

On phase segregation in nonlocal two-particle Hartree systems

Research Article

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Abstract: We prove the phase segregation phenomenon to occur in the ground state solutions of an interacting system of two self-coupled repulsive Hartree equations for large nonlinear and nonlocal interactions. A self-consistent numerical investigation visualizes the approach to this segregated regime.

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1. Introduction

In this paper, we study the phase segregation phenomenon in the ground states of the eigenvalue system consisting of two interacting repulsive Hartree equations whose interaction, as well as the respective self-couplings, are nonlinear and nonlocal,

$$\begin{cases} -\Delta\phi_1 + V_1(x)\phi_1 + \vartheta_1 (V * |\phi_1|^2) \phi_1 + \kappa (V * |\phi_2|^2) \phi_1 = \mu_1 \phi_1 & \text{in } \mathbb{R}^N, \\ -\Delta\phi_2 + V_2(x)\phi_2 + \vartheta_2 (V * |\phi_2|^2) \phi_2 + \kappa (V * |\phi_1|^2) \phi_2 = \mu_2 \phi_2 & \text{in } \mathbb{R}^N, \\ \|\phi_1\|_{L^2}^2 = N_1, \\ \|\phi_2\|_{L^2}^2 = N_2. \end{cases} \quad (1)$$

Here, the external potentials V_1 and V_2 are assumed to be nonnegative and confining, whereas the interaction potential V is, for example, of Coulomb type. Moreover, the system is purely repulsive, i.e. the self-coupling constants and the interaction strength are nonnegative,

$$\vartheta_1, \vartheta_2 \geq 0, \quad \kappa \geq 0.$$

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For fixed $\vartheta_1, \vartheta_2 \geq 0$ and fixed $N_1, N_2 > 0$, the phase segregation phenomenon in the ground state (ϕ_1, ϕ_2) with ground state energy (μ_1, μ_2) of the system (1) is characterized by the decay to zero of the Coulomb energy functional

$$\mathbb{D}(\phi_1, \phi_2) = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} |\phi_1(x)|^2 V(x-y) |\phi_2(y)|^2 dx dy \quad (2)$$

in the regime of large interaction strength κ , i.e. by

$$\mathbb{D}(\phi_1, \phi_2) = o(1) \quad \text{for } \kappa \rightarrow \infty.$$

This study is not only of independent mathematical interest but it can also be motivated by various physical applications like, e.g., electromagnetic waves in a Kerr medium in nonlinear optics, surface gravity waves in hydrodynamics, and ground states in Bose-Einstein condensed bosonic quantum mechanical many-body systems (see also [1]). The latter domain has been a subject of great interest since many years, both on the experimental and the theoretical side, starting off from a series of successful experimental realizations of Bose-Einstein condensation for atomic gases, first achieved in 1995 for a single condensate (see e.g. [2]), then, in 1997, for a mixture of two interacting atomic species with equal masses (see e.g. [13]), and, finally, in 2003 for triplet species states (see e.g. [17]). On the theoretical side, the standard scenario of two interacting Bose-Einstein condensates for a very dilute system of repulsive bosons uses the description based on a system of two coupled Gross-Pitaevskii equations (see e.g. [10, 11, 14, 15]). These equations are formally contained in (1) for the case of the zero range interaction potential $V = \delta$, i.e. in the case of local nonlinearities.¹ For a complete survey paper, we also refer the reader to [8] and references therein. One may argue that, for higher density regimes, it is sensible to capture more of the boson-boson interaction by allowing for its nonlocal and, hence, less coarse grained resolution by use of a potential $V \neq \delta$ (see e.g. [4]). The phase segregation phenomenon has been studied e.g. in [14, 16, 18] for Gross-Pitaevskii equations, and it has been given a general variational framework in [7]. Recently, the second author, jointly with M. Caliri, has investigated both numerically and analytically the behavior of ground state solutions² highlighting their location³ and the occurring phase segregation phenomena in the highly interacting regime (see [6]).⁴

In the present paper, we extend the analysis to the nonlocal system (1) and give a proof of the phase segregation phenomenon in the variational calculus setup. Moreover, in contradistinction to [6], we adopt a classical self-consistent numerical approach to the solution of the ground state of (1) in order to compute the phase segregated states and to monitor the decay of the Coulomb interaction (2).

As we aim at keeping the paper self-contained and easily readable also for those readers who are more acquainted with the physical or the numerical side, we will provide rather detailed mathematical arguments throughout the paper.

2. Strong interaction and phase segregation

Throughout this section, we shall denote by C a generic positive constant which can vary from line to line inside the proofs.

2.1. Functional setting

As described in the introduction, we are interested in the case of nonnegative confining external potentials V_1 and V_2 . More precisely, we make the following assumption.

¹ For the case of a single condensate, the stationary and dynamical Gross-Pitaevskii equation has been rigorously derived from the many-body bosonic Schrödinger equation in the weak coupling limit, see e.g. [12] and [9], respectively.

² And, in some particular cases, also excited state solutions.

³ With respect to the off-centering of the confining potentials V_i .

⁴ For a complete numerical study of ground states for vector like nonlinear Schrödinger systems with cubic coupling, we also refer to [5].

Assumption 2.1.

The external potentials V_i are nonnegative, continuous, and confining, i.e. for $i = 1, 2$, we have $V_i \in C(\mathbb{R}^N, \mathbb{R}_0^+)$ with

$$\lim_{|x| \rightarrow \infty} V_i(x) = \infty.$$

The functional setting we want to apply makes use of the following Hilbert space.

Definition 2.1.

Let the external potentials V_i satisfy Assumption 2.1 and let \mathcal{H} be the Hilbert subspace of $H^1(\mathbb{R}^N) \times H^1(\mathbb{R}^N)$ defined by

$$\mathcal{H} = \left\{ (\phi_1, \phi_2) \in H^1(\mathbb{R}^N) \times H^1(\mathbb{R}^N) : \int_{\mathbb{R}^N} V_i(x) |\phi_i(x)|^2 dx < \infty, \quad i = 1, 2 \right\}, \quad (3)$$

where the scalar product of $\phi = (\phi_1, \phi_2) \in \mathcal{H}$ with $\psi = (\psi_1, \psi_2) \in \mathcal{H}$ is given by

$$\langle \phi, \psi \rangle_{\mathcal{H}} = \sum_{i=1}^2 \left(\int_{\mathbb{R}^N} \overline{\nabla \phi_i(x)} \cdot \nabla \psi_i(x) dx + \int_{\mathbb{R}^N} V_i(x) \overline{\phi_i(x)} \psi_i(x) dx \right). \quad (4)$$

This functional setting is the natural framework for the study of bound states of systems (1) in external potentials as it allows (together with Lemma 2.2) the associated energy functional (see (11)) to be well-defined and finite.

Lemma 2.1.

Under Assumption 2.1, for any $N \geq 3$, the embedding

$$\mathcal{H} \hookrightarrow L^2(\mathbb{R}^N) \oplus L^2(\mathbb{R}^N)$$

is compact, \mathcal{H} being the Hilbert space (3) equipped with the norm from (4). Also, for $3 \leq N \leq 5$, the embedding

$$\mathcal{H} \hookrightarrow L^{\frac{4N}{N+2}}(\mathbb{R}^N) \oplus L^{\frac{4N}{N+2}}(\mathbb{R}^N)$$

is compact.

Proof. Let (ϕ_1^h, ϕ_2^h) be a bounded sequence in \mathcal{H} , say $\|(\phi_1^h, \phi_2^h)\|_{\mathcal{H}} \leq C$ for all $h \in \mathbb{N}$. Up to a subsequence, it converges weakly in \mathcal{H} to some $(\phi_1, \phi_2) \in \mathcal{H}$. Moreover, by the Rellich-Kondrachov compactness theorem, up to a further subsequence, (ϕ_1^h, ϕ_2^h) converges strongly to (ϕ_1, ϕ_2) in $L^2(B_R) \oplus L^2(B_R)$ for any $R > 0$, where B_R denotes the open ball in \mathbb{R}^N of radius R , centered at the origin. Let now $M > 0$ be an arbitrary number. Then, by Assumption 2.1, there exists an $R > 0$ such that $V_i(x) \geq M$ for all $x \in \mathbb{R}^N \setminus B_R$ and any $i = 1, 2$. Hence, we can write

$$\begin{aligned} \int_{\mathbb{R}^N} |\phi_i^h(x) - \phi_i(x)|^2 dx &= \int_{B_R} |\phi_i^h(x) - \phi_i(x)|^2 dx + \int_{\mathbb{R}^N \setminus B_R} |\phi_i^h(x) - \phi_i(x)|^2 dx \\ &\leq \int_{B_R} |\phi_i^h(x) - \phi_i(x)|^2 dx + \frac{1}{M} \int_{\mathbb{R}^N \setminus B_R} V_i(x) |\phi_i^h(x) - \phi_i(x)|^2 dx \\ &\leq \int_{B_R} |\phi_i^h(x) - \phi_i(x)|^2 dx + \frac{4C^2}{M}. \end{aligned}$$

Let now $\varepsilon > 0$ be given and choose an $M_0 > 0$ such that $4C^2/M_0 < \varepsilon/2$. Then, as the corresponding radius $R_0 > 0$ is fixed, take $h_0 \geq 1$ such that $\int_{B_{R_0}} |\phi_i^h(x) - \phi_i(x)|^2 dx < \varepsilon/2$ for any $h \geq h_0$. This yields $\|\phi_i^h - \phi_i\|_{L^2} \rightarrow 0$ for $h \rightarrow \infty$ and proves the first assertion. Moreover, by the Gagliardo-Nirenberg inequality and the boundedness in \mathcal{H} , we have

$$\|\phi_i^h - \phi_i\|_{L^{\frac{4N}{N+2}}}^4 \leq C \|\phi_i^h - \phi_i\|_{L^2}^{6-N} \|\phi_i^h - \phi_i\|_{H^1}^{N-2} \leq C \|\phi_i^h - \phi_i\|_{L^2}^{6-N},$$

from which it follows that

$$\lim_{h \rightarrow \infty} \|\phi_i^h - \phi_i\|_{L^{\frac{4N}{N+2}}} = 0.$$

This completes the proof. \square

The interaction between the components ϕ_1 and ϕ_2 is described by the following Coulomb energy functional which is well-known from classical Hartree theory.

Definition 2.2.

The Coulomb energy functional ⁵

$$\mathbb{D}: H^1(\mathbb{R}^N) \times H^1(\mathbb{R}^N) \rightarrow \mathbb{R}$$

is defined by

$$\mathbb{D}(\phi_1, \phi_2) = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} |\phi_1(x)|^2 V(x-y) |\phi_2(y)|^2 dx dy, \tag{5}$$

where the interaction potential V is the Coulomb potential in \mathbb{R}^N for $N \geq 3$,

$$V(x) = \frac{1}{|x|^{N-2}}. \tag{6}$$

Due to the following lemma, for any $3 \leq N \leq 6$, the Coulomb energy functional with potential (6) is well-defined.

Lemma 2.2.

Let $3 \leq N \leq 6$ and let $\phi_i \in H^1(\mathbb{R}^N)$ with $\|\phi_i\|_{L^2}^2 = N_i > 0$ for $i = 1, 2$. Then, there exists a constant C such that

$$\mathbb{D}(\phi_1, \phi_2) \leq C(N_1 N_2)^{\frac{6-N}{4}} \|\phi_1\|_{H^1}^{\frac{N-2}{2}} \|\phi_2\|_{H^1}^{\frac{N-2}{2}}.$$

Proof. Due to Schwarz' inequality, we have

$$\mathbb{D}(\phi_1, \phi_2)^2 \leq \mathbb{D}(\phi_1, \phi_1) \mathbb{D}(\phi_2, \phi_2). \tag{7}$$

Hence, by the Hardy-Littlewood-Sobolev inequality (for $N \geq 3$) and the Gagliardo-Nirenberg inequality (for $2 \leq N \leq 6$), we get

$$\mathbb{D}(\phi_i, \phi_i) \leq C \|\phi_i\|_{L^{\frac{4N}{N+2}}}^4 \leq C \|\phi_i\|_{L^2}^{6-N} \|\phi_i\|_{H^1}^{N-2} = C N_i^{\frac{6-N}{2}} \|\phi_i\|_{H^1}^{N-2},$$

which yields the assertion. □

Remark 2.1.

If $N \geq 2$ and the interaction potential is of the form

$$V_\lambda(x) = \frac{1}{|x|^\lambda} \text{ for some } 0 < \lambda < \min\{4, N\}, \tag{8}$$

we can again estimate the energy functional

$$\mathbb{D}_\lambda(\phi_1, \phi_2) := \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} |\phi_1(x)|^2 V_\lambda(x-y) |\phi_2(y)|^2 dx dy \tag{9}$$

by virtue of the Hardy-Littlewood-Sobolev inequality (for any $0 < \lambda < N$) and the Gagliardo-Nirenberg inequality (for any $0 < \lambda \leq 4$) as

$$\mathbb{D}_\lambda(\phi_1, \phi_2) \leq C \|\phi_1\|_{L^{\frac{4N}{2N-\lambda}}}^2 \|\phi_2\|_{L^{\frac{4N}{2N-\lambda}}}^2 \leq C(N_1 N_2)^{\frac{4-\lambda}{4}} \|\phi_1\|_{H^1}^{\lambda/2} \|\phi_2\|_{H^1}^{\lambda/2}.$$

In particular, if $N = 2$ and $\lambda = 1$, we have

$$\mathbb{D}_1(\phi_1, \phi_2) \leq C(N_1 N_2)^{3/4} \|\phi_1\|_{H^1}^{1/2} \|\phi_2\|_{H^1}^{1/2}.$$

If $\lambda = N - 2$ with $N \geq 3$ then $\mathbb{D}_{N-2} = \mathbb{D}$ and one recovers the estimate of the previous Lemma 2.2.

⁵ Also called direct term in the Hartree (-Fock) theory.

2.2. Existence of a minimizer

Let us consider the following two component Hartree eigenvalue system in \mathbb{R}^N for $3 \leq N \leq 6$ with Coulomb interaction V from (6) and $N_1, N_2 > 0$,

$$\begin{cases} -\Delta\phi_1 + V_1(x)\phi_1 + \vartheta_1 (V * |\phi_1|^2) \phi_1 + \kappa (V * |\phi_2|^2) \phi_1 = \mu_1 \phi_1, \\ -\Delta\phi_2 + V_2(x)\phi_2 + \vartheta_2 (V * |\phi_2|^2) \phi_2 + \kappa (V * |\phi_1|^2) \phi_2 = \mu_2 \phi_2, \\ \|\phi_1\|_{L^2}^2 = N_1, \\ \|\phi_2\|_{L^2}^2 = N_2. \end{cases} \quad (10)$$

Since we are interested in the phase segregation phenomenon in the case of a purely repulsive Hartree system, we make the following assumption.

Assumption 2.2.

The self-coupling constants ϑ_1, ϑ_2 and the interaction strength κ are nonnegative,

$$\vartheta_1, \vartheta_2 \geq 0, \quad \kappa \geq 0.$$

Remark 2.2.

In the case of coupled Bose–Einstein condensates discussed in the introduction (where the nonlinearities are local, i.e. $V = \delta$), the self-coupling constants ϑ_1, ϑ_2 as well as the interaction strength κ are explicitly related to the scattering lengths and the masses of the atomic species in the condensates (see e.g. [10]).

In order to study the nonlinear ground states of the Hartree system (10), we make use of the following energy functional.⁶

Definition 2.3.

The Hartree energy functional $\mathcal{E}_\kappa : \mathcal{H} \rightarrow [0, \infty)$ is defined by

$$\mathcal{E}_\kappa(\phi_1, \phi_2) = \mathcal{E}_\infty(\phi_1, \phi_2) + \kappa \mathbb{D}(\phi_1, \phi_2), \quad (11)$$

where the decoupled energy functional $\mathcal{E}_\infty : \mathcal{H} \rightarrow [0, \infty)$ consists of the sum of the two single particle energies $\mathcal{E}_i : \mathcal{H} \rightarrow [0, \infty)$,

$$\mathcal{E}_\infty(\phi_1, \phi_2) = \sum_{i=1}^2 \mathcal{E}_i(\phi_i), \quad (12)$$

$$\mathcal{E}_i(\phi_i) = \int_{\mathbb{R}^N} |\nabla \phi_i(x)|^2 dx + \int_{\mathbb{R}^N} V_i(x) |\phi_i(x)|^2 dx + \frac{\vartheta_i}{2} \mathbb{D}(\phi_i, \phi_i). \quad (13)$$

In view of Lemma 2.2, the functional \mathcal{E}_κ is well-defined for $3 \leq N \leq 6$. Moreover, it is readily seen that \mathcal{E}_κ is a C^1 smooth functional and that its critical points constrained to the set $\{(\phi_1, \phi_2) \in \mathcal{H} : \|\phi_i\|_{L^2}^2 = N_i \text{ for } i = 1, 2\}$ are weak solutions of (10).

Remark 2.3.

The case $\kappa = 0$ corresponds to a noninteracting Hartree system (10) consisting of two independent Hartree equations, each describing a repulsive single particle self-coupling.

⁶ From here on, since $\vartheta_1, \vartheta_2 \geq 0$ and $N_1, N_2 > 0$ are fixed, we display the dependence of the energy functionals and the ground state energies on the interaction strength κ only.

Definition 2.4.

The ground state energy $E_\kappa \geq 0$ of the Hartree functional (11) at interaction strength $\kappa \in [0, \infty)$ is defined by

$$E_\kappa = \inf_{(\phi_1, \phi_2) \in \mathcal{S}} \mathcal{E}_\kappa(\phi_1, \phi_2), \quad (14)$$

where the infimum is taken over the set

$$\mathcal{S} = \{(\phi_1, \phi_2) \in \mathcal{H} : \|\phi_i\|_{L^2}^2 = N_i \text{ for } i = 1, 2\}. \quad (15)$$

Moreover, the segregated ground state energy $E_\infty \geq 0$ is defined by

$$E_\infty = \inf_{(\phi_1, \phi_2) \in \mathcal{S}_\infty} \mathcal{E}_\infty(\phi_1, \phi_2),$$

where now the infimum is taken over the set

$$\mathcal{S}_\infty = \{(\phi_1, \phi_2) \in \mathcal{S} : \mathbb{D}(\phi_1, \phi_2) = 0\}.$$

Let us now prove that the Hartree functional (11) admits a real and positive minimizer for any positive interaction strength κ .

Proposition 2.1.

Let $\kappa \in (0, \infty)$ and $3 \leq N \leq 6$. Then, there exists a positive minimizer $(\phi_1^\kappa, \phi_2^\kappa) \in \mathcal{S}$ of the Hartree functional (11) with ground state energy E_κ given in (14).

Proof. In order to prove the assertion, we make use of the direct method in the calculus of variations. Hence, we verify the three standard assumptions implying the existence of a minimizer. First, since by Lemma 2.1, the normed space \mathcal{H} from (3) with the norm from (4) is compactly embedded in $L^2(\mathbb{R}^N) \oplus L^2(\mathbb{R}^N)$, it follows that the set \mathcal{S} from (15) is weakly closed in \mathcal{H} . Second, since

$$\|(\phi_1, \phi_2)\|_{\mathcal{H}}^2 \leq \mathcal{E}_\kappa(\phi_1, \phi_2) = \|(\phi_1, \phi_2)\|_{\mathcal{H}}^2 + \sum_{i=1}^2 \frac{\partial_i}{2} \mathbb{D}(\phi_i, \phi_i) + \kappa \mathbb{D}(\phi_1, \phi_2), \quad (16)$$

the set $\{(\phi_1, \phi_2) \in \mathcal{S} : \mathcal{E}_\kappa(\phi_1, \phi_2) \leq a\}$ is a bounded nonempty subset of \mathcal{S} for any positive number a . Third, we have to show that the functional \mathcal{E}_κ is weakly lower semicontinuous on \mathcal{S} . For this purpose, consider a sequence of elements $(\phi_1^h, \phi_2^h) \in \mathcal{S}$ which converges for $h \rightarrow \infty$ weakly in \mathcal{H} to some $(\phi_1, \phi_2) \in \mathcal{S}$. Since, for any $i, j = 1, 2$,

$$\frac{|\phi_i^h(x)|^2 |\phi_j^h(y)|^2}{|x-y|^{N-2}} \rightarrow \frac{|\phi_i(x)|^2 |\phi_j(y)|^2}{|x-y|^{N-2}} \quad \text{for a.e. } (x, y) \in \mathbb{R}^{2N},$$

Fatou's Lemma implies

$$\mathbb{D}(\phi_1, \phi_2) \leq \liminf_{h \rightarrow \infty} \mathbb{D}(\phi_1^h, \phi_2^h), \quad \mathbb{D}(\phi_i, \phi_i) \leq \liminf_{h \rightarrow \infty} \mathbb{D}(\phi_i^h, \phi_i^h). \quad (17)$$

Therefore, due to (16), the fact that the norm $\|\cdot\|_{\mathcal{H}}$ from (4) on \mathcal{H} is weakly lower semicontinuous on \mathcal{S} , and (17), the Hartree functional \mathcal{E}_κ is indeed weakly lower semicontinuous on \mathcal{S} . Hence, the three assumptions are verified and the existence of a minimizer is proven. Moreover, due to the convexity inequality for gradients,

$$\int_{\mathbb{R}^N} |\nabla |\phi_i|(x)|^2 dx \leq \int_{\mathbb{R}^N} |\nabla \phi_i(x)|^2 dx,$$

the Hartree functional \mathcal{E}_κ satisfies the following inequality for any $(\phi_1, \phi_2) \in \mathcal{S}$,

$$\mathcal{E}_\kappa(|\phi_1|, |\phi_2|) \leq \mathcal{E}_\kappa(\phi_1, \phi_2).$$

Consequently, with no loss of generality, we can assume that any minimizer of \mathcal{E}_κ is positive. \square

Remark 2.4.

Note that, for $3 \leq N \leq 5$, the Coulomb energy functional \mathbb{D} is not only weakly lower semicontinuous as given in (17), but even weakly continuous over \mathcal{H} , i.e. for any sequence of elements $(\phi_1^h, \phi_2^h) \in \mathcal{S}$ which converges for $h \rightarrow \infty$ weakly in \mathcal{H} to some $(\phi_1, \phi_2) \in \mathcal{S}$, we have

$$\lim_{h \rightarrow \infty} \mathbb{D}(\phi_1^h, \phi_2^h) = \mathbb{D}(\phi_1, \phi_2), \quad \lim_{h \rightarrow \infty} \mathbb{D}(\phi_i^h, \phi_i^h) = \mathbb{D}(\phi_i, \phi_i). \quad (18)$$

In order to prove this claim, we make use of Lemma 2.1, which states that the embedding $\mathcal{H} \hookrightarrow L^{\frac{4N}{N+2}}(\mathbb{R}^N) \oplus L^{\frac{4N}{N+2}}(\mathbb{R}^N)$ is compact. Hence, up to a subsequence, it follows that, for $i = 1, 2$,

$$\lim_{h \rightarrow \infty} \|\phi_i^h - \phi_i\|_{L^{\frac{4N}{N+2}}} = 0. \quad (19)$$

Using (19), we want to show that $\mathbb{D}(\phi_i^h, \phi_i^h) \rightarrow \mathbb{D}(\phi_i, \phi_i)$ as $h \rightarrow \infty$. To this end, we use that the Coulomb potential V from (6) is even and write

$$|\mathbb{D}(\phi_i^h, \phi_i^h) - \mathbb{D}(\phi_i, \phi_i)| \leq \mathbb{D}(|\phi_i^h|^2 - |\phi_i|^2)^{1/2}, (|\phi_i^h|^2 + |\phi_i|^2)^{1/2}.$$

By inequality (7), the Hardy-Littlewood-Sobolev inequality, and Hölder's inequality, it follows that there exist a constant C with

$$|\mathbb{D}(\phi_i^h, \phi_i^h) - \mathbb{D}(\phi_i, \phi_i)|^2 \leq C \| |\phi_i^h|^2 - |\phi_i|^2 \|_{L^{\frac{4N}{N+2}}}^4 \| (|\phi_i^h|^2 + |\phi_i|^2)^{1/2} \|_{L^{\frac{4N}{N+2}}}^4 \leq C \|\phi_i^h - \phi_i\|_{L^{\frac{4N}{N+2}}}^2.$$

This implies, via (19), the desired convergence of $\mathbb{D}(\phi_i^h, \phi_i^h)$ to $\mathbb{D}(\phi_i, \phi_i)$.⁷ Hence, it follows that all the terms in \mathcal{E}_κ containing the Coulomb energy functional \mathbb{D} are weakly continuous on \mathcal{S} . Notice that, as a consequence of (18), the weak lower semicontinuity of \mathcal{E}_κ over \mathcal{S} also holds in the case of attractive self-coupling or attractive interaction, i.e. for $\vartheta_1, \vartheta_2 \leq 0$ or $\kappa \leq 0$. In fact, this case amounts to the replacement of some (or all) \mathbb{D} terms (with positive coupling) in the Hartree functional by $-\mathbb{D}$.

2.3. Phase segregation

As pointed out in the introduction, we are interested in the situation where the values of the self-coupling constants ϑ_1, ϑ_2 (and N_1, N_2) remain fixed whereas the interaction strength κ becomes very large.

Definition 2.5.

A sequence of minimizers $(\phi_1^\kappa, \phi_2^\kappa) \in \mathcal{S}$ of the Hartree energy functional \mathcal{E}_κ from (11) is said to be *phase segregating* if

$$\mathbb{D}(\phi_1^\kappa, \phi_2^\kappa) = o(1) \quad \text{for } \kappa \rightarrow \infty.$$

Remark 2.5.

If the phase segregating sequence $(\phi_1^\kappa, \phi_2^\kappa)$ is convergent in \mathcal{H} , then the limiting configuration $(\phi_1^\infty, \phi_2^\infty)$ satisfies $\mathbb{D}(\phi_1^\infty, \phi_2^\infty) = 0$.

Let us now state our main assertion.

Theorem 2.1.

Let $3 \leq N \leq 6$ and let \mathbb{D} be the Coulomb energy functional from (5). Then, for $\kappa \in (0, \infty)$, any sequence of minimizers $(\phi_1^\kappa, \phi_2^\kappa) \in \mathcal{S}$ of the Hartree energy functional \mathcal{E}_κ from (11) is phase segregating for $\kappa \rightarrow \infty$, and

$$\mathbb{D}(\phi_1^\kappa, \phi_2^\kappa) = o(\kappa^{-1}).$$

In addition, such a sequence converges in the \mathcal{H} -norm to a minimizer $(\phi_1^\infty, \phi_2^\infty) \in \mathcal{S}_\infty$ of the decoupled functional \mathcal{E}_∞ from (12) and (13).

⁷ The convergence $\mathbb{D}(\phi_1^h, \phi_2^h) \rightarrow \mathbb{D}(\phi_1, \phi_2)$ as $h \rightarrow \infty$ can be proved in a similar fashion.

Corollary 2.1.

Under the assumptions of Theorem 2.1, the limiting configuration satisfies the following set of uncoupled variational inequalities,

$$-\Delta\phi_i^\infty + V_i(x)\phi_i^\infty + \vartheta_i \left(V * |\phi_i^\infty|^2 \right) \phi_i^\infty \leq \mu_i^\infty \phi_i^\infty, \quad (20)$$

where $N_i\mu_i^\infty = \mathcal{E}_i(\phi_i^\infty) + \frac{\vartheta_i}{2} \mathbb{D}(\phi_i^\infty, \phi_i^\infty)$ and $i = 1, 2$.

Remark 2.6.

Although we stated Theorem 2.1 for minimizers of the Hartree functional in \mathbb{R}^N with $3 \leq N \leq 6$ containing the Coulomb energy functional \mathbb{D} , it also holds for minimizers of the Hartree functional in \mathbb{R}^N with $0 < \lambda < \min\{4, N\}$ containing instead \mathbb{D}_λ from (9). This corresponds to the system

$$\begin{cases} -\Delta\phi_1 + V_1(x)\phi_1 + \vartheta_1 (V_\lambda * |\phi_1|^2) \phi_1 + \kappa (V_\lambda * |\phi_2|^2) \phi_1 = \mu_1 \phi_1, \\ -\Delta\phi_2 + V_2(x)\phi_2 + \vartheta_2 (V_\lambda * |\phi_2|^2) \phi_2 + \kappa (V_\lambda * |\phi_1|^2) \phi_2 = \mu_2 \phi_2, \\ \|\phi_1\|_{L^2}^2 = N_1, \\ \|\phi_2\|_{L^2}^2 = N_2, \end{cases} \quad (21)$$

where V_λ stems from (8). In particular, in view of the numerical setup, the case $N = 2$ and $\lambda = 1$ is covered.

Proof. Consider a sequence of minimizers $(\phi_1^\kappa, \phi_2^\kappa) \in \mathcal{S}$ for $\kappa \rightarrow \infty$ whose existence is assured by Proposition 2.1. Note first that, in the light of Definition 2.4, the sequence of corresponding ground state energies (E_κ) is uniformly bounded because

$$E_\kappa = \inf_{(\phi_1, \phi_2) \in \mathcal{S}} \mathcal{E}_\kappa(\phi_1, \phi_2) \leq \inf_{(\phi_1, \phi_2) \in \mathcal{S}_\infty} \mathcal{E}_\kappa(\phi_1, \phi_2) = \inf_{(\phi_1, \phi_2) \in \mathcal{S}_\infty} \mathcal{E}_\infty(\phi_1, \phi_2) = E_\infty. \quad (22)$$

In particular, due to (16) and the definition of a minimizer, the sequence $(\phi_1^\kappa, \phi_2^\kappa)$ is uniformly bounded in \mathcal{H} with respect to κ ,

$$\|(\phi_1^\kappa, \phi_2^\kappa)\|_{\mathcal{H}}^2 \leq \mathcal{E}_\kappa(\phi_1^\kappa, \phi_2^\kappa) = E_\kappa \leq E_\infty.$$

Hence, since \mathcal{H} is weakly sequentially compact, there exists a pair $(\phi_1^\infty, \phi_2^\infty) \in \mathcal{H}$ and a subsequence of $(\phi_1^\kappa, \phi_2^\kappa)$, again denoted by $(\phi_1^\kappa, \phi_2^\kappa)$ which, for $\kappa \rightarrow \infty$, converges weakly in \mathcal{H} to $(\phi_1^\infty, \phi_2^\infty)$. Next, we want to show that $(\phi_1^\infty, \phi_2^\infty) \in \mathcal{S}_\infty$. Since $(\phi_1^\kappa, \phi_2^\kappa) \in \mathcal{S}$ and the embedding $\mathcal{H} \hookrightarrow L^2(\mathbb{R}^N) \oplus L^2(\mathbb{R}^N)$ is compact, we have, for $i = 1, 2$,

$$\|\phi_i^\infty\|_{L^2}^2 = N_i.$$

Hence, $(\phi_1^\infty, \phi_2^\infty) \in \mathcal{S}$. Moreover, again due (16) and (22), we have

$$\kappa \mathbb{D}(\phi_1^\kappa, \phi_2^\kappa) \leq \mathcal{E}_\kappa(\phi_1^\kappa, \phi_2^\kappa) \leq E_\infty, \quad (23)$$

which implies that the sequence $(\phi_1^\kappa, \phi_2^\kappa)$ is phase segregating for $\kappa \rightarrow \infty$,

$$\mathbb{D}(\phi_1^\kappa, \phi_2^\kappa) = O(\kappa^{-1}).$$

Also, since we know from the proof of Proposition 2.1 that the Coulomb energy \mathbb{D} is weakly lower semicontinuous on \mathcal{S} , we get

$$\mathbb{D}(\phi_1^\infty, \phi_2^\infty) = 0,$$

and, therefore, $(\phi_1^\infty, \phi_2^\infty) \in \mathcal{S}_\infty$. In order to prove that $(\phi_1^\infty, \phi_2^\infty)$ is a minimizer of \mathcal{E}_∞ and that $(\phi_1^\kappa, \phi_2^\kappa)$ converges strongly in \mathcal{H} to $(\phi_1^\infty, \phi_2^\infty)$, we next show that $\mathbb{D}(\phi_1^\kappa, \phi_2^\kappa) = o(\kappa^{-1})$. To this end, consider the sequence $\kappa \mathbb{D}(\phi_1^\kappa, \phi_2^\kappa)$ which is

bounded due to (23), and pick a convergent subsequence, denoted by $\kappa_n \mathbb{D}(\phi_1^{\kappa_n}, \phi_2^{\kappa_n})$. Then, using that $(\phi_1^\infty, \phi_2^\infty) \in \mathcal{S}_\infty$, the weak lower semicontinuity of the decoupled energy functional \mathcal{E}_∞ on \mathcal{S} , and (22), we get

$$\mathcal{E}_\infty(\phi_1^\infty, \phi_2^\infty) + \lim_{n \rightarrow \infty} \kappa_n \mathbb{D}(\phi_1^{\kappa_n}, \phi_2^{\kappa_n}) \leq \liminf_{n \rightarrow \infty} \mathcal{E}_{\kappa_n}(\phi_1^{\kappa_n}, \phi_2^{\kappa_n}) \leq E_\infty \leq \mathcal{E}_\infty(\phi_1^\infty, \phi_2^\infty), \quad (24)$$

with the consequence that $\kappa_n \mathbb{D}(\phi_1^{\kappa_n}, \phi_2^{\kappa_n}) = 0$ as $n \rightarrow \infty$. Therefore, since this holds for all convergent subsequences of $\kappa \mathbb{D}(\phi_1^\kappa, \phi_2^\kappa)$, we arrive at

$$\mathbb{D}(\phi_1^\kappa, \phi_2^\kappa) = o(\kappa^{-1}). \quad (25)$$

This implies, on one hand, that $(\phi_1^\kappa, \phi_2^\kappa)$ converges strongly in \mathcal{H} to $(\phi_1^\infty, \phi_2^\infty)$ since from $E_\kappa \leq \mathcal{E}_\infty(\phi_1^\infty, \phi_2^\infty)$, (25), and the weak continuity of $\mathbb{D}(\phi_1^\kappa, \phi_2^\kappa)$, we get

$$\limsup_{\kappa \rightarrow \infty} \|(\phi_1^\kappa, \phi_2^\kappa)\|_{\mathcal{H}}^2 \leq \|(\phi_1^\infty, \phi_2^\infty)\|_{\mathcal{H}}^2.$$

On the other hand, using (24) and (25), we see that $(\phi_1^\infty, \phi_2^\infty)$ is a minimizer of \mathcal{E}_∞ , that is $E_\infty = \mathcal{E}_\infty(\phi_1^\infty, \phi_2^\infty)$. Finally, we note that, again due to (24), we have $E_\kappa \rightarrow E_\infty$ as $\kappa \rightarrow \infty$. This brings the proof of Theorem 2.1 to an end. \square

Finally, we prove the assertion of Corollary 2.1.

Proof. Observe that, by virtue of

$$\mu_i^\kappa = \frac{1}{N_i} \left\{ \mathcal{E}_i(\phi_i^\kappa) + \frac{\vartheta_i}{2} \mathbb{D}(\phi_i^\kappa, \phi_i^\kappa) + \kappa \mathbb{D}(\phi_1^\kappa, \phi_2^\kappa) \right\}, \quad (26)$$

the inequality (23) and $\mathcal{E}_i(\phi_i^\kappa) \leq E_\infty$, we get

$$\sup_{\kappa \geq 1} \mu_i^\kappa < \infty,$$

where μ_i^κ denotes the nonlinear eigenvalue of the minimizer ϕ_i^κ as the weak nonlinear ground state in the corresponding nonlinear eigenvalue system (10). Then, up to a subsequence, $\mu_i^\kappa \rightarrow \mu_i^\infty$ as $\kappa \rightarrow \infty$. Testing the equations of (10) with arbitrary nonnegative functions η of compact support, we get, recalling that $\phi_i \geq 0$,

$$\begin{aligned} & \int_{\mathbb{R}^N} \nabla \phi_i^\kappa(x) \cdot \nabla \eta(x) \, dx + \int_{\mathbb{R}^N} V_i(x) \phi_i^\kappa(x) \eta(x) \, dx + \vartheta_i \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \frac{\phi_i^\kappa(y)^2 \phi_i^\kappa(x) \eta(x)}{|x-y|^{N-2}} \, dx \, dy \\ & \leq \mu_i^\kappa \int_{\mathbb{R}^N} \phi_i^\kappa(x) \eta(x) \, dx. \end{aligned}$$

Hence, letting $\kappa \rightarrow \infty$, it turns out that ϕ_i^∞ satisfies the variational inequality (20). Finally, the strong convergence and (26) yields, for $i = 1, 2$,

$$N_i \mu_i^\infty = \mathcal{E}_i(\phi_i^\infty) + \frac{\vartheta_i}{2} \mathbb{D}(\phi_i^\infty, \phi_i^\infty).$$

This ends the proof of Corollary 2.1. \square

3. Numerical approach

3.1. Galerkin approximation of the nonlinear eigenvalue system

In order to carry out the numerical simulation, we treat the Hartree system in the plane from (21) with $N = 2$ and $\lambda = 1$ in the framework of the following finite element approximation. As physical subdomain of \mathbb{R}^2 , we choose the open square

$$\Omega = (0, D)^{\times 2} \tag{27}$$

with $D > 0$ whose closure is the union of the $(m - 1)^2$ congruent closed subsquares generated by dividing each side of Ω equidistantly into $m - 1$ intervals. Let us denote by $M = (m - 2)^2$ the total number of interior vertices of this lattice and by $h = D/(m - 1)$ the lattice spacing.⁸ Moreover, let us choose the Galerkin space S_h to be spanned by the bilinear Lagrange rectangle finite elements $\varphi_j \in C(\bar{\Omega})$.⁹

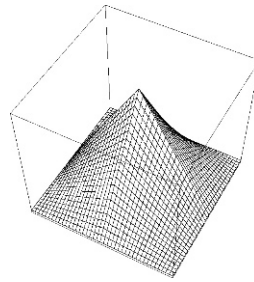


Figure 1. $\varphi_0(x, y)$ on its support $[0, 2h]^{\times 2}$ with maximum at vertex (h, h) .

Hence, with this choice, we have

$$S_h \subset C(\bar{\Omega}) \cap H_0^1(\Omega),$$

and $\dim S_h = (m - 2)^2$. The Hartree system (21) in its weak finite element approximation form reads, for all $\varphi \in S_h$,¹⁰

$$\begin{cases} (\nabla \varphi, \nabla \phi_1) + (\varphi, V_1 \phi_1) + (\varphi, (V * [\vartheta_1 |\phi_1|^2 + \kappa |\phi_2|^2]) \phi_1) = \mu_{1,0}(\varphi, \phi_1), \\ (\nabla \varphi, \nabla \phi_2) + (\varphi, V_2 \phi_2) + (\varphi, (V * [\vartheta_2 |\phi_2|^2 + \kappa |\phi_1|^2]) \phi_2) = \mu_{2,0}(\varphi, \phi_2), \\ \|\phi_1\|_{L^2}^2 = N_1, \\ \|\phi_2\|_{L^2}^2 = N_2. \end{cases} \tag{29}$$

⁸ As bijection from the one-dimensional to the two-dimensional lattice numbering, we may use the mapping $\tau : \{0, \dots, m - 1\}^{\times 2} \rightarrow \{0, \dots, m^2 - 1\}$ with $j = \tau(m_1, m_2) := m_1 + m_2 m$.

⁹ The reference basis function $\varphi_0 : \bar{\Omega} \rightarrow [0, \infty)$ is defined on its support $[0, 2h]^{\times 2}$ by

$$\varphi_0(x, y) := \frac{1}{h^2} \begin{cases} xy, & \text{if } (x, y) \in [0, h]^{\times 2}, \\ (2h - x)y, & \text{if } (x, y) \in [h, 2h] \times [0, h], \\ (2h - x)(2h - y), & \text{if } (x, y) \in [h, 2h]^{\times 2}, \\ x(2h - y), & \text{if } (x, y) \in [0, h] \times [h, 2h], \end{cases} \tag{28}$$

see Figure 1. The functions φ_j are then defined to be of the form (28) having their support translated by $(m_1 h, m_2 h)$ with $m_1, m_2 = 0, \dots, m - 3$.

¹⁰ In this section, (\cdot, \cdot) and $\|\cdot\|$ stand for the $L^2(\Omega)$ -scalar product and $L^2(\Omega)$ -norm, respectively. Moreover, the convolution on the finite domain Ω is defined, for any $(x, y) \in \Omega$, by $(V * \phi)(x, y) := \int_{\Omega} V(x - x', y - y') \phi(x', y') dx' dy'$. See also [3] for the analysis of the continuum, the semidiscrete, and the fully discrete setting for the dynamical single particle Hartree equation.

If we expand $\phi_\alpha \in S_h$ with expansion coefficients $z_\alpha = (z_{\alpha,1}, \dots, z_{\alpha,M}) \in \mathbb{C}^M$ w.r.t. the finite element basis $\{\varphi_j\}_{j=1}^M$ of S_h ,

$$\phi_\alpha = \sum_{j=1}^M z_{\alpha,j} \varphi_j, \quad (30)$$

and if we plug this expansion together with $\varphi = \varphi_i$, $i = 1, \dots, M$, into (29), we get the following coupled matrix system on \mathbb{C}^M ,¹¹

$$\begin{cases} Q_1[z_1, z_2]z_1 = \mu_{0,1}z_1, \\ Q_2[z_1, z_2]z_2 = \mu_{0,2}z_2, \\ |z_1|_2^2 = N_1, \\ |z_2|_2^2 = N_2. \end{cases} \quad (31)$$

Here, the matrix-valued mappings $Q_1, Q_2 : \mathbb{C}^M \times \mathbb{C}^M \rightarrow \mathbb{C}^{M \times M}$ are defined by

$$\begin{aligned} Q_1[z_1, z_2] &:= A^{-1}(B + Y_1 + \vartheta_1 G[z_1] + \kappa G[z_2]), \\ Q_2[z_1, z_2] &:= A^{-1}(B + Y_2 + \vartheta_2 G[z_2] + \kappa G[z_1]), \end{aligned}$$

and $A \in \mathbb{C}^{M \times M}$ is the mass matrix, $B \in \mathbb{C}^{M \times M}$ the stiffness matrix, and $Y_\alpha \in \mathbb{C}^{M \times M}$ the matrices generated by the external potentials V_α ,

$$A_{ij} := (\varphi_i, \varphi_j), \quad B_{ij} := (\nabla \varphi_i, \nabla \varphi_j), \quad (Y_\alpha)_{ij} := (\varphi_i, V_\alpha \varphi_j). \quad (32)$$

Moreover, the matrix-valued mapping $G : \mathbb{C}^M \rightarrow \mathbb{C}^{M \times M}$ is defined on $w = (w_1, \dots, w_M) \in \mathbb{C}^M$ by

$$G[w]_{ij} := \left(\varphi_i, g \left[\sum_{k=1}^M w_k \varphi_k \right] \varphi_j \right) = \sum_{k,l=1}^M \bar{w}_k w_l V_{iklj},$$

where the function g and the Hartree convolution term V_{iklj} are defined by

$$g[\phi] := V * |\phi|^2, \quad V_{iklj} := (\varphi_i, V * (\bar{\varphi}_k \varphi_l) \varphi_j). \quad (33)$$

Remark 3.1.

We avoid the inversion of the mass matrix A and simplify the evaluation of the double integral in the Hartree convolution term (33) by approximating the integrals over Ω by the standard mass lumping quadrature procedure.

In order to simplify the eigenvalue system (31) with the help of Remark 3.1, let us introduce the mappings $H_1, H_2 : \mathbb{C}^M \times \mathbb{C}^M \rightarrow \mathbb{C}^{M \times M}$ defined by

$$\begin{aligned} H_1[z_1, z_2] &:= \frac{1}{h^2} (B + Y_1 + \vartheta_1 \text{diag}(G_0[z_1]) + \kappa \text{diag}(G_0[z_2])), \\ H_2[z_1, z_2] &:= \frac{1}{h^2} (B + Y_2 + \vartheta_2 \text{diag}(G_0[z_2]) + \kappa \text{diag}(G_0[z_1])), \end{aligned}$$

¹¹ $|z|_2^2 := \langle z, z \rangle_2$ denotes the L^2 -norm on \mathbb{C}^M , where $\langle z, w \rangle := \sum_{j=1}^M \bar{z}_j w_j$ and $\langle z, w \rangle_2 := \langle z, Aw \rangle$ are the Euclidean and the L^2 -scalar product on \mathbb{C}^M , respectively. For ϕ_α from (30), we have $\|\phi_\alpha\|^2 = \langle z_\alpha, Az_\alpha \rangle = |z_\alpha|_2^2 = N_\alpha$ for $\alpha = 1, 2$.

where $\text{diag} : \mathbb{C}^M \rightarrow \mathbb{C}^{M \times M}$ is defined to be the matrix-valued mapping on $w = (w_1, \dots, w_M) \in \mathbb{C}^M$ defined by $\text{diag}(w)_{ij} := \delta_{ij} w_j$ for all $i, j = 1, \dots, M$, and $G_0 : \mathbb{C}^M \rightarrow \mathbb{C}^M$ is defined by

$$G_0[w]_i := h^4 \sum_{j=1}^M |w_j|^2 V(h(\tau^{-1}(i) - \tau^{-1}(j))),$$

where τ is the grid numbering bijection from footnote 8. Hence, Remark 3.1 amounts to the replacement $G[z] \mapsto \text{diag}(G_0[z])$ and we get the approximated Hartree system

$$\begin{cases} H_1[z_1, z_2]z_1 = \mu_{0,1}z_1, \\ H_2[z_1, z_2]z_2 = \mu_{0,2}z_2, \\ |z_1|_2^2 = N_1, \\ |z_2|_2^2 = N_2. \end{cases} \quad (34)$$

3.2. Algorithms

In order to solve the nonlinear coupled eigenvalue system (34), we make use of the method of successive substitution¹² whose fixed-point map is constructed with the help of the power method used for the solution of the corresponding linearized problem. In the following, we briefly describe the basic ideas of these algorithms.

Method of successive substitution (MSS)

Let \mathcal{M} be the compact set

$$\mathcal{M} := \{[z_1, z_2] \in \mathbb{C}^M \times \mathbb{C}^M \mid |z_1|_2^2 = N_1, |z_2|_2^2 = N_2\}.$$

The MSS is an iterative method of the form

$$[z_1^{(n+1)}, z_2^{(n+1)}] = F[z_1^{(n)}, z_2^{(n)}], \quad (35)$$

where the fixed point map $F : \mathcal{M} \rightarrow \mathcal{M}$ is constructed as follows. Given an approximate nonlinear system ground state $[z_1^{(n)}, z_2^{(n)}] \in \mathcal{M}$ at iteration level $n \in \mathbb{N}$, the approximate nonlinear system ground state $[z_1^{(n+1)}, z_2^{(n+1)}] \in \mathcal{M}$ at iteration level $n+1$ is defined to be the linear system ground state of the linearized eigenvalue system

$$\begin{cases} H_1[z_1^{(n)}, z_2^{(n)}]z_1^{(n+1)} = \epsilon_{0,1}^{(n+1)} z_1^{(n+1)}, \\ H_2[z_1^{(n)}, z_2^{(n)}]z_2^{(n+1)} = \epsilon_{0,2}^{(n+1)} z_2^{(n+1)}, \\ |z_1^{(n+1)}|_2^2 = N_1, \\ |z_2^{(n+1)}|_2^2 = N_2. \end{cases} \quad (36)$$

Remark 3.2.

Here and in the following, we make the assumption that $H_\alpha[z_1^{(n)}, z_2^{(n)}]$ has a unique linear ground state. E.g., using perturbation theory in the regime of small nonlinear couplings, this holds as soon as the linear operator $H_\alpha[0, 0]$ has a nondegenerate ground state energy.

¹² Also called nonlinear Richardson iteration or Picard iteration.

Remark 3.3.

We can write the fixed point map $F_\alpha[z_1^{(n)}, z_2^{(n)}]$ from (35) with the help of the linear ground state projection

$$P_\alpha[z_1, z_2] = -\frac{1}{2\pi i} \oint_{\Gamma_\alpha[z_1, z_2]} (H_\alpha[z_1, z_2] - \zeta)^{-1} d\zeta,$$

where $\Gamma_\alpha[z_1, z_2]$ is a path which encircles the linear ground state energy of $H_\alpha[z_1, z_2]$ in the positive direction and no other point of the spectrum of $H_\alpha[z_1, z_2]$. The map F can now be written as

$$F_\alpha[z_1^{(n)}, z_2^{(n)}] = \sqrt{N_\alpha} \frac{P_\alpha[z_1^{(n)}, z_2^{(n)}]z_\alpha^{(n)}}{|P_\alpha[z_1^{(n)}, z_2^{(n)}]z_\alpha^{(n)}|_2}. \quad (37)$$

Since $H_\alpha[\cdot, \cdot]$ is Lipschitz continuous on \mathcal{M} , the map F has a not necessarily unique fixed point due to Schauder's fixed point theorem.

The system (36) being not only linearized but also decoupled, we can solve the two linear eigenvalue problems separately. In order to approximately determine the ground states of the linear eigenvalue problems, we make use of the power method which works as follows.

Power method (PM)

The PM computes the eigenvector of $H_\alpha[z_1^{(n)}, z_2^{(n)}]$ whose eigenvalue has largest modulus amongst all the eigenvalues whose eigenvectors appear in the eigenvector expansion of the starting approximation. To access the ground state of $H_\alpha[z_1^{(n)}, z_2^{(n)}]$, we apply the following spectral shift¹³

$$s_\alpha^{(n)} := |H_\alpha[z_1^{(n)}, z_2^{(n)}]|_1 + 1.$$

Moreover, we define the shifted operator by

$$\hat{H}_\alpha[z_1^{(n)}, z_2^{(n)}] := H_\alpha[z_1^{(n)}, z_2^{(n)}] - s_\alpha^{(n)}.$$

Now, the p -th iterate of the PM iteration is defined by¹⁴

$$z_\alpha^{(n+1), p} := \frac{\hat{H}_\alpha[z_1^{(n)}, z_2^{(n)}]^p z_\alpha^{(n)}}{|\hat{H}_\alpha[z_1^{(n)}, z_2^{(n)}]^p z_\alpha^{(n)}|}. \quad (38)$$

Remark 3.4.

Since $\hat{H}_\alpha[z_1^{(n)}, z_2^{(n)}]$ is real symmetric, the spectral theorem implies the existence of an orthonormal basis of \mathbb{C}^M of eigenvectors $\{w_{\alpha, k}\}_{k=0}^{M-1}$ of $\hat{H}_\alpha[z_1^{(n)}, z_2^{(n)}]$.¹⁵ Moreover, since the spectral radius of $\hat{H}_\alpha[z_1^{(n)}, z_2^{(n)}]$ is smaller than $s_\alpha^{(n)}$, we have for all eigenvalues of the shifted operator $\hat{e}_{\alpha, k} \in \text{spec}(H_\alpha[z_1^{(n)}, z_2^{(n)}]) - s_\alpha^{(n)}$ that

$$-2s_\alpha^{(n)} < \hat{e}_{\alpha, 0} < \hat{e}_{\alpha, 1} \leq \dots \leq \hat{e}_{\alpha, M-1} < 0.$$

¹³ For $A = [a_{ij}] \in \mathbb{C}^{M \times M}$, we define the ℓ^1 -matrix norm by $|A|_1 := \sum_{i,j=1}^M |a_{ij}|$.

¹⁴ $|z| := \langle z, z \rangle^{1/2}$ denotes the Euclidean norm of $z \in \mathbb{C}^M$.

¹⁵ We suppress the superscript n in the eigenvectors, eigenvalues, and in the expansion coefficients, since the PM iteration acts at a fixed n . Moreover, the numbering starts at 0 being the index of the ground state.

Let us expand $z_\alpha^{(n)}$ w.r.t. the orthonormal basis $\{w_{\alpha,k}\}_{k=0}^{M-1}$ as

$$z_\alpha^{(n)} = \sum_{k=0}^{M-1} \xi_{\alpha,k} w_{\alpha,k},$$

use that $\widehat{H}_\alpha[z_1^{(n)}, z_2^{(n)}]w_{\alpha,k} = \widehat{\epsilon}_{\alpha,k} w_{\alpha,k}$, and divide the numerator and the denominator in (38) by $|\widehat{\epsilon}_{\alpha,0}|^p$. Moreover, let us assume that $\xi_{\alpha,0} \neq 0$. Then, in the large p limit, $(-1)^p z_\alpha^{(n+1),p}$ converges to a multiple of the ground state of $H_\alpha[z_1^{(n)}, z_2^{(n)}]$,

$$z_\alpha^{(n+1),p} = (-1)^p \frac{\xi_{0,\alpha}}{|\xi_{0,\alpha}|} w_{\alpha,0} + o(1). \quad (39)$$

Remark 3.5.

Using formula (39), the fixed point map F from (35), (37) can also be written as

$$F_\alpha[z_1^{(n)}, z_2^{(n)}] = \sqrt{N_\alpha} \lim_{p \rightarrow \infty} \frac{(-1)^p z_\alpha^{(n+1),p}}{|z_\alpha^{(n+1),p}|_2}.$$

Stopping criteria

Both for the inner PM iteration and the outer MSS iteration, we use a relative error stopping criterion in the numerical computation. For the PM iteration, let us define the energy

$$\widehat{\epsilon}_{\alpha,0}^{(n+1),p} := \langle z_\alpha^{(n+1),p}, \widehat{H}_\alpha[z_1^{(n)}, z_2^{(n)}] z_\alpha^{(n+1),p} \rangle. \quad (40)$$

Then, for suitably chosen accuracy tolerance $\delta_{\text{PM}} > 0$, we stop the PM iteration for each component $\alpha = 1, 2$ as soon as

$$\frac{|(\widehat{H}_\alpha[z_1^{(n)}, z_2^{(n)}] - \widehat{\epsilon}_{\alpha,0}^{(n+1),p}) z_\alpha^{(n+1),p}|}{|\widehat{\epsilon}_{\alpha,0}^{(n+1),p} + s_\alpha^{(n)}|} \leq \delta_{\text{PM}}. \quad (41)$$

Remark 3.6.

Note that the quotient (41) does not depend on the shift $s_\alpha^{(n)}$, since the iterates $z_\alpha^{(n+1),p}$ are normalized w.r.t. the Euclidean norm on \mathbb{C}^M .

Remark 3.7.

Clearly, the stopping criterion (41) is satisfied for any eigenvector of $\widehat{H}_\alpha[z_1^{(n)}, z_2^{(n)}]$. But as soon as $\xi_{\alpha,0} \neq 0$, e.g. due to finite precision arithmetic, the PM iterate $z_\alpha^{(n+1),p}$ converges to a multiple of the ground state $w_{\alpha,0}$. But note that the chosen accuracy may be reached before a nonvanishing $\xi_{\alpha,0}$ is generated.

For the MSS iteration, we implement a similar stopping criterion. To this end, we define the approximate nonlinear ground state energies as

$$\mu_{\alpha,0}^{(n+1)} := \frac{1}{N_\alpha} \langle z_\alpha^{(n+1)}, H_\alpha[z_1^{(n+1)}, z_2^{(n+1)}] z_\alpha^{(n+1)} \rangle_2,$$

where, compared to (40), the Hartree energy H_α depends on iteration level $n+1$ instead of level n . We stop the MSS iteration as soon as

$$\frac{|(H_\alpha[z_1^{(n+1)}, z_2^{(n+1)}] - \mu_{0,\alpha}^{(n+1)}) z_\alpha^{(n+1)}|_2}{|\mu_{0,\alpha}^{(n+1)}|} \leq \delta_{\text{MSS}},$$

where $\delta_{\text{MSS}} > 0$ is some suitably chosen accuracy tolerance.

3.3. Phase segregation

As it has been defined above in Definition 2.5, a sequence of nonlinear ground state solutions $(\phi_1^\kappa, \phi_2^\kappa)$ is phase segregating if its Coulomb energy vanishes in the limit of large interaction strength κ , i.e.

$$\mathbb{D}(\phi_1^\kappa, \phi_2^\kappa) = (\phi_1^\kappa, (V * |\phi_2^\kappa|^2)\phi_1^\kappa) \rightarrow 0 \quad \text{for } \kappa \rightarrow \infty. \quad (42)$$

Plugging the expansions (30) into (42), we get

$$\mathbb{D}\left(\sum_{i=1}^M z_{1,i} \varphi_i, \sum_{j=1}^M z_{2,j} \varphi_j\right) = \langle z_1, G[z_2]z_1 \rangle.$$

Hence, making use of Remark 3.1, we define the approximated Coulomb energy $\mathbb{D}_0 : \mathbb{C}^M \times \mathbb{C}^M \rightarrow \mathbb{R}$ by

$$\mathbb{D}_0[z_1, z_2] := \langle z_1, \text{diag}(G_0[z_2])z_1 \rangle. \quad (43)$$

Below, we will use this approximation in the numerical computation of the Coulomb energy.

4. Figures

The numerical computations leading to the following figures visualize the qualitative picture of the approach to the segregated regime. First, we exhibit the densities of the wave functions ϕ_1 and ϕ_2 for increasing values of the interaction strength κ approaching the segregated regime. Second, we report on the decay of the Coulomb energy (43).

We choose the external potentials V_α for $\alpha = 1, 2$ to be isotropic harmonic potentials,

$$V_\alpha(x, y) = c_\alpha \left((x - a_\alpha)^2 + (y - b_\alpha)^2 \right), \quad (44)$$

and the interaction potential V to be a regularized Yukawa potential,

$$V(x, y) = \frac{e^{-\Gamma \sqrt{x^2 + y^2}}}{\sqrt{x^2 + y^2 + \gamma}}. \quad (45)$$

Remark 4.1.

The potential (45) being the regularized three-dimensional Yukawa potential, it may be argued that we consider a physically three-dimensional system constrained to a two-dimensional submanifold of the three-dimensional configuration space.

The specification of the parameters used in the simulations below is summarized in the following table (cf. (27), (29), (44), and (45)).¹⁶

N_1	N_2	a_1	b_1	c_1	a_2	b_2	c_2	ϑ_1	ϑ_2	κ	Γ	γ
1	1	$D/2$	$D/2$	10^5	$D/2$	$D/2$	10^3	0	0	cf. below	10^2	10^{-1}

Remark 4.2.

All the qualitative features of the following simulations have been tested for stability in different physical and numerical parameter ranges.

¹⁶ The code is part of our Hartree package written in C++.

4.1. $\kappa = 0$

For the interaction strength $\kappa = 0$, the system is uncoupled and linear, and we find the ground state wave functions of the harmonic oscillator. The supports are fully overlapping, see Figure 2.¹⁷

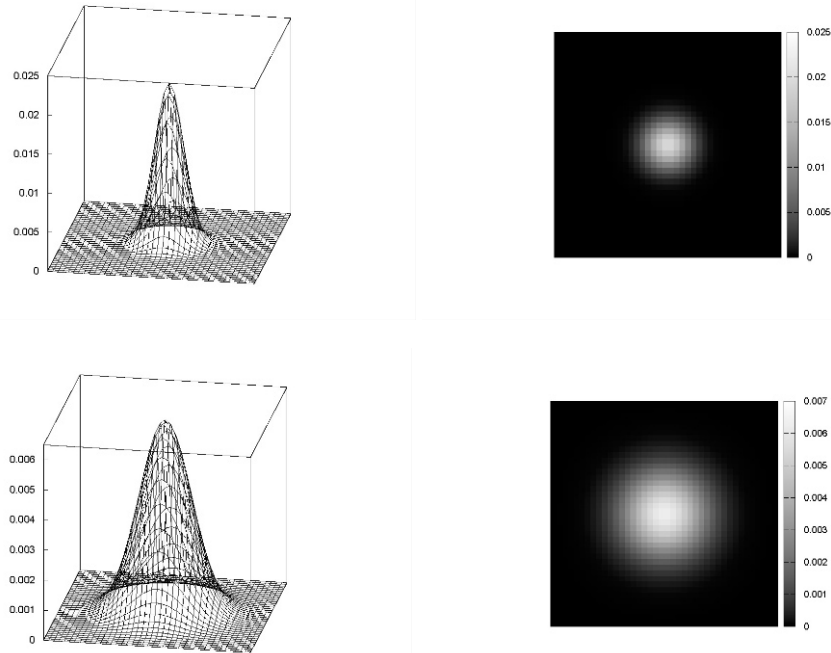


Figure 2. The wave function densities $|z_\alpha|^2$ and their contours with $\alpha = 1$ above and $\alpha = 2$ below for the interaction strength $\kappa = 0$.

4.2. $\kappa = 0.5$

The wave functions ϕ_1 and ϕ_2 start to feel their respective repulsion. The support of ϕ_1 is retracting whereas the one of ϕ_2 gets pushed outwards. The supports are still heavily overlapping, see Figure 3.

4.3. $\kappa = 10$

In the regime of large interaction strength κ , the segregation phenomenon occurs: the supports get more and more disjoint, see Figure 4.

Remark 4.3.

Up to the shape of the support of ϕ_i , there is no qualitative change in the picture if the two harmonic potentials are slightly dislocated with respect to each other.

¹⁷ All the figures have been produced with the help of gnuplot.

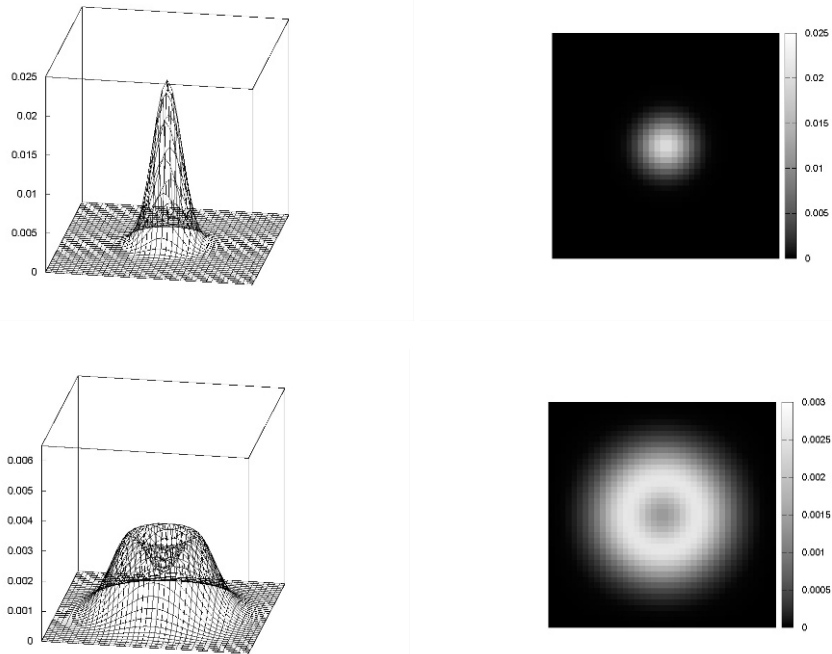


Figure 3. The interaction strength is $\kappa = 0.5$.

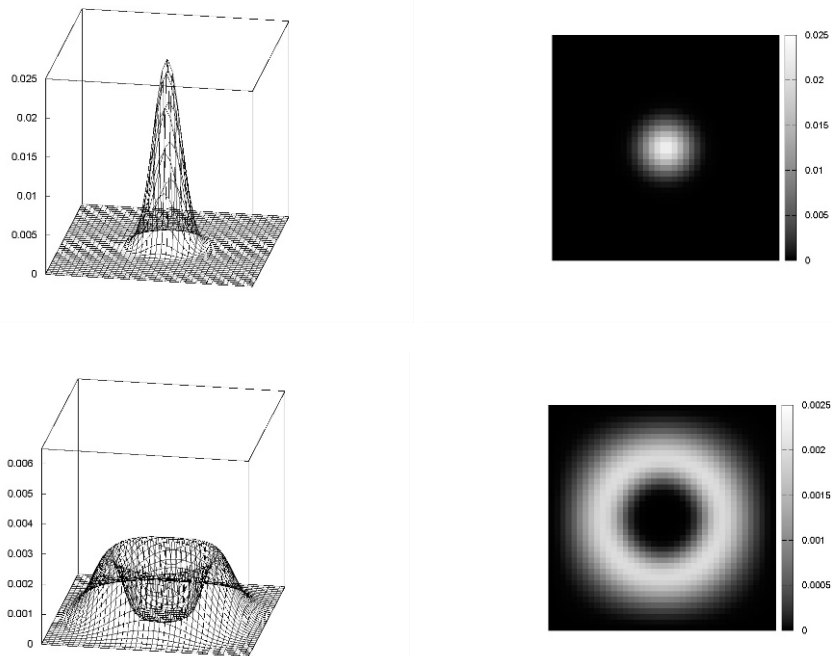


Figure 4. The interaction strength is $\kappa = 10$.

4.4. Coulomb energy

Finally, we monitor the decay of the Coulomb energy from formula (43), see Figure 5.

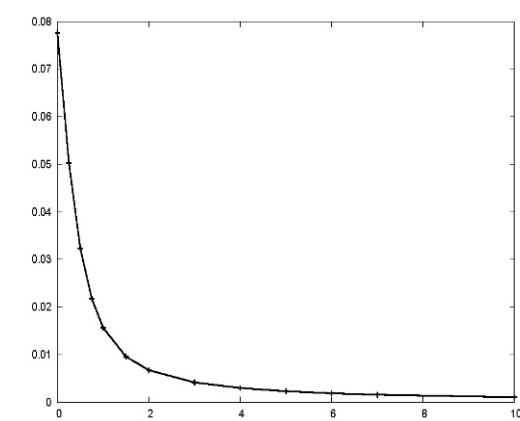


Figure 5. The decay of $\mathbb{D}_0[z_1^\kappa, z_2^\kappa]$ as a function of κ .

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