Symmetry Breaking Regime in the Nonlinear Hartree Equation

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Abstract

The present paper is concerned with minimizers Φ of the Hartree energy functional $\mathcal{H}_g[\bar{\psi}, \psi] = \frac{1}{2}\|\nabla\psi\|_2^2 + (\psi, v\psi)_2 + g(\psi, V * |\psi|^2\psi)_2$ with $g < 0$ on the configuration space $\mathbb{R}^d$, $d \geq 2$, for a general class of external potentials v and two-body potentials V. We prove that a minimizer Φ does not have the symmetry properties of the potential v for $|g|$ strictly larger than a critical $g_* > 0$. A numerical investigation visualizes this symmetry breaking regime in the simple case of an external double well potential. As a particular application of these results and as a motivation for the investigation of the Hartree functional, we propose a generalization of the Gross-Pitaevskii functional of Bose-Einstein condensation for *attractive* interatomic forces that overcomes the break-down of this theory at the collapse point of the condensate.

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1 Introduction

Bose-Einstein condensation (BEC) has been attracting growing attention in recent years, due to a series of seminal experiments essentially carried out in 1995 on rubidium $^{87}_{37}$Rb, sodium $^{23}_{11}$Na, and lithium $^{7}_{3}$Li, in which 10^3 to 10^6 atoms have been confined in magnetic traps with a characteristic length scale of $\sim 10^{-4}\, m$, cooled down to $\sim 10^{-6}\, K$. First evidence of BEC was found in time-of-flight measurements below a critical temperature, which, with the help of optical methods, recorded a sharp peak in the velocity distribution of atoms released to free expansion after having switched off the confining trap, cf. [1].

A description of BEC for very dilute gases can be based on an analysis of the *weak coupling limit of large bosonic systems*, cf. [2], [3], [4]. It reduces to the *nonlinear* Hartree theory whose ground state describes the condensate wave function,

$$\begin{aligned} \left(-\frac{\hbar^2}{2m}\Delta + v + \gamma V * |\psi|^2\right)\psi &= E\psi \\ \|\psi\|_2^2 &= N, \end{aligned} \tag{1}$$

where m denotes the mass of a boson, N is the number of bosons in the system, v is the external potential (trap), and V is the two-body interaction potential between the bosons.

In the standard BEC scenario (i.e., V *repulsive*, $\gamma > 0$), where the mean interboson distance d is much larger than the range of the two-body potential V, the Hartree nonlinearity is assumed to be *local*, $V = \delta$. Namely, in the regime of a very dilute and cold gas, low energy scattering theory implies that the details of the two-body potential are irrelevant and that the boson-boson interaction is characterized by the *s-wave scattering length* a alone,

$$\gamma = \frac{4\pi\hbar^2}{m}\, a.$$

We rescale the physical quantities in (1) to dimensionless variables with the help of the ground state energy $\hbar\omega_v$ of the *linear* operator $-\frac{\hbar^2}{2m}\Delta + v$ as a natural energy unit with corresponding length unit $\Delta_v = \hbar^{1/2}(m\omega_v)^{-1/2}$. This leads to a Hartree coupling constant g in the rescaled eigenvalue problem,

$$g \propto \frac{a}{\Delta_v}\, N. \tag{2}$$

We are mainly interested in the case of *attractive* interatomic forces, e.g. for lithium $^{7}_{3}$Li whose scattering length equals

$$a = -1.45 \cdot 10^{-9} m$$

as has been measured by [5]. (Note that the mean density ρ of the atoms in the trap v is $\rho \approx 10^{18}\, m^{-3}$, so that $d \approx 10^{-6}\, m$ is three orders of magnitude larger than $a \approx 10^{-9}\, m$.)

Since bosons with *attractive* interactions may collapse into clusters of *very high density*, we propose the use of a two-body potential V which provides a less coarse-grained resolution of the boson-boson interaction (compared to $V = \delta$). This is motivated by experiments [6], [7], which show that, for a fixed trap, the ${}^7_3$Li gas undergoes a collective collapse as soon as the number of condensate atoms exceeds a critical value (e.g. ~ 1400 atoms for the trap specified in [1]).

In Gross-Pitaevskii theory the condensate wave function for *attractive* inter-atomic forces is related to a *local* minimum of the Gross-Pitaevskii functional

$$\mathcal{H}_g^{GP}[\bar{\psi}, \psi] := \frac{1}{2}\|\nabla\psi\|_2^2 + g\,\|\psi\|_{p+1}^{p+1}, \quad p = 3, \tag{3}$$

since *no global* minimizer of (3) exists for $g < 0$!
More precisely, plugging the dilate wave function $\psi_\lambda(x) := \lambda^{\frac{d}{2}}\psi(\lambda x)$, $\lambda \in \mathbb{R}^+$, into (3), we arrive at

$$\mathcal{H}_g^{GP}[\bar{\psi}_\lambda, \psi_\lambda] = \lambda^2\,\frac{1}{2}\|\nabla\psi\|_2^2 + g\,\lambda^{\frac{d}{2}(p-1)}\,\|\psi\|_{p+1}^{p+1}. \tag{4}$$

For *attractive* interaction, $g < 0$, the scaled functional (4) diverges to $-\infty$ in the limit $\lambda \to \infty$ if

$$p > 1 + \frac{4}{d} \tag{5}$$

in d dimensions. But for $d \geq 3$ and $p = 3$ inequality (5) is satisfied (and (4) goes to $-\infty$ in the limit $\lambda \to \infty$ for $d = 2$ if $|g|$ is sufficiently large) !

But, unlike in Gross-Pitaevskii theory, minimizers of the Hartree functional

$$\mathcal{H}_g\,[\bar{\psi}, \psi] = \frac{1}{2}\|\nabla\psi\|_2^2 + (\psi, v\psi)_2 + g\,(\psi, V * |\psi|^2\psi)_2 \tag{6}$$

exist for all $g < 0$ as soon as $|g|$ exceeds some critical threshold value $g_* \geq 0$, $|g| \geq g_*$, and this even holds when $v = 0$!
The *existence* of a g_* follows from standard arguments in the calculus of variations (cf. below) whereas the *size* of g_* can be determined with the help of Birman-Schwinger theory of binding in quantum mechanics. It implies, in the case $v = 0$, that for $d = 1, 2$ the critical coupling vanishes, $g_* = 0$, as well as for $d \geq 3$ in the case of *long range* two-body potentials V. For *short range* potentials V the threshold is *strictly above zero*, $g_* > 0$, for $d \geq 3$ (e.g. by the Cwikel-Lieb-Rozenblujm bound).
In the case of a nonvanishing *confining* trap, $v \neq 0$, a minimizer *always* exists (i.e., for all $g \geq g_* = 0$). Nevertheless, there is a new *strictly positive* critical

coupling, say g_v, which relates the length scale Δ_H set by a minimizer to the length scale Δ_v of the trap by

$$\begin{array}{rclcl} \Delta_H & \approx & \Delta_v & \text{for} & |g| < g_v, \\ \Delta_H & \ll & \Delta_v & \text{for} & |g| > g_v, \end{array}$$

and Δ_H is *independent* of the trap v.

We realize that, for a system of bosonic atoms close to collapse, inelastic collision processes and recombination that heat up the system tend to become important, see e.g. [1]. Such processes and the interactions of electrons and nuclei with the radiation field are not taken into account in a description of the system in terms of Hartree theory. Furthermore, if we neglect short range repulsive (soft core or hard core) interactions between the atoms such that the two-body forces are *purely attractive*, we are dealing with a system that is *not* thermodynamically stable (for a fixed value of $g < 0$, the ground state energy scales like $-O(N^2)$, as $N \to \infty$!).
However, as mentioned above, in the *mean-field regime*, a dilute gas of bosonic atoms is well described by Hartree theory. But this theory continues to be meaningful, mathematically, as the collapse point of the system is approached and even beyond ! It may thus serve to describe *qualitatively* features of the system close to collapse. For example, it should reproduce the main features of *structure formation* in a gas of bosonic atoms close to collapse (Hartree theory with *attractive* Newtonian two-body interactions may be expected to provide a useful approach towards understanding *structure formation in the universe*, possibly for models of bosonic dark matter).

None of these processes can be described by means of Gross-Pitaevskii theory with a self-focussing, *local* nonlinearity.

2 Symmetry Breaking Regime at Finite Coupling

In this section we will prove that for large enough negative coupling g the minimizer of the functional (6) will break very general symmetries possibly induced by the external potential v. For convenience, we will formulate this statement for $N = \|\psi\|_2^2$ instead of g, which without loss of generality will be set equal to -1. Theorem 1 will be worked out for the case where V is a Coulomb potential, but at the end of the proof we will shortly discuss other potentials.

Our main Theorem is:

Theorem 1. *Let V be the Coulomb potential in $\mathbb{R}^d$, $V = |x|^{-1}$, and $v \in C_b(\mathbb{R}^d)$, $d \geq 2$. Let $E(d)$ be the Euclidean group in d dimensions.*
If for some $R \in E(d)$, any minimizing sequence $x_k \in \mathbb{R}^d$ for the external potential v

$$\lim_{k\to\infty} v(x_k) = \inf_{x\in\mathbb{R}^d} v(x) \tag{7}$$

fulfills

$$\liminf_{k\to\infty} |Rx_k - x_k| > 0,$$

then, for sufficiently large N, any minimizer Φ of the Hartree functional (6) satisfies

$$|\Phi \circ R|^2 \neq |\Phi|^2.$$

Remark
If the infimum of v is attained on its set X of minimima only, i.e., if (7) implies $\lim_{k\to\infty} \mathrm{dist}(x_k, X) = 0$, then the hypothesis simply means: $\inf\{|Rx_* - x_*|\,|x_* \in X\} > 0$.

Corollary 1 (Symmetry Breaking).
If $v \in C_b(\mathbb{R}^d)$ has a symmetry $R \in E(d)$, then Theorem 1 predicts symmetry breaking in the sense that no ground state wave function Φ is invariant under R.

The formulation of Theorem 1 is quite general. For illustration we consider more closely the particular cases of a) a nonvanishing external potential consisting in a double well which has as discrete symmetry respective to the reflection at the axis orthogonal to the line between its two separate minima, b) the mexican hat and c) a periodic potential. Case a) is considered also in view of our numerical simulations. Note that Theorem 1 is not restricted to discrete symmetries at all. The corollary now tells us that for sufficiently large coupling g the ground state

Φ of the case considered will not have the symmetry properties of a) the double well, b) the mexican hat resp. c) the periodic potential. In the cases a) and b) this means that Φ can be localized either in the one or the other well resp. part of the mexican hat. We mention that for a single well potential the hypotheses of the theorem are not fulfilled for any R which is a symmetry of the potential.

Proof of Theorem 1
The proof of Theorem 1 will be done in three steps corresponding to lemma 1, lemma 2 and the proof of the theorem itself: The first step of our proof is to show that an approximate minimizer of the *free* energy functional (i.e. without external potential)

$$\mathcal{E}_g\left[\bar{\psi}, \psi\right] = \frac{1}{2}\|\nabla\psi\|_2^2 + g(\psi, V * |\psi|^2\psi)_2, \quad g < 0 \tag{8}$$

will be concentrated in a ball in space whose size can be arranged by varying the size of N. This is stated somewhat more accurately in the following lemma. There the term *η-approximate minimizer* (of the *free* functional) is used: Let $\eta > 0$. An *η-approximate minimizer* is defined as a wave function ψ that satisfies:

$$\|\psi\|_2^2 = N \quad , \quad \mathcal{E}_{-1}\left[\bar{\psi}, \psi\right] \leq (1-\eta)\, E_N, \quad E_N := E[N, -1]$$

where

$$E[N, g] := \inf\{\mathcal{E}_g[\bar{\psi}, \psi] \mid \psi \in W^{1,2}(\mathbb{R}^d), \|\psi\|_2^2 = N\}$$

Lemma 1 (Concentration of approximate minimizer).
Given $\delta > 0$, there is $\eta > 0$ such that, for N large enough any η-approximate minimizer ψ obeys

$$\int_{B(y,\delta)} d^dx\, |\psi(x)|^2 \geq (1-\delta)\, N \qquad \textit{for some} \quad y \in \mathbb{R}^d. \tag{9}$$

It will then be shown that the minimizer of the full energy functional (6) are approximate minimizer of the free energy functional, in the sense of lemma 1, and that they are localized around the minima of the potential:

Lemma 2 (Localization).
Let $v \in C_b(\mathbb{R}^d)$ and $\epsilon, \delta > 0$ be fixed. Then, for N large enough, any minimizer Φ of

$$\mathcal{H}_{-1}\left[\bar{\psi}, \psi\right] = \mathcal{E}_{-1}\left[\bar{\psi}, \psi\right] + \int_{\mathbb{R}^d} d^dx\, v(x)|\psi(x)|^2, \quad \|\psi\|_2^2 = N \tag{10}$$

satisfies

$$\int_{B(y,\delta)} d^d x \, |\Phi(x)|^2 \geq (1-\delta)N \tag{11}$$

and

$$\inf_{x \in B(y,\delta)} v(x) \leq \inf_{x \in \mathbb{R}^d} v(x) + \epsilon \tag{12}$$

The last step of our proof will explicitly prove symmetry breaking. In the following a scaling property of the wave function and the ground state energy will be used: The scaled function $\psi_{N,g}(x) = |g|^{d/2} N^{\frac{1+d}{2}} \psi_{1,1}(|g|Nx)$ satisfies for $d \geq 2$

$$||\psi_{N,g}||_2^2 = N||\psi_{1,1}||_2^2, \quad E[N,g] = g^2 N^3 E[1,-1], \quad E[1,-1] < 0 \tag{13}$$

The key ingredient for the proof of lemma 1 is a partition of unity in the following form: For some $\chi \in C_0^\infty(\mathbb{R}^d)$ with $0 \leq \chi \leq 1$, $||\chi||_2 = 1$, $\mathrm{supp}(\chi) \subset B(0,1)$, the ball of radius 1 with center at 0, the convolution of these approximate characteristic functions satisfies

$$\int_{\mathbb{R}^d} d^d y \, \chi^2(x-y) \, \chi^2(x'-y) \geq 1-\gamma, \tag{14}$$

for any $0 < \gamma \leq 1$ and for $|x - x'| < \epsilon(\gamma)$ small enough. The functions

$$j_y(x) = \delta^{-\frac{d}{2}} \chi(\delta^{-1}(x-y)) \equiv \delta^{-\frac{d}{2}} \chi_{y,\delta}(x)$$

indexed by $y \in \mathbb{R}^d$ form a partition of unity:

$$\int_{\mathbb{R}^d} d^d y \, j_y^2(x) = 1$$

Using the IMS-localization formula [9]

$$p^2 = \int dy j_y p^2 j_y - \int dy (\nabla j_y)^2$$

with p being the momentum operator, we get for the kinetic energy:

$$\frac{1}{2}||\nabla\psi||_2^2 = \frac{\delta^{-d}}{2}\int\limits_{\mathbb{R}^d} d^d y\, ||\nabla(\chi_{y,\delta}\psi)||_2^2 - \frac{\delta^{-2}}{2}||\nabla\chi||_2^2||\psi||_2^2 \tag{15}$$

Proof of Lemma 1
Using (14) and taking $|x-x'| < \epsilon(\gamma)\delta$ we write for the nonlinearity:

$$\begin{aligned}(\psi, V * |\psi|^2\psi)_2 \leq \quad & -g\delta^{-d} \int\limits_{|x-x'|<\epsilon\delta} \int\limits_{\mathbb{R}^d} d^d y\, \frac{d^d x\; d^d x'}{|x-x'|} \left|\chi_{y,\delta}(x)\psi(x)\right|^2 \left|\chi_{y,\delta}(x')\psi(x')\right|^2 + \\ & + \int\limits_{|x-x'|\geq\epsilon\delta} \frac{d^d x\; d^d x'}{|x-x'|} \left|\psi(x)\right|^2 \left|\psi(x')\right|^2\end{aligned}$$

where we have set $0 > g = -(1-\gamma)^{-1}$. The last term is obviously bounded by $(\epsilon\delta)^{-1}N^2$. Using (15) and extending the double integral in the first term to the whole space, which can be done because the integrand is positive, we get:

$$\mathcal{E}_{-1}[\bar{\psi}, \psi] \geq \delta^{-d} \int\limits_{\mathbb{R}^d} d^d y\; \mathcal{E}_g[\overline{\chi_{y,\delta}\psi}, \chi_{y,\delta}\psi] - (\epsilon\delta)^{-1}N^2 - \frac{\delta^{-2}}{2}\|\nabla\chi\|_2^2 N \tag{16}$$

with $g = -(1-\gamma)^{-1}$. Now we use (13) and obtain:

$$\begin{aligned}\mathcal{E}_{-1}[\bar{\psi}, \psi] \quad + \quad & (\epsilon\delta)^{-1}N^2 + \frac{\delta^{-2}}{2}\|\nabla\chi\|_2^2 N \geq g^2\delta^{-d}\left(\int\limits_{\mathbb{R}^d} d^d y\; \|\chi_{y,\delta}\psi\|_2^6 E[1,-1]\right) \\ \geq \quad & g^2\delta^{-d}\sup_y \|\chi_{y,\delta}\psi\|_2^4 \left(\int\limits_{\mathbb{R}^d} d^d y\; (\|\chi_{y,\delta}\psi\|_2^2) E[1,-1]\right) \\ = \quad & g^2 N \sup_y \|\chi_{y,\delta}\psi\|_2^4 E[1,-1]\end{aligned}$$

By assumption $(1-\eta)N^3 E[1,-1] \geq \mathcal{E}_{-1}[\bar{\psi}, \psi]$ and since $E[1,-1] < 0$

$$N^{-2}(\sup_y \|\chi_{y,\delta}\psi\|_2)^4 g^2 \geq (1-\eta) + \left((\epsilon\delta)^{-1}N^{-1} + \frac{\delta^{-2}}{2}\|\nabla\chi\|_2^2 N^{-2}\right) E[1,-1]^{-1}$$

Choose now $\gamma(\eta)$ such that

$$g^{-2} = (1-\gamma)^2 \geq 1-\eta$$

For $N > N_0(\eta)$ sufficiently large:

$$\left((\epsilon\delta)^{-1}N^{-1} + \frac{\delta^{-2}}{2}N^{-2}\|\nabla\chi\|_2^2\right) E[1,-1]^{-1} \geq -\eta$$

So one gets

$$(\sup_y \|\chi_{y,\delta}\psi\|_2)^4 N^{-2} \geq (1-2\eta)(1-\eta) \geq (1-\frac{\delta}{2})^2$$

for $\eta(\delta)$ small enough. And finally:

$$\int\limits_{B(y,\delta)} d^d x \, |\psi(x)|^2 \geq \|\chi_{y,\delta}\psi\|_2^2 \geq (1-\delta)N \tag{17}$$

for some $y \in \mathbb{R}^d$.

Proof of Lemma 2

It is enough to prove this lemma for a $\delta_0 = O(\epsilon)$ because it then holds for any $\delta \geq \delta_0$ as well.

We first show that that a minimizer Φ of (6) is an approximate minimizer of (8) and so by lemma 1 the first statement holds.

For any ψ with $||\psi||_2^2 = N$ one has by assumption: $\mathcal{H}_{-1}[\bar{\Phi}, \Phi] \leq \mathcal{H}_{-1}[\bar{\psi}, \psi]$. This gives:

$$\mathcal{E}_{-1}[\bar{\Phi}, \Phi] - \mathcal{E}_{-1}[\bar{\psi}, \psi] \leq \int\limits_{\mathbb{R}^d} d^d x \, v(x)(|\psi(x)|^2 - |\Phi(x)|^2) \leq 2||v||_\infty N$$

and by passing to the infimum over ψ

$$\mathcal{E}_{-1}[\bar{\Phi}, \Phi] \leq E_N \left(1 - \frac{2||v||_\infty N}{(-E_N)}\right) = E_N \left(1 - \frac{2||v||_\infty}{N^2|E[1,-1]|}\right)$$

For N large enough the bracket is $\geq (1-\eta)$, where η is as in lemma 1, and so:

$$\mathcal{E}_{-1}[\bar{\Phi}, \Phi] \leq E_N(1-\eta)$$

Hence (9) holds true.

The second statement of lemma 2 will be proved by contradiction:

In the following we denote $\inf\limits_{x\in\mathbb{R}^d} v(x)$ by v_*. Pick $y_0 \in \mathbb{R}^d$ and $\delta > 0$ small enough, so that

$$v(x) \leq v_* + \frac{\epsilon}{2} \qquad \forall\, x \in B(y_0, \delta)$$

and assume the second statement is false. For

$$\tilde{\Phi}(x) = \Phi(x - (y_0 - y)),$$

the translate of Φ by $(y_0 - y)$, one has

$$\int\limits_{B(y_0,\delta)} d^d x \, |\tilde{\Phi}(x)|^2 \geq (1-\delta)N$$

and, since $\int\limits_{\mathbb{R}^d \setminus B(y_0,\delta)} d^d x \, |\tilde{\Phi}(x)|^2 \leq \delta N$,

$$\int\limits_{\mathbb{R}^d} d^d x \, (v(x) - v_*)|\tilde{\Phi}(x)|^2 \leq \frac{\epsilon}{2} N + \|v - v_*\|_\infty \delta N$$

On the other hand, if (12) were false,

$$\int\limits_{\mathbb{R}^d} d^d x \, (v(x) - v_*)|\Phi(x)|^2 > \epsilon(1-\delta)N - \|v - v_*\|_\infty \delta N$$

This gives:

$$\begin{aligned}
\mathcal{H}_{-1}[\bar{\tilde{\Phi}}, \tilde{\Phi}] - \mathcal{H}_{-1}[\bar{\Phi}, \Phi] &= \int\limits_{\mathbb{R}^d} d^d x \, (v(x) - v_*)(|\tilde{\Phi}(x)|^2 - |\Phi(x)|^2) \\
&\leq -\frac{\epsilon}{2}(1 - 2\delta)N + 2\|v - v_*\|_\infty \delta N \\
&= -\left(\frac{\epsilon}{2} - \delta(2\|v - v_*\|_\infty + \epsilon)\right) N < 0
\end{aligned}$$

for $\delta < \frac{\epsilon}{4\|v - v_*\| + 2\epsilon}$. This contradicts Φ being a minimizer and proves lemma 2.

Proof of Theorem 1
By assumption, there is $0 < \delta < 1/2$ for ϵ sufficiently small such that

$$v(x) \leq \inf_{x'} v(x') + 2\epsilon$$

implies

$$|Rx - x| > 4\delta$$

By lemma 2,

$$\int\limits_{B(y,\delta)} d^d x \, |\Phi(x)|^2 \geq (1-\delta)N$$

holds for some y with

$$|Ry - y| > 4\delta - 2\delta = 2\delta$$

Assume $|\Phi(Rx)| \equiv |\Phi(x)|$. Then (11) also holds for y replaced by Ry. This leads to

$$N = \int_{\mathbb{R}^d} d^d x\, |\Phi(x)|^2 \geq \int_{B(y,\delta)} d^d x\, |\Phi(x)|^2 + \int_{B(Ry,\delta)} d^d x\, |\Phi(x)|^2 \geq 2(1-\delta)N > N$$

since $B(y,\delta)$ and $B(Ry,\delta)$ are disjoint, which is a contradiction.
This proves Theorem 1.

We will now show how Theorem 1 can easily be extended to other potentials like the case where the two-body potential V is a potential of the form $V \in C_b(\mathbb{R}^d)$ such that $V(x) \to \sup V$ implies $x \to 0$. We first note that we have the following inequality for the energy of the minimizer:

$$E[N,-1] = E_N \leq -V(0)N^2 + \rho \qquad \text{where } \rho = o(N^2) \text{ as } N \to \infty \tag{18}$$

The validity of this inequality can easily be seen by noting that the scaled function $\tilde{\phi}(x) = N^{\frac{1}{2}} a^{-\frac{d}{2}} \phi(a^{-1}x)$, $\|\phi\|_2^2 = 1$, satisfies

$$N^{-2}\mathcal{E}_g(\tilde{\phi}) = a^{-2}N^{-1}\|\nabla\phi\|_2^2 - \int_{\mathbb{R}^{2d}} d^d\tilde{x}\, d^d\tilde{x}'\, V(|\tilde{x} - \tilde{x}'|a)\, |\phi(\tilde{x})|^2\, |\phi(\tilde{x}')|^2, \;\; \tilde{x} = a^{-1}x$$

and $||\tilde{\phi}||_2 = N$. Setting $a = N^{-\frac{1}{3}}$ and using dominated convergence in the limit of large N, one gets (18).
For the proof of lemma 1 we note the following: We again split up the nonlinearity in (8) into two terms, one involving the integration over $|x - x'| < \epsilon\delta$ (with $\epsilon = \epsilon(\gamma)$ as in (14)) and the other over its complement. Noting that $\sup V := V(0) > V(x)$ for $x \neq 0$ by assumption, we set $f(x,x') = |\psi(x)|^2\, |\psi(x')|^2$ and write:

$$\begin{aligned}
(\psi, V * |\psi|^2\psi)_2 &\leq V(0) \int_{|x-x'|<\epsilon\delta} d^d x\, d^d x'\, f(x,x') + V^* \int_{|x-x'|\geq\epsilon\delta} d^d x\, d^d x'\, f(x,x') \\
&= (V(0) - V^*) \int_{|x-x'|<\epsilon\delta} d^d x\, d^d x'\, f(x,x') + V^* N^2 \\
&= (V(0) - V^*) \left(\int_{|x-x'|<\epsilon\delta} d^d x\, d^d x'\, f(x,x') - N^2 \right) + V(0)N^2
\end{aligned}$$

where we have set $V^* := \sup\limits_{|x-x'|\geq\epsilon\delta} V(x-x')$. Now we use (14) to get

$$(\psi, V * |\psi|^2\psi)_2 \leq (V(0)-V^*)\left(-g \sup_{y\in\mathbb{R}^d}\left(\|\chi_{y,\delta}\psi\|_2^2\right) N - N^2\right) + V(0)N^2$$

where again $g = -(1-\gamma)^{-1}$ and the first integral was evaluated as:

$$\delta^{-d} \int\limits_{|x-x'|<\epsilon\delta} \int\limits_{\mathbb{R}^d} d^d y\, d^d x\ d^d x'\, |\chi_{y,\delta}(x)\psi(x)|^2\, |\chi_{y,\delta}(x')\psi(x')|^2 \leq \sup_{y\in\mathbb{R}^d}\left(\|\chi_{y,\delta}\psi\|_2^2\right) N$$

By assumption $(1-\eta)E[N,-1] \geq \mathcal{E}_{-1}(\bar{\psi},\psi)$ for an η-approximate ground state and using (18) we arrive at:

$$(1-\eta)(V(0)N^2-\rho) \leq (V(0)-V^*)\left(-gN \sup_{y\in\mathbb{R}^d}\left(\|\chi_{y,\delta}\psi\|_2^2\right) - N^2\right) + V(0)N^2$$

This is rewritten as:

$$-g^{-1}\left(1 - \frac{\eta V(0) + \rho N^{-2}}{V(0)-V^*}\right) \leq N^{-1} \sup_{y\in\mathbb{R}^d}\left(\|\chi_{y,\delta}\psi\|_2^2\right)$$

Setting now $\gamma = c^{-1}\delta$ with $c \gg \delta$ and choosing η small and N large enough, such that

$$\frac{\eta V(0) + \rho N^{-2}}{V(0)-V^*} < c^{-1}\delta$$

we get:

$$N^{-1} \sup_{y\in\mathbb{R}^d}\left(\|\chi_{y,\delta}\psi\|_2^2\right) \geq (1-c^{-1}\delta)^2 \geq 1-\delta$$

which gives the first lemma.
The proofs of the second lemma and of theorem 1 are almost the same as before.

Remark
This is complemented by the following result, which conversely implies that no symmetry breaking of the ground state occurs at small coupling. This feature is reproduced by our numerical simulations.

Theorem 2 (Positive Critical Coupling for $d \geq 1$).
Let the two-body potential $V \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ be real-valued, and the external potential $v \in C_b(\mathbb{R}^d)$, $d \geq 1$, such that

$$H_0 = -\frac{1}{2}\Delta + v \tag{19}$$

has an isolated ground state.
Then, for sufficiently small coupling $|g|$, there exists a unique nonlinear ground state ψ, $\|\psi\|_2 = 1$, of

$$H_g^{(\psi)} = H_0 + gV * |\psi|^2. \tag{20}$$

This implies that, in any dimension $d \geq 1$, symmetry breaking occurs above a strictly positive critical coupling g_* only, $|g| > g_*$.

Proof of Theorem 2
The ground state energy E_0 of H_0 is nondegenerate by the Perron–Frobenius theorem (see e.g. [10]). Let ψ_0 (with $\|\psi_0\| \equiv \|\psi_0\|_2 = 1$) be the corresponding ground state, and P_0 its eigenprojection. The perturbation in (29) is bounded in operator norm since $\|V * |\psi|^2\| \leq \|V\|_\infty \|\psi\|^2$; hence, $H_g^{(\psi)}$ is an analytic family of type A. By the Kato-Rellich theorem [10] and its proof, we have the following.

(i) Let Γ be a circle around E_0 of small enough radius r, so that no other point in $\sigma(H_0)$ is encircled. Then

$$C \equiv \sup \|(H_g^{(\psi)} - z)^{-1}\| < \infty ,$$

where the supremum is over $z \in \Gamma$, $|g| < g_*$ and $\|\psi\| \leq 1$, provided g_* is small enough.

(ii) For such g and ψ there is precisely one (nondegenerate) eigenvalue of $H_g^{(\psi)}$ within Γ. It is the ground state energy, and its eigenprojection is

$$P_g^{(\psi)} = -(2\pi i)^{-1} \oint_\Gamma dz \, (H_g^{(\psi)} - z)^{-1} .$$

A nonlinear ground state is the same (up to the phase) as a fixed point of the map

$$T : \ \mathcal{S} = \{\|\psi\| = 1\} \to \mathcal{S} , \qquad \psi \mapsto \frac{P_g^{(\psi)}\psi_0}{\|P_g^{(\psi)}\psi_0\|}. \tag{21}$$

By the contraction mapping principle [11], it suffices to prove that T is a *strict contraction.* Indeed,

$$P_g^{(\psi)} - P_g^{(\phi)} = (2\pi i)^{-1} \oint_\Gamma dz \, (H_g^{(\psi)} - z)^{-1} (gV * (|\psi|^2 - |\phi|^2))(H_g^{(\phi)} - z)^{-1}$$

is estimated for $\|\psi\|$, $\|\phi\| \leq 1$ as

$$\|P_g^{(\psi)} - P_g^{(\phi)}\| \leq |g|C^2 r\|V\|_\infty\| \, |\psi|^2 - |\phi|^2\|_1 \leq 2|g|C^2 r\|V\|_\infty\|\psi - \phi\| \, ,$$

where the triangle inequality has been used on $|\psi|^2 - |\phi|^2 = \psi(\bar{\psi} - \bar{\phi}) - (\psi - \phi)\bar{\phi}$. The same bound applies to

$$\big| \|P_g^{(\psi)}\psi_0\| - \|P_g^{(\phi)}\psi_0\| \big| \leq \|(P_g^{(\psi)} - P_g^{(\phi)})\psi_0\| \, .$$

In particular for $\phi = 0$, and hence $P_g^{(\phi)} = P_0$, $\|P_g^{(\phi)}\psi_0\| = 1$, this shows that $\|P_g^{(\psi)}\psi_0\| \geq 1/2$ for g_* small enough. Thus (21) is well–defined. From

$$\begin{aligned} T(\psi) - T(\phi) &= \|P_g^{(\psi)}\psi_0\|^{-1}(P_g^{(\psi)} - P_g^{(\phi)})\psi_0 \\ &\quad + \|P_g^{(\psi)}\psi_0\|^{-1}\|P_g^{(\phi)}\psi_0\|^{-1}(\|P_g^{(\psi)}\psi_0\| - \|P_g^{(\phi)}\psi_0\|)P_g^{(\phi)}\psi_0 \end{aligned}$$

T is now seen to be a strict contraction on $\mathcal{S}$.
This proves theorem 2.

3 Numerical Investigation

The following simulation performed by a branch of our C++ HARTREE package [12] (using the extension BLITZ++, cf. [13]) is built on a bilinear Lagrange finite element discretization of the numerical configuration space $\Omega \subset \mathbb{R}^2$, $\Omega =]0, D[^{\times 2}$, $D > 0$, endowed with homogeneous Dirichlet boundary conditions leading to a Galerkin space of globally continuous functions in $W_0^{1,2}(\Omega)$.

Discretizing the scaled version of (1) by means of these bilinear finite elements, we arrive at the following nonlinear eigenvalue problem,

$$\frac{1}{(h^{(n)})^2}\left(\frac{1}{2}A^{(N)} + v^{(N)} + g\, W^{(N)}\left[\underline{\psi}^{(N)}\right]\right)\underline{\psi}^{(N)} = E^{(N)}\,\underline{\psi}^{(N)} \tag{22}$$

where $A^{(N)}$, $v^{(N)}$ and $W^{(N)}$ denote the finite element discretizations of the Laplacian $-\Delta$, the external potential v, and the Hartree energy $V * |\psi|^2$, respectively, on the square grid of $N = n^2$ vertices, and mass lumping saves us the inversion of the massmatrix. $\underline{\psi}^{(N)}$ denotes the component vector gained by expanding $\psi^{(N)}$ with respect to the finite element basis in the Galerkin space, and $h^{(n)} := \frac{D}{n-1}$. Since we would like to use a version of the Fast Fourier Transform algorithm (MFFT, cf. [14]) for the fast evaluation of the Hartree energy term $W^{(N)}$, we depart from the finite element framework in the treatment of $W^{(N)}$ using a quadrature scheme for its computation. We denote by $\tilde{W}^{(N)}$ this nonconforming discretization. The two-body potentials V considered here are three-dimensional regularized Coulomb and Yukawa potentials

$$\tilde{W}^{(N)}\left[\underline{\psi}^{(N)}\right]_{(i,j),(k,l)} = \delta_{ik}\delta_{jl}\,(h^{(n)})^4 \sum_{i',j'=0}^{n-1} \left|\psi_{i'j'}^{(N)}\right|^2 \frac{e^{-(\alpha h^{(n)}\sqrt{(i-i')^2+(j-j')^2})}}{h^{(n)}\sqrt{(i-i')^2+(j-j')^2}+\delta} \tag{23}$$

depending on the falloff parameter α and the regularization δ. Here, the indices represent pairs of coordinates of the vertices in the two-dimensional grid.
The external potential v is chosen to consist of two smooth potential wells. The y-coordinates of their minima are equal whereas the x-coordinates are connected by a reflection at the axis orthogonal to the line joining the two local minimima of v. Hence, this external potential possesses a discrete symmetry, cf. Figure 1.

The nonlinear eigenvalue problem (22) is solved by means of two interlocking iterative procedures

$$\Psi^{(N),p,q} \overset{\mathsf{PM}}{\underset{}{\xrightarrow{q\to\infty}}} \Psi^{(N),p} \overset{\mathsf{PC}}{\underset{}{\xrightarrow{p\to\infty}}} \Psi^{(N)} \tag{24}$$

for $\Psi^{(N),p,q} := (E^{(N),p,q}, \underline{\Phi}^{(N),p,q})$ and analogously for $\Psi^{(N),p}$ and $\Psi^{(N)}$. The superscript p is index of the Picard (PC) iteration sequence $\Psi^{(N),p}$ whose elements are the solutions of the sequence of *linearized* problems

$$\frac{1}{(h^{(n)})^2}\left(\frac{1}{2}A^{(N)} + v^{(N)} + g\,\tilde{W}^{(N)}\left[\underline{\Phi}^{(N),p}\right]\right)\underline{\Phi}^{(N),p+1} = E^{(N),p+1}\,\underline{\Phi}^{(N),p+1} \tag{25}$$

for some suitably chosen starting guess $\underline{\Phi}^{(N),0}$. Note, that the Hartree energy $\tilde{W}^{(N)}$ depends on p only, and not on $p+1$!
Each element of this sequence of linear problems is solved by use of the Power Method (PM) consisting simply in a repeated application of the linearized operator on the rhs of (25) on a starting guess $\underline{\Phi}^{(N),p,0}$ for the linear problem, for all $p \in \mathbb{N}_0$. Subsequently, the iterate is normalized. This PM iteration is assigned the superscript q in $\Psi^{(N),p,q}$.

Although there is a *Lanczos algorithm* implemented in the HARTREE package [12] we discuss the elementary PM iteration for reasons of monitoring the iterates directly. For the Lanczos algorithm, cf. [15], [16].

The PM iteration procedure works as follows. Given a linear real symmetric operator H on a complex finite N-dimensional Hilbert space $\mathcal{H}$ and a vector $\psi^0 \in \mathcal{H}$, PM provides us with the eigenvector whose corresponding eigenvalue is the eigenvalue with largest modulus of H restricted to the subspace determined by ψ^0. More precisely, if $\{\phi_k\}_{k=0}^{N-1}$ is an orthonormal eigenbasis of H in $\mathcal{H}$, $H\phi_k = E_k\phi_k$, in which ψ^0 may be expanded, $\psi^0 = \sum_{k=0}^{N-1} c_k\phi_k$, then PM computes a multiple of the eigenfunction $\phi_* \in \{\phi_k\}_{k=0}^{N-1}$ with eigenvalue E_*, for which

$$|E_*| = \max\left\{|E_k| \mid E_k \in \sigma\left(H|_{span\{\phi_k \mid c_k \neq 0\}}\right)\right\} \tag{26}$$

holds (provided they are unique). This is achieved by iterating the application of H on ψ^0 with subsequent normalization of the iterate.

$$\begin{aligned}
\psi^j &:= \frac{H^j\psi^0}{\|H^j\psi^0\|} \\
&= \sum_{k=0}^{N-1} \frac{c_k\left(\frac{E_k}{E_*}\right)^j}{\left(|c_*|^2 + \sum_{l=0,l\neq *}^{N-1}|c_l|^2\left(\frac{E_l}{E_*}\right)^{2j}\right)^{\frac{1}{2}}}\,\phi_k \overset{j\to\infty}{\to} \frac{c_*}{|c_*|}\phi_* \qquad (27)\\
(\psi^j, H\psi^j) &= \sum_{k=0}^{N-1} \frac{|c_k|^2\left(\frac{E_k}{E_*}\right)^{2j}}{|c_*|^2 + \sum_{l=0,l\neq *}^{N-1}|c_l|^2\left(\frac{E_l}{E_*}\right)^{2j}}\,E_k \overset{j\to\infty}{\to} E_* \qquad (28)
\end{aligned}$$

As we can see in (26) the restriction to a subspace of $\mathcal{H}$ is determined by the choice of non-vanishing components in the eigenbasis expansion of the starting seed ψ^0. Now, depending on the location of the spectrum, we have to shift the linear operator H by an amount $s \in \mathbb{R}$ which, in our case, reads as

$$\begin{aligned} H_s^{(N)}\left[\underline{\Phi}^{(N),p}\right]\underline{\Phi}^{(N),p+1} &:= \left[\frac{1}{h^{(n)2}}\left(\frac{1}{2}A^{(N)} + v^{(N)} + g\,\tilde{W}^{(N)}\left[\underline{\Phi}^{(N),p}\right]\right) + s\,\mathbb{I}^{(N)}\right]\underline{\Phi}^{(N),p+1} \\ &= \left(E^{(N),p+1} + s\right)\underline{\Phi}^{(N),p+1} \end{aligned} \tag{29}$$

such that for the computation of the ground state energy, at most,

$$|\min\sigma\left(H_s^{(N)}\left[\underline{\Phi}^{(N),p}\right]\right)| > |\max\sigma\left(H_s^{(N)}\left[\underline{\Phi}^{(N),p}\right]\right)| \tag{30}$$

Then, the ground state energy of $H_s^{(N)}[\underline{\Phi}^{(N),p}]$ has maximal modulus among all energies of $H_s^{(N)}[\underline{\Phi}^{(N),p}]$.

The *convergence speed characteristic* is determined by the quotient $q_{\hat{k}}(s)$ in the numerator of (27) shifted by s, where $\hat{k} \in \{0, ..., N-1\}$ denotes the energy level for which the quotient $q_{\hat{k}}(s)$ is closest to one among all existing $q_k(s)$, $k \in \{0, ..., N-1\}$,

$$q_{\hat{k}}(s) := \left(\frac{E_{\hat{k}} + s}{E_* + s}\right)^j. \tag{31}$$

The length and energy scales l and E set by a minimizer are $l \propto |g|^{-1}$, and $E \propto g^2$. For numerical reasons, we have to allow grid resolutions with $l \gg h$ only ($h := h^{(n)}$ for some n). But the maximal kinetic energy on such a grid is roughly proportional to h^{-2} which determines the scale of the coupling g, $|g| \ll h^{-1}$. This implies the existence of positive energy states on the grid since the depth of the Hartree energy well is $O(g^2)$. Hence,

$$\max\sigma(H^{(N)}[\underline{\Phi}^{(N),p}]) = O\left(h^{-2}\right) > 0.$$

Approximating the Hartree energy well around its minimum by a harmonic potential, we find the *level spacing* ΔE to be

$$\Delta E = O(g^2),$$

since, on the length scale $|g|^{-1}$, the quadratic function changes as g^2 (depth of the energy well), it is of the form $O(g^4)x^2$ which results in a harmonic oscillator frequency $\omega = O(g^2)$. Therefore, we can set $E_0 = -\alpha_0 g^2$ and the first excited state $E_1 = -\alpha_1 g^2$ with $\alpha_0 - \alpha_1 > 0$. The convergence speed characteristic $q_1(s)$ from (31) is now expanded in $g^2h^2 \ll 1$, with $(\alpha_0 - \alpha_1)$ is of order $O(1)$:

$$q_1(-h^{-2})^{\frac{1}{j}} = 1 - (\alpha_0 - \alpha_1)g^2h^2 + O(g^4h^4). \tag{32}$$

Now, in order to get an idea for the *size* of j, we can expand ψ^j up to first order, $k = 0, 1$, for example, and compute j approximately from

$$\left\|\frac{H_s\psi^j - (\psi^j, H_s\psi^j)\,\psi^j}{(\psi^j, (H_s - s\mathbb{I})\psi^j)}\right\| \le \epsilon_{rel} \tag{33}$$

which is the chosen *stopping criterion* for the PM iteration, given the relative error ϵ_{rel} (with $H_s := H + s1$). Note that this criterion does not depend on the shift $s \in \mathbb{R}$ if ψ^j is normalized for all j.

Clearly, (33) is satisfied for *any* eigenstate of H. But as soon as the $*$-component in the expansion of ψ^0 is nonvanishing (e.g. due to *finite precision arithmetic*), $c_* \neq 0$, the sequence ψ^j will eventually converge to a multiple of ϕ_*.

But note, that the chosen accuracy may be reached *before* a nonvanishing c_* is generated !

4 Figures

In Figure 1 we visualize some instructive elements of the PC iteration sequence $\{\Phi^{(N),p}\}_{p=0}^{\infty}$. The data specification for the simulation in Figures 1 and 2 is as follows.

The grid is generated by six bisections leading to $n = 2^6 = 64$.
The external potential $v(x, y)$ is chosen to be a double well potential composed of two wells of the form

$$v(x, y) = V_0/\cosh((x - x_0)^2/a^2 + (y - y_0)^2/b^2)$$

localized at
$((x_1)_0, (y_1)_0) = (0.35, 0.5)$ and
$((x_2)_0, (y_2)_0) = (0.65, 0.5)$ with widths
$(a_1, b_1) = (a_2, b_2) = (0.03, 0.03)$ and strengths
$(V_1)_0 = (V_2)_0 = -0.1$.
The two-body potential V has the form (23) with
$\alpha = 0$ and
$\delta = 0.1$.
This Hartree energy is coupled by a coupling constant
$g = -16$.

The starting guess $\Phi^{(N),0}$ for the iteration is chosen to be the ground state for the pure kinetic energy in Ω. With the additional rule

$$\underline{\Phi}^{(N),p+1,0} := \underline{\Phi}^{(N),p,\infty}, \tag{34}$$

all the necessary starting approximations are determined, where $p \in \mathbb{N}_0$, and $\underline{\Phi}^{(N),0,\infty} := \underline{\Phi}^{(N),0}$.

In the following simulation, $q = \infty$ means $q = O(10) - O(10^2)$ iterations, whereas $p = \infty$ is $p = O(10)$.

Figure 1 visualizes the density contours of selected iterates from the PC iteration sequence. The first picture shows the ground state for the pure kinetic energy. After a while, a state similar to the ground state of the linear operator $-\frac{1}{2}\Delta + v$ is approached. This state becomes unstable, such that, finally, one of the two possible nonlinear ground states results. The decision for the left or the right potential well is made by finite precision arithmetic.

The qualitative behavior of Figure 1 is confirmed for different grid resolutions $n = 2^m$, $m \in \mathbb{N}$, where the location and strength of the external potential v has been kept fixed.
On the chosen level of accuracy, $\epsilon_{rel} = 10^{-6}$, and on this space discretization level, $n = 64$, the critical coupling lies around

$$g_* \approx 16$$

(we are only interested in the qualitative behavior). Above g_*, the minimizer density looks as in the second picture of Figure 1.

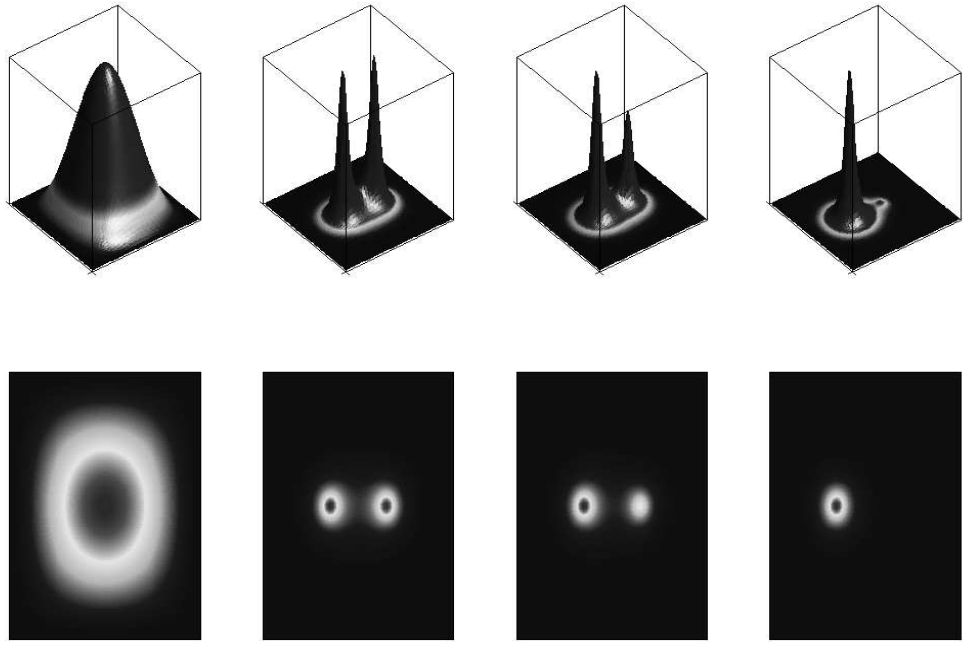

Figure 1: Modulus squared of selected wave function iterates from the PC sequence converging to a symmetry broken minimizer. For the reason of visibility, the volumes of the boxes are determined by the maximal value of the modulus of the iterate.

In Figure 2 the expectation value of $H^{(N)}$ in the PC states from Figure 1 and their underlying PM states is monitored. We note that the energy minimum for all these states is in fact reached in the final configuration.

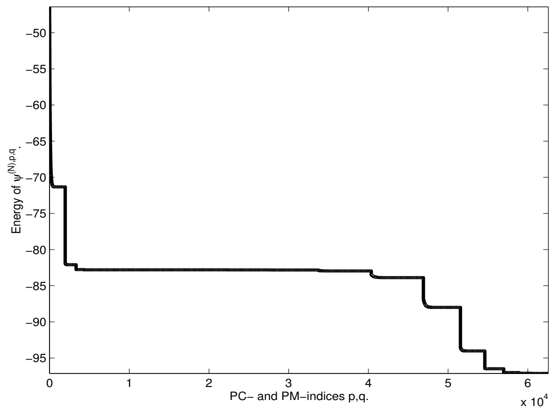

Figure 2: Total energy of the interlocking PC iterates and PM iterates for the sequence in Figure 1 .

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