a function $(\phi_1^\infty,\phi_2^\infty,\phi_3^\infty) \in \mathscr{S}^\infty_{i_0 j_0}$ at energy level $c_\infty^{i_0 j_0}$. Moreover, there exist $\mu_i^\infty > 0$ such that the variational inequalities hold*

$$-\frac{\hbar^2}{2m_i}\Delta\phi_i^\infty + V_i(x_1,x_2)\phi_i^\infty + \theta_{ii}\hbar^2|\phi_i^\infty|^2\phi_i^\infty \leq \mu_i^\infty\phi_i^\infty \quad \text{in } \mathbb{R}^2, \tag{3.4}$$

for all $i = 1,2,3$.

Remark 3.2. *It is natural to wonder if the limit function ϕ_i^∞ solves the equation*

$$-\frac{\hbar^2}{2m_i}\Delta\phi_i^\infty + V_i(x_1,x_2)\phi_i^\infty + \theta_{ii}\hbar^2(\phi_i^\infty)^3 = \mu_i^\infty\phi_i^\infty \quad \text{in } \Omega_i = \{\phi_i^\infty > 0\}$$

when $\Omega_i \subset \mathbb{R}^2$ is an open set. In other words, taken any positive compactly supported function φ with support in Ω_i does it holds $\kappa\int_{\mathbb{R}^2}|\phi_j^\kappa|^2\phi_i^\kappa\varphi \to 0$ as $\kappa\to\infty$? This will be the subject of further investigations.

Proof of Proposition 3.1. In light of the first inequality of (3.3), if $(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa) \in \mathscr{H}$, $\phi_i^\kappa \not\equiv 0$ for any i is the ground state solution, we have $E_\kappa(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa) = c_\kappa^{i_0 j_0}$ and

$$\begin{aligned}\kappa\hbar^2\int_{\mathbb{R}^2}|\phi_{i_0}^\kappa|^2|\phi_{j_0}^\kappa|^2 &\leq \sum_{n\neq m}^{3}\theta_{nm}\hbar^2\int_{\mathbb{R}^2}|\phi_n|^2|\phi_m|^2 \\ &\leq (J_\kappa + E_\infty)(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa) = c_\kappa^{i_0 j_0} \leq c_\infty^{i_0 j_0},\end{aligned}$$

for every κ. As a consequence, we obtain $\int_{\mathbb{R}^2}|\phi_{i_0}^\kappa|^2|\phi_{j_0}^\kappa|^2 \to 0$ as $\kappa\to\infty$. In addition, we have $\|(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa)\|^2_{\mathscr{H}} \leq E_\kappa(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa) \leq c_\infty^{i_0 j_0}$ for any κ. Hence, the sequences $(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa)$ is bounded in $\mathscr{H}$, with respect to κ. In particular, up to a subsequence, there exist $(\phi_1^\infty,\phi_2^\infty,\phi_3^\kappa)$ in $\mathscr{H}$ such that $(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa) \rightharpoonup (\phi_1^\infty,\phi_2^\infty,\phi_3^\infty)$ in $\mathscr{H}$ as $\kappa\to\infty$ and $\phi_i^\kappa(x_1,x_2) \to \phi_i^\infty(x_1,x_2)$ a.e. in $\mathbb{R}^2$. Hence, by Fatou's Lemma, we get $\int_{\mathbb{R}^2}(\phi_{i_0}^\infty)^2(\phi_{j_0}^\infty)^2 = 0$, namely $\phi_{i_0}^\infty\phi_{j_0}^\infty = 0$ a.e. in $\mathbb{R}^2$. Moreover if by contradiction we had $\int_{\mathbb{R}^2}(\phi_i^\infty)^2(\phi_j^\infty)^2 = 0$ for any other index $i \neq j$, by definition, it follows that $(\phi_1^\infty,\phi_2^\infty,\phi_3^\infty) \in \mathscr{S}^\infty$ and by (3.1) and (3.2), we have

$$c_\infty = \inf_{(\phi_1,\phi_2,\phi_3)\in\mathscr{S}^\infty} E_\infty(\phi_1,\phi_2,\phi_3) \leq E_\infty(\phi_1^\infty,\phi_2^\infty,\phi_3^\infty) \leq c_\infty^{i_0 j_0} \leq c_\infty.$$

Therefore, $c_\infty^{i_0 j_0} = c_\infty$, which is not possible. Since by definition $\int_{\mathbb{R}^2}|\phi_i^\kappa|^2 = N_i$ for any $\kappa > 0$ and $\mathscr{H}$ in compactly embedded into $L^r(\mathbb{R}^2)\times L^r(\mathbb{R}^2)$ for any $r \geq 2$ (via (3.7) and

Gagliardo–Nirenberg inequalities), up to a further subsequence, we have $\int_{\mathbb{R}^2}|\phi_i^\infty|^2 = N_i$ for $i = 1,2,3$. Whence

$$(\phi_1^\infty,\phi_2^\infty,\phi_3^\infty) \in \mathscr{S}^\infty_{i_0 j_0}. \tag{3.5}$$

Observe also that $E^i_\infty(\phi_i^\kappa) \le c_\infty^{i_0 j_0}$ for any $i = 1,2,3$ and

$$\sup_{\kappa\ge 1}\mu_i^\kappa = \frac{1}{N_i}\sup_{\kappa\ge 1}\left\{E^i_\infty(\phi_i^\kappa) + \frac{\theta_{ii}\hbar^2}{2}\int_{\mathbb{R}^2}|\phi_i^\kappa|^4 + \sum_{m\ne i}^3 \theta_{im}\hbar^2\int_{\mathbb{R}^2}|\phi_m^\kappa|^2|\phi_i^\kappa|^2\right\} < \infty,$$

denoting μ_i^κ the eigenvalues corresponding to ϕ_i^κ. Hence, up to a subsequence, $\mu_i^\kappa \to \mu_i^\infty$ as $\kappa\to\infty$. By testing the equations of the system by an arbitrary compactly supported positive function η, we get

$$\frac{\hbar^2}{2m_i}\int_{\mathbb{R}^2}\nabla\phi_i^\kappa\cdot\nabla\eta + \int_{\mathbb{R}^2}V_i(x_1,x_2)\phi_i^\kappa\eta + \theta_{ii}\int_{\mathbb{R}^2}|\phi_i^\kappa|^2\phi_i^\kappa\eta \le \mu_i^\kappa\int_{\mathbb{R}^2}\phi_i^\kappa\eta,$$

for all $\kappa > 0$. Hence, letting $\kappa\to\infty$, it turns out that ϕ_i^∞ satisfies the variational inequalities (3.4). Notice that, by Fatou's lemma and the first inequality of (3.3), we have

$$\begin{aligned}
&\sum_{i=1}^3\frac{\hbar^2}{2m_i}\int_{\mathbb{R}^2}|\nabla\phi_i^\infty|^2 + \sum_{i=1}^3\int_{\mathbb{R}^2}V_i|\phi_i^\infty|^2 + \sum_{i=1}^3\frac{\theta_{ii}\hbar^2}{2}\int_{\mathbb{R}^2}|\phi_i^\infty|^4\\
&+\lim_{\kappa\to\infty}\kappa\hbar^2\int_{\mathbb{R}^2}|\phi_{i_0}^\kappa|^2|\phi_{j_0}^\kappa|^2 + \sum_{n\ne m,\,n\ne i_0,\,m\ne j_0}^3 J^{nm}(\phi_n^\infty,\phi_m^\infty)\\
&\le \sum_{i=1}^3\frac{\hbar^2}{2m_i}\liminf_{\kappa\to\infty}\int_{\mathbb{R}^2}|\nabla\phi_i^\kappa|^2 + \sum_{i=1}^3\liminf_{\kappa\to\infty}\int_{\mathbb{R}^2}V_i|\phi_i^\kappa|^2 + \sum_{i=1}^3\frac{\theta_{ii}\hbar^2}{2}\liminf_{\kappa\to\infty}\int_{\mathbb{R}^2}|\phi_i^\kappa|^4\\
&+\lim_{\kappa\to\infty}\kappa\hbar^2\int_{\mathbb{R}^2}|\phi_{i_0}^\kappa|^2|\phi_{j_0}^\kappa|^2 + \sum_{n\ne m,\,n\ne i_0,\,m\ne j_0}^3 \liminf_{\kappa\to\infty}J^{nm}(\phi_n^\kappa,\phi_m^\kappa)\\
&\le \liminf_{\kappa\to\infty}E_\kappa(\phi_1^\kappa,\phi_2^\kappa,\phi_3^\kappa) = \liminf_{\kappa\to\infty}c_\kappa^{i_0 j_0} \le c_\infty^{i_0 j_0}.
\end{aligned}$$

Recalling formula (3.5), by the definition of $c_\infty^{i_0 j_0}$ the above inequalities rewrite as

$$\begin{aligned}
&E_\infty(\phi_1^\infty,\phi_2^\infty,\phi_3^\infty) + \lim_{\kappa\to\infty}\kappa\hbar^2\int_{\mathbb{R}^2}|\phi_{i_0}^\kappa|^2|\phi_{j_0}^\kappa|^2 + \sum_{n\ne m,\,n\ne i_0,\,m\ne j_0}^3 J^{nm}(\phi_n^\infty,\phi_m^\infty)\\
&\le c_\infty^{i_0 j_0} \le E_\infty(\phi_1^\infty,\phi_2^\infty,\phi_3^\infty) + \sum_{n\ne m,\,n\ne i_0,\,m\ne j_0}^3 J^{nm}(\phi_n^\infty,\phi_m^\infty)
\end{aligned}$$

which yields

$$\lim_{\kappa\to\infty}\kappa\int_{\mathbb{R}^2}|\phi_{i_0}^\kappa|^2|\phi_{j_0}^\kappa|^2 = 0. \tag{3.6}$$

Therefore, the convergence of ϕ_i^κ to ϕ_i^∞ in $\mathscr{H}$ is strong, otherwise, assuming by contradiction that this is not the case, the previous inequalities would become strict, yielding immediately a contradiction with (3.6). Finally, as a further consequence, $c_\infty^{i_0 j_0} = E_\infty(\phi_1^\infty,\phi_2^\infty,\phi_3^\infty)$, concluding the proof. □

Remark 3.3. *The strong convergence of ϕ_i^κ to ϕ_i^∞ in $\mathscr{H}$,* (2.4) *and* (3.5) *yield*

$$N_i\mu_i = E^i_\infty(\phi_i^\infty) + \frac{\theta_{ii}\hbar^2}{2}\int_{\mathbb{R}^2}|\phi_i^\infty|^4 + \sum_{m\neq i}^{3} J^{im}(\phi_i^\infty,\phi_m^\infty), \quad i\neq i_0,$$

$$N_{i_0}\mu_{i_0} = E^{i_0}_\infty(\phi_{i_0}^\infty) + \frac{\theta_{i_0i_0}\hbar^2}{2}\int_{\mathbb{R}^2}|\phi_{i_0}^\infty|^4 + \sum_{m\neq i_0,j_0}^{3} J^{i_0m}(\phi_{i_0}^\infty,\phi_m^\infty).$$

Remark 3.4. *Assume that one of the parameters ω_i in the trapping potentials gets very large, say $\omega_{i_0x}=\Lambda\to+\infty$ while the other remain bounded, say $\omega_{ix},\omega_{iy}\in(0,1]$ for any $i=1,2,3$ with $i\neq i_0$. Then, numerical simulations show that the corresponding component $\phi_{i_0}^\Lambda$ of the ground state tends to assume a cigar-like shape along the vertical direction, and the bigger is Λ, the thinner is the profile of ϕ_{i_0} (see Figure 1). We show that, in the asymptotic process $\lambda\to+\infty$, contrary to what happens in the strong interaction limit $\kappa\to\infty$, the energies of the ground state solutions cannot remain bounded. More precisely, set*

$$V_{i_0}^\Lambda(x_1,x_2)=\frac{m_{i_0}}{2}\big(\Lambda^2(x_1-x_1^{i_0})^2+\omega_{i_0y}^2(x_2-x_2^{i_0})^2\big).$$

Hence, we denote the least energy of the ground state solution as follows

$$c_\Lambda = \inf_{(\phi_1,\phi_2,\phi_3)\in\mathscr{S}} E^{i_0}_\Lambda(\phi_{i_0}) + \sum_{i\neq i_0}^{3} E^i_\infty(\phi_i) + J(\phi_1,\phi_2,\phi_3),$$

where $E^{i_0}_\Lambda = E^{i_0}_\infty$ with $V_{i_0}=V_{i_0}^\Lambda$. We want to prove that

$$\Gamma := \sup_{\Lambda>0} c_\Lambda = +\infty.$$

Assume by contradiction that this is not the case, namely $\Gamma<\infty$. Hence, it is readily seen that the sequence of ground state solutions $(\phi_1^\Lambda,\phi_2^\Lambda,\phi_3^\Lambda)$ is bounded in $H^1(\mathbb{R}^2,\mathbb{R}^3)$. In particular, up to a subsequence, it converges weakly in $H^1(\mathbb{R}^2,\mathbb{R}^3)$ and pointwise to a function $(\phi_1^\infty,\phi_2^\infty,\phi_3^\infty)$. Moreover, since for any $\varrho>0$ it holds

$$\sup_{\Lambda\geq 1}\varrho^2\int_{\mathbb{R}^2\setminus B_\varrho(x_1^i,x_2^i)}|\phi_i^\Lambda|^2<\infty, \tag{3.7}$$

for $i=1,2,3$, it follows that $(\phi_1^\Lambda,\phi_2^\Lambda,\phi_3^\Lambda)$ also converges, strongly, in $L^2(\mathbb{R}^2,\mathbb{R}^3)$. Since, for any $\Lambda>0$ and $i=1,2,3$,

$$\int_{\mathbb{R}^2}|\phi_i^\Lambda|^2 = N_i,$$

taking the limit as $\Lambda\to+\infty$ entails $\int_{\mathbb{R}^2}|\phi_i^\infty|^2=N_i$. Whence $\phi_i\neq 0$ in $H^1(\mathbb{R}^2)$ for every $i=1,2,3$. On the other hand, as all the terms in the energy functional are positive, we have

$$\int_{\mathbb{R}^2}V_{i_0}^\Lambda(x_1,x_2)|\phi_{i_0}^\Lambda|^2\leq\Gamma,$$

for all $\Lambda>0$, yielding in particular

$$\int_{\mathbb{R}^2}\frac{m_{i_0}}{2}(x_1-x_1^{i_0})^2|\phi_{i_0}^\Lambda|^2\leq\frac{\Gamma}{\Lambda^2}.$$

By Fatou's lemma this entails $|x_1-x_1^{i_0}||\phi_{i_0}^\infty(x_1,x_2)|=0$ a.e. $(x_1,x_2)\in\mathbb{R}^2$, namely $\phi_{i_0}^\infty=0$ in $H^1(\mathbb{R}^2)$, which produces a contradiction.

4. LOCATION OF COMPONENTS

In the so called Thomas–Fermi regime, a very good approximation of the ground state solutions of (2.3) which holds for sufficiently large values of the coupling constants θ_{ij}, can be obtained by simply dropping the diffusion terms $-\Delta\phi_i$, namely the kinetic contributions, thus assuming the wave functions to be slowly varying (cf. [10, 18, 13]). In turn, system (2.3) reduces to the algebraic system (here we let $\hbar = m_i = 1$)

$$\begin{cases} \theta_{11}|\phi_1|^2 + \theta_{12}|\phi_2|^2 + \theta_{13}|\phi_3|^2 = \mu_1 - V_1(x_1,x_2), \\ \theta_{21}|\phi_1|^2 + \theta_{22}|\phi_2|^2 + \theta_{23}|\phi_3|^2 = \mu_2 - V_2(x_1,x_2), \\ \theta_{31}|\phi_1|^2 + \theta_{32}|\phi_2|^2 + \theta_{33}|\phi_3|^2 = \mu_3 - V_3(x_1,x_2). \end{cases} \tag{4.1}$$

Let us denote by $\Theta = (\theta_{ij})$ the symmetric coupling matrix and set $\eta_i = \phi_i^2$ and $\chi_i(x_1,x_2) = \mu_i - V_i(x_1,x_2)$, where the μ_is should be computed through the normalization conditions (2.1). Moreover, assume that $|\Theta| > 0$ (positive determinant). Think, for instance, to the case where the diagonal coefficients θ_{ii} are much larger that the θ_{ij}s, i.e. $\theta_{ii} \gg \theta_{ij} \gg 1$. Then, we obtain

$$|\Theta|\,\eta_1(x_1,x_2) = \begin{vmatrix} \chi_1(x_1,x_2) & \theta_{12} & \theta_{13} \\ \chi_2(x_1,x_2) & \theta_{22} & \theta_{23} \\ \chi_3(x_1,x_2) & \theta_{32} & \theta_{33} \end{vmatrix},$$

$$|\Theta|\,\eta_2(x_1,x_2) = \begin{vmatrix} \theta_{11} & \chi_1(x_1,x_2) & \theta_{13} \\ \theta_{21} & \chi_2(x_1,x_2) & \theta_{23} \\ \theta_{31} & \chi_3(x_1,x_2) & \theta_{33} \end{vmatrix},$$

$$|\Theta|\,\eta_3(x_1,x_2) = \begin{vmatrix} \theta_{11} & \theta_{12} & \chi_1(x_1,x_2) \\ \theta_{21} & \theta_{22} & \chi_2(x_1,x_2) \\ \theta_{31} & \theta_{32} & \chi_3(x_1,x_2) \end{vmatrix}.$$

As the coupling coefficients are positive, if we set $r_i = \sqrt{2\mu_i}$ for $i = 1,2,3$, it is evident that system (4.1) makes sense only if the right hand sides of each equation in it is positive, that is in the set

$$\mathscr{D} = \bigcap_{i=1}^{3} \mathscr{D}_i, \quad \mathscr{D}_i = \left\{(x_1,x_2) \in \mathbb{R}^2 :\ \omega_{ix}^2(x_1 - x_{i1})^2 + \omega_{iy}^2(x_2 - x_{i2})^2 \le r_i^2\right\}.$$

Furthermore, taking into account that, for any i, the η_is are positive and are a combination of quadratic polynomials (due to the structure of χ_i), there exist positive constants Ω_{ix}, Ω_{iy} and R_i and centers (y_{i1}, y_{i2}) which allow to define the (possibly empty) overlap region of the components of the wave functions

$$\mathscr{O} = \bigcap_{i=1}^{3} \mathscr{O}_i, \quad \mathscr{O}_i = \left\{(x_1,x_2) \in \mathscr{D} :\ \Omega_{ix}^2(x_1 - y_{i1})^2 + \Omega_{iy}^2(x_2 - y_{i2})^2 \le R_i^2\right\}.$$

Then, for $\mathscr{O} \neq \emptyset$, there is $\alpha_i > 0$ such that a non-smooth approximation of the i-th component of the ground state is given by

$$\phi_i^2(x_1,x_2) := \begin{cases} \alpha_i(R_i^2 - \Omega_{ix}^2(x_1 - y_{i1})^2 - \Omega_{iy}^2(x_2 - y_{i2})^2), & \text{in } \mathscr{O}, \\ \frac{r_i^2 - \omega_{ix}^2(x_1 - x_{i1})^2 - \omega_{iy}^2(x_2 - x_{i2})^2}{2\theta_{ii}}, & \text{in } \mathscr{D}_i \setminus \mathscr{O}, \\ 0, & \text{in } \mathbb{R}^2 \setminus \mathscr{D}_i. \end{cases} \tag{4.2}$$

Notice that, since $\theta_{ij} \ll \theta_{ii}$, we have (e.g. for the first component ϕ_1)

$$\theta_{11}\theta_{22}\theta_{33}\phi_1^2(x_1,x_2) \approx \begin{vmatrix} \chi_1(x_1,x_2) & 0 & 0 \\ \chi_2(x_1,x_2) & \theta_{22} & 0 \\ \chi_3(x_1,x_2) & 0 & \theta_{33} \end{vmatrix} = \chi_1(x_1,x_2)\theta_{22}\theta_{33}.$$

This clarifies why it makes sense to extend to the set $\mathscr{D}_i \setminus \mathscr{O}$ the Thomas–Fermi approximation defined in $\mathscr{O}$ according to formula (4.2).

5. Numerical computation of solutions

We briefly describe the numerical algorithm used for the computation of the ground states. For more details, we refer the reader to [5]. It is sufficient to consider the single one-dimensional Gross–Pitaevskii equation. In fact the extension to the case with any number of equations is straightforward. Moreover, without loss of generality, we reduce to the case $\hbar = m = 1$. The main idea is to directly minimize the energy $E(\phi)$ associated to a wave function $\psi(x) = e^{-i\mu t}\phi(x)$, discretized by Hermite functions, with a normalization constraint for the wave function. As it is known, the Hermite functions $(\mathscr{H}_l^\beta)_{l\in\mathbb{N}}$ are defined by

$$\mathscr{H}_l^\beta(x) = H_l^\beta(x)e^{-\frac{1}{2}\beta^2x^2}, \quad l \in \mathbb{N},$$

where $(H_l^\beta)_{l\in\mathbb{N}}$ are the *Hermite polynomials* [4], orthonormal in L^2 with respect to the weight $e^{-\beta^2x^2}$. The Hermite functions are the solutions (ground state, for $l = 0$, and excited states, if else) to the eigenvalue problem for the linear Schrödinger equation with *standard* harmonic potential

$$\frac{1}{2}\left(-\frac{d^2}{dx^2} + (\beta^2x)^2\right)\mathscr{H}_l = \lambda_l\mathscr{H}_l, \qquad \lambda_l = \beta^2\left(l + \frac{1}{2}\right).$$

If we set

$$\phi = \sum_{l\in\mathbb{N}} \phi_l\mathscr{H}_l,$$

where

$$\phi_l = (\phi, \mathscr{H}_l)_{L^2} = \int_{\mathbb{R}} \phi\mathscr{H}_l,$$

the energy functional rewrites as

$$E(\phi) = \sum_{l\in\mathbb{N}} \lambda_l\phi_l^2 + \int_{\mathbb{R}}\left(V(x) - \frac{(\beta^2x)^2}{2}\right)\left(\sum_{l\in\mathbb{N}}\phi_l\mathscr{H}_l\right)^2 + \frac{1}{2}\theta\int_{\mathbb{R}}\left(\sum_{l\in\mathbb{N}}\phi_l\mathscr{H}_l\right)^4,$$

and the chemical potential turns into

$$N\mu = E(\phi) + \frac{1}{2}\theta\int_{\mathbb{R}}\left(\sum_{l\in\mathbb{N}}\phi_l\mathscr{H}_l\right)^4 \tag{5.1}$$

By minimizing E, under the constraint $\|\phi\|_{L^2}^2 = N$, we look for local minima of

$$E(\phi;\lambda) = E(\phi) + \lambda\left(N - \sum_{l\in\mathbb{N}}\phi_l^2\right)$$

which solve the system, with $k \in \mathbb{N}$,

$$\begin{cases} (\lambda_\kappa - \lambda)\phi_\kappa + \int_{\mathbb{R}} \left(V(x) - \frac{(\beta^2 x)^2}{2} \right) \mathcal{H}_k \left(\sum_{l\in\mathbb{N}} \phi_l \mathcal{H}_l \right) + \theta \int_{\mathbb{R}} \mathcal{H}_k \left(\sum_{l\in\mathbb{N}} \phi_l \mathcal{H}_l \right)^3 = 0, \\ \sum_{l\in\mathbb{N}} \phi_l^2 = N. \end{cases}$$

We notice that, if ϕ is a solution of the above system, then it is immediately seen, by multiplying times ϕ_k, summing up over k and using (5.1), that the Lagrange multiplier λ equals the chemical potential μ. Next, we truncate the Hermite series to degree $L-1$ and introduce an additional parameter $\rho = 1$ in front of the first integral (its usage will be clear later), to obtain a corresponding truncated energy functional $E_L(\phi;\lambda;\rho)$, whose local minima solve the system, with $0 \le k \le L-1$,

$$\begin{cases} (\lambda_\kappa - \lambda)\phi_\kappa + \rho \int_{\mathbb{R}} \left(V(x) - \frac{(\beta^2 x)^2}{2} \right) \mathcal{H}_k \left(\sum_{l=0}^{L-1} \phi_l \mathcal{H}_l \right) + \theta \int_{\mathbb{R}} \mathcal{H}_k \left(\sum_{l=0}^{L-1} \phi_l \mathcal{H}_l \right)^3 = 0, \\ \sum_{l=0}^{L-1} \phi_l^2 = N. \end{cases}$$

In order to approximate the integrals, we used a Gauss–Hermite quadrature formula with $2L-1$ nodes relative to the weight $e^{-2\beta^2 x^2}$. The system is solved by a modified Newton method with backtracking line-search, which guarantees global convergence to the ground states. We refer to [3, 7] and, in particular, to [5] for the details. Here we just mention that the initial guess for the Newton iteration is obtained by a continuation technique over ρ and θ, starting from the ground state of the Schrödinger equation with the standard harmonic potential, which corresponds to $\rho = \theta = 0$. Using the tensor basis of the Hermite functions, the extension to the two-dimensional case is straightforward.

In the following figures we show some typical spatial patters of the ground states solution triplet with respect some relevant features as:

(1) the anisotropy of the trapping potentials (Figure 1);
(2) the phase separation via potential off-centering (Figure 2);
(3) the phase separation via large inter-atomic interactions (Figure 3);
(4) the shape of supports with respect to the number of atoms N_i (Figure 4);
(5) the shape of supports with respect to the size of the masses m_i (Figure 5).

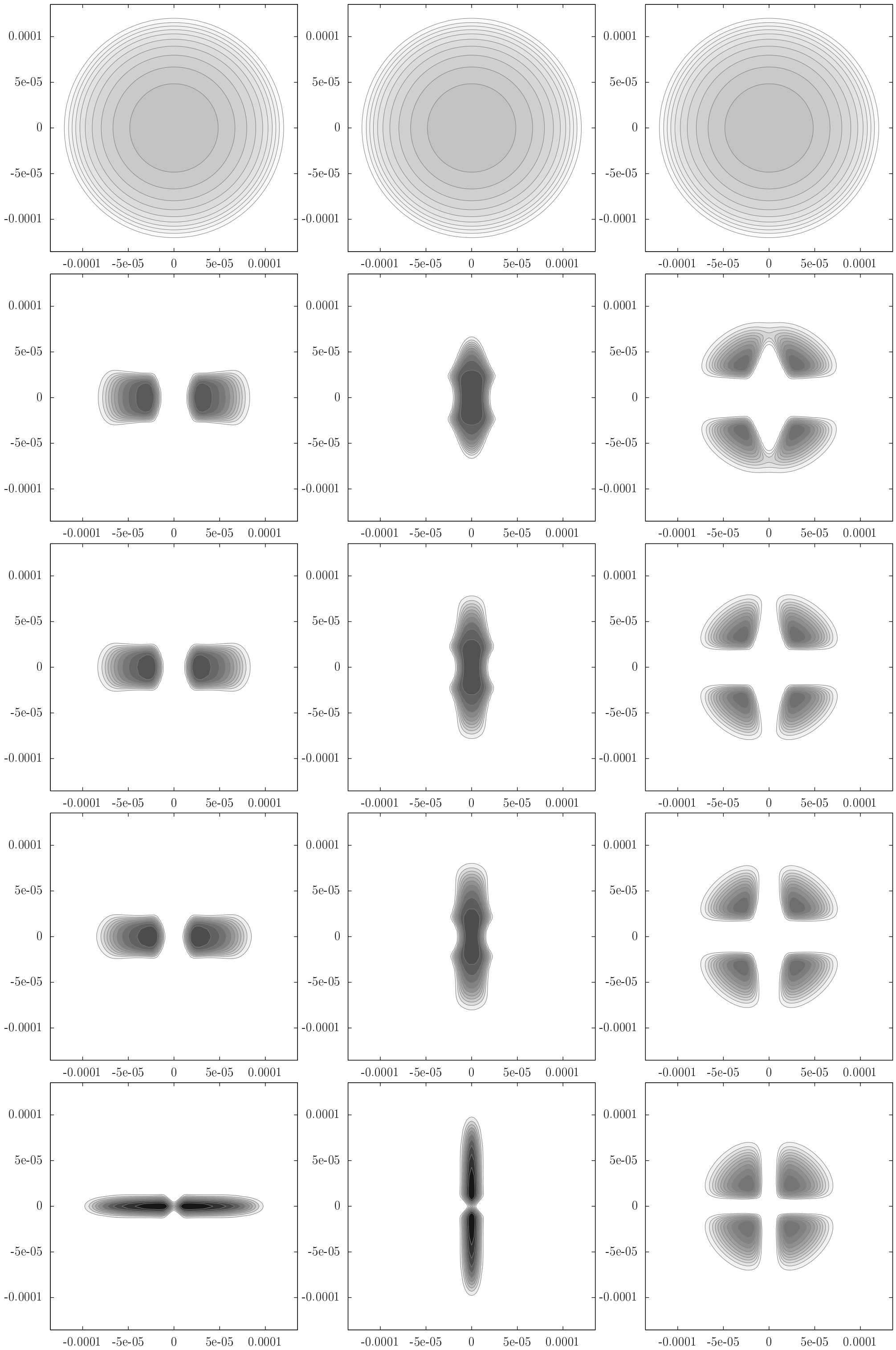

FIGURE 1. (anisotropy) ground state (ϕ_1, ϕ_2, ϕ_3) (left to right); ω_{y1} and ω_{x2} assume values $\pi, 1.1\pi, 1.5\pi, 2\pi, 10\pi$ (top to bottom), other $\omega_{yi} = \pi$, $\omega_{xi} = \pi$, $m_i = 1.44 \cdot 10^{-25}$, $N_i = 10^7$, $\sigma_{11} = \sigma_{22} = \sigma_{33} = 10^{-6}$ and $\sigma_{12} = \sigma_{23} = \sigma_{13} = 10\sigma_{ii}$.

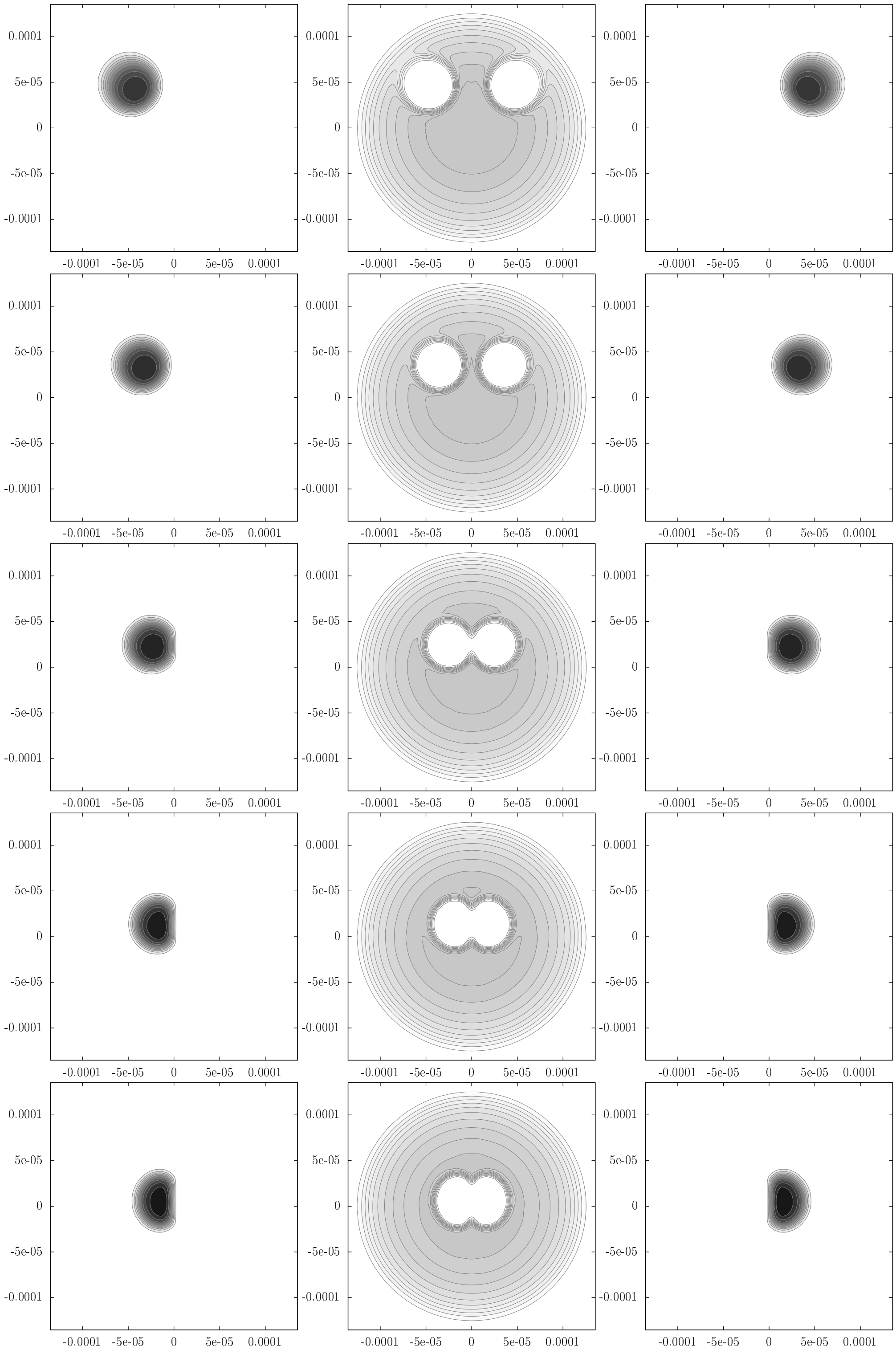

FIGURE 2. (off-centering) ground state (ϕ_1, ϕ_2, ϕ_3) (left to right); V_2 with center $(0,0)$; V_1 with centers $(-4,4)$, $(-3,3)$, $(-2,2)$, $(-1,1)$, $(-0.4,0.4)$ and V_3 with centers $(4,4)$, $(3,3)$, $(2,2)$, $(1,1)$, $(0.4,0.4)$ (up to 10^{-5}, top to bottom); $\omega_{yi} = \omega_{xi} = \pi$, $m_i = 1.44 \cdot 10^{-25}$, $N_i = 10^7$, $\sigma_{11} = \sigma_{33} = 2 \cdot 10^{-7}$, $\sigma_{22} = 100\sigma_{11}$ and $\sigma_{ij} = 50\sigma_{11}$.

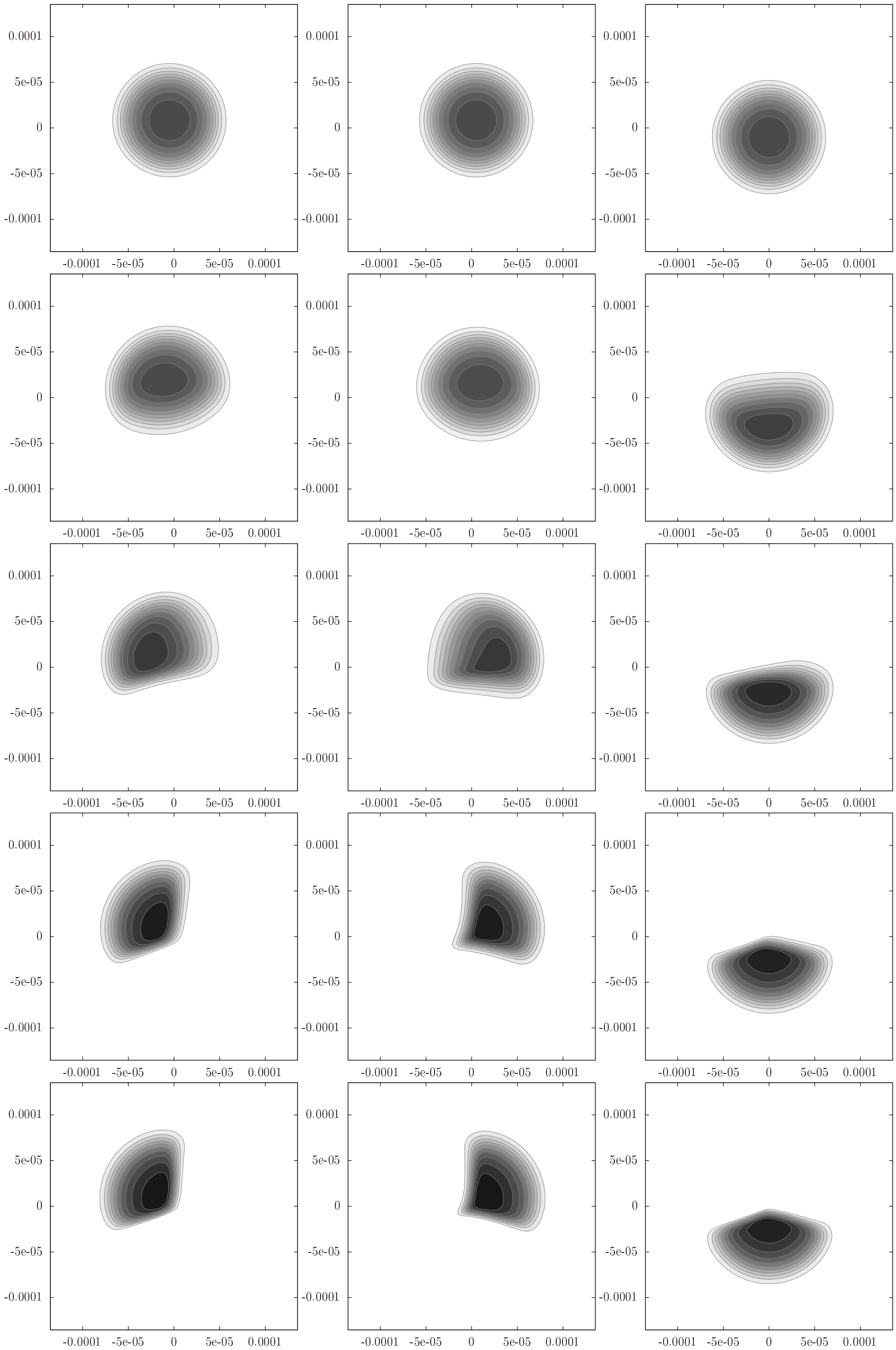

FIGURE 3. (phase segregation) ground state (ϕ_1, ϕ_2, ϕ_3) (left to right); $\omega_{yi} = \omega_{xi} = \pi$, $m_i = 1.44 \cdot 10^{-25}$, $N_i = 10^7$, $\sigma_{11} = \sigma_{22} = \sigma_{33} = 10^{-6}$ and $\sigma_{12} = 0, 0.3, 0.8, 1.4, 2 \cdot 10^{-6}$, $\sigma_{23} = 0, 0.5, 1, 1.8, 5 \cdot 10^{-6}$, $\sigma_{13} = 0, 0.7, 1.8, 5, 50 \cdot 10^{-6}$ (top to bottom).

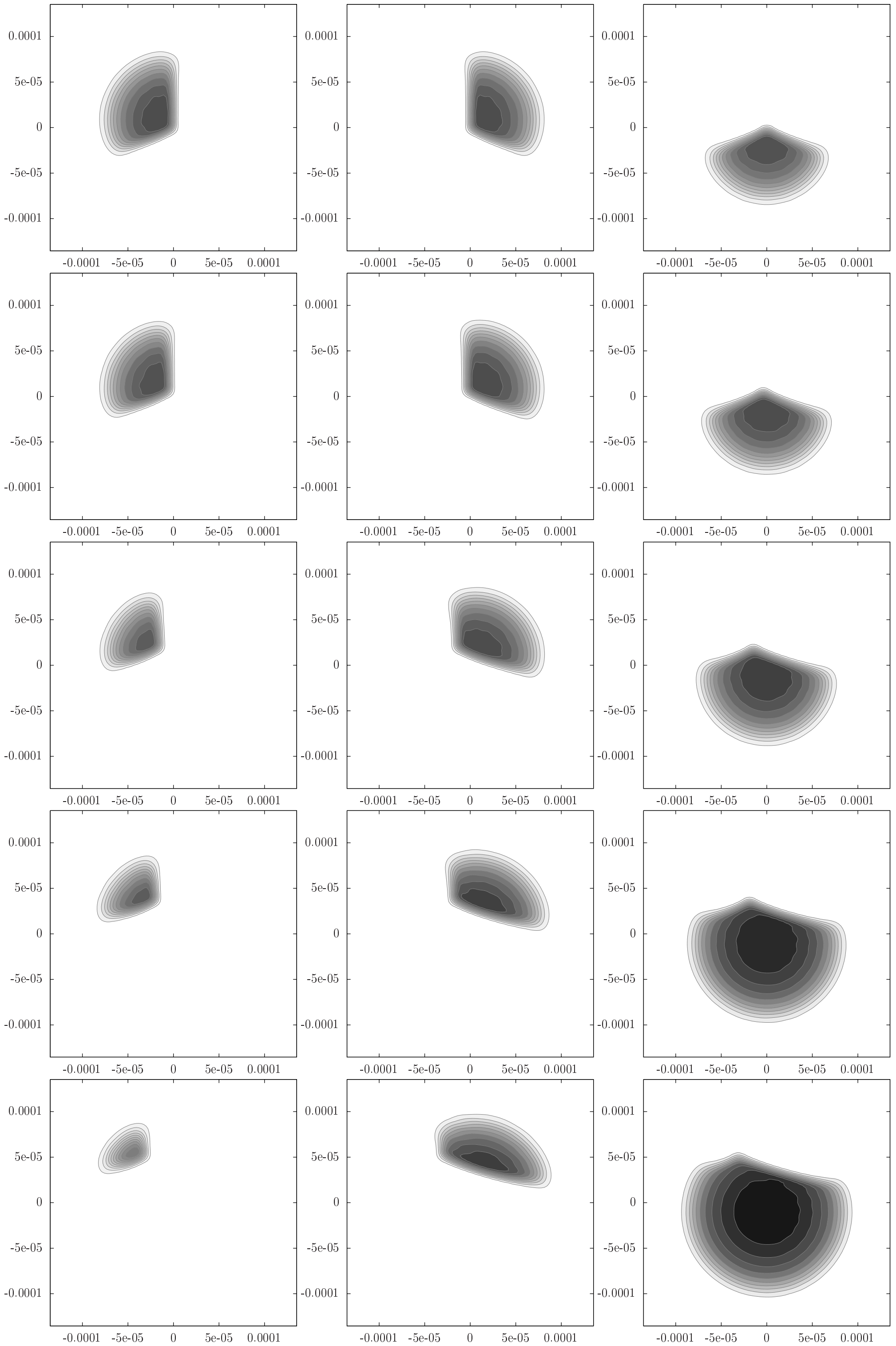

FIGURE 4. (numbers of atoms) ground state (ϕ_1, ϕ_2, ϕ_3) (left to right); $\omega_{yi} = \omega_{xi} = \pi$, $m_i = 1.44 \cdot 10^{-25}$, $\sigma_{ii} = 10^{-6}$, $\sigma_{ij} = 4\sigma_{ii}$, $N_1 = 1, 0.8, 0.4, 0.3, 0.1 \cdot 10^7$ and $N_3 = 1, 1.3, 2, 4, 6 \cdot 10^7$ (top to bottom).

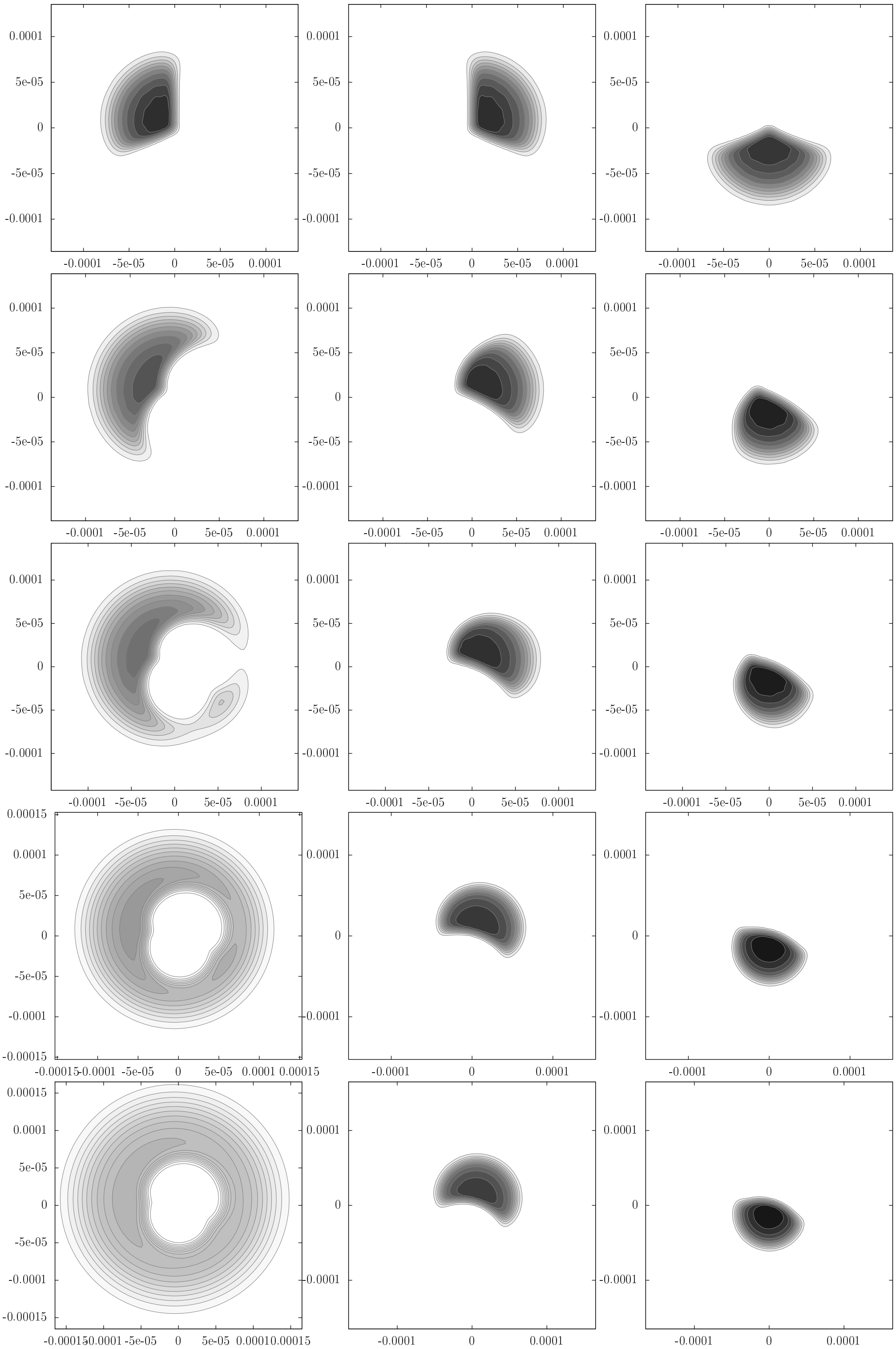

FIGURE 5. (atomic masses) ground state (ϕ_1, ϕ_2, ϕ_3) (left to right); $\omega_{yi} = \omega_{xi} = \pi$, $N_i = 10^7$, $\sigma_{ii} = 10^{-6}$, $\sigma_{ij} = 4\sigma_{ii}$, $m_1 = 1.44, 1, 0.8, 0.5, 0.3 \cdot 10^{-25}$, $m_2 = 1.44 \cdot 10^{-25}$ and $m_3 = 1.44, 1.8, 1.9, 2, 2.1 \cdot 10^{-25}$ (top to bottom).

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