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ON THE GROSS–PITAEVSKII EQUATION WITH STRONGLY ANISOTROPIC CONFINEMENT: FORMAL ASYMPTOTICS AND NUMERICAL EXPERIMENTS

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The three-dimensional (3D) Gross–Pitaevskii equation with strongly anisotropic confining potential is analyzed. The formal limit as the ratio of the frequencies ϵ tends to zero provides a denumerable system of two-dimensional Gross–Pitaevskii equations, strongly coupled through the cubic nonlinearities. To numerically solve the asymptotic approximation only a finite number of limiting equations is considered. Finally, the approximation error for a fixed number of equations is compared for different ϵ tending to zero. On the other hand, the approximation error for an increasing number of terms in the approximation is observed.

Keywords: Gross–Pitaevskii equation; spectral decomposition; Fourier expansion; time splitting-spectral techniques; approximation error.

AMS Subject Classification: 35Q55, 65M70, 65M15

1. Description of the Problem

We analyze the 3D Gross–Pitaevskii equation (GPE), which is a nonlinear Schrödinger equation with confining potential. More precisely we focus on the case when the potential is quadratic and strongly anisotropic. Thus, we consider the following problem:

$$i\psi_t = -\frac{1}{2}\Delta\psi + \left(\frac{|x|^2}{2} + \frac{z^2}{2\varepsilon^4}\right)\psi + \delta|\psi|^2\psi,$$
$$\psi(0,x,z) = \psi_I(x,z), \quad x \in \mathbb{R}^2, \quad z \in \mathbb{R},$$

where the parameter ε, which determines the strength of the anisotropy, tends to zero. Note that $1/\varepsilon^2$ is the harmonic oscillator frequency in z-direction. Furthermore, we impose the normalization condition:

$$\int_{\mathbb{R}^3} |\psi_I|^2 \, dx\, dz = 1, \tag{1.1}$$

at time $t = 0$, which is then maintained by the equation.

As will be shown below, by expanding the solution with respect to the eigenstates of the Hamiltonian in the strongly confined direction, the formal asymptotic analysis yields in the limit (of "infinite" confinement in z-direction) a denumerable system of NLS equations.

In particular, when the initial data belongs to the eigenspace of the ground state of the dominating Hamiltonian, it can then be proven rigorously that there is only one limiting equation, whose solution remains concentrated on the ground state.[3]

The stationary case is treated in Ref. 7. There, the limit of the three-dimensional ground state energy is carried out (for $z \in \mathbb{R}^2$ and $x \in \mathbb{R}$).

In the present paper we are interested in the numerical approximation of the limiting equations. For this porpose, we truncate the expansion at a finite index N considering only a finite number of limiting equations, whose well-posedness will be proven in Sec. 2. The subsequent section presents the numerical procedure for solving the limiting system for different $N = 1, 2, 3$ and 4. Accordingly, a multistep time splitting scheme, second order in time and of spectral accurancy in space, is introduced. Finally, the numerical simulations are presented in Sec. 4.

At first we perform the rescaling $z \to \varepsilon z$. In order to keep the wave function normalized in $L^2(\mathbb{R}^3)$ we have to rescale $\psi \to \varepsilon^{-1/2}\psi$. As we want to balance the nonlinearity with the terms of order 1 we choose $\delta = \mathcal{O}(\varepsilon)$, thus we consider weak nonlinearities. After the rescaling we obtain

$$i\psi_t = H^{\perp}\psi + \frac{1}{\varepsilon^2}H\psi + |\psi|^2\psi,$$
$$\psi(t=0,x,z) = \psi_I(x,z), \quad x \in \mathbb{R}^2, \quad z \in \mathbb{R}, \tag{1.2}$$

where $H^{\perp} = -\frac{1}{2}\Delta_x + \frac{|x|^2}{2}$ and $H = -\frac{1}{2}\partial_{zz} + \frac{z^2}{2}$ are harmonic oscillator Hamiltonians in x and z directions, respectively.

We introduce the fast time scale $\tau = t/\varepsilon^2$, characteristics for oscillations in the z-direction, and make the two scale ansatz $\psi = \psi(t, \tau, x, z)$ leading to

$$i\psi_t + i\frac{1}{\varepsilon^2}\psi_\tau = H^\perp\psi + \frac{1}{\varepsilon^2}H\psi + |\psi|^2\psi. \tag{1.3}$$

If we let $\varepsilon \to 0$, we formally obtain the equation

$$i\Psi_\tau = H\Psi, \tag{1.4}$$

which can be solved explicitly in terms of the spectral decomposition:

$$\Psi = \sum_{k\geq 0} \phi_k e^{-i\mu_k\tau}\omega_k(z). \tag{1.5}$$

Here $(\omega_k(z))_{k\geq 0}$ are eigenfunctions, normalized in $L^2(\mathbb{R})$, of the self-adjoint, non-negative operator H, defined on $L^2(\mathbb{R})$ with the domain

$$X_H = \{u \in H^1(\mathbb{R});\ zu \in L^2(\mathbb{R})\}.$$

The eigenvalue problem

$$H\omega_k = \mu_k\omega_k,$$

can be solved explicitly with

$$\mu_k = k + \frac{1}{2}, \quad \omega_k(z) = (2^k k!)^{-1/2}\left(\frac{1}{\pi}\right)^{1/4} H_k(z), \qquad k = 0, 1, \ldots$$

denoting the eigenvalues and eigenfunctions respectively.[9] Here $H_k(z)$ are the standard Hermite polynomials. By modulation, we let ϕ_k depend on the slow variables (t, x). This motivates the expansion of the solution ψ^ε of (1.2) with respect to the eigenstates of H:

$$\psi^\varepsilon(t, x, z) = \sum_{k\geq 0} e^{-i\mu_k t/\varepsilon^2}\phi_k^\varepsilon(t, x)\omega_k(z), \tag{1.6}$$

where $\phi_k^\varepsilon(t, x) = \int_{\mathbb{R}} \psi^\varepsilon(x, z, t)\omega_k(z)\,dz$ are the Fourier coefficients. Substitute the expansion (1.6) into (1.2), multiply the equation by $\omega_k e^{i\mu_k t/\varepsilon^2}$, and integrate with respect to z, we obtain:

$$i\partial_t\phi_k^\varepsilon = H^\perp\phi_k^\varepsilon + \sum_{l,m,n\geq 0} \gamma_{klmn} e^{-i(\mu_n+\mu_l-\mu_m-\mu_k)t/\varepsilon^2}\phi_l^\varepsilon\overline{\phi_m^\varepsilon}\phi_n^\varepsilon, \quad k \geq 0, \tag{1.7}$$

where $\gamma_{klmn} = \int_{\mathbb{R}} \omega_k(z)\omega_l(z)\omega_m(z)\omega_n(z)\,dz$. Note that all coefficients in the sum, for which $\mu_n + \mu_l - \mu_m - \mu_k$ is different from 0, tend to zero weakly. Thus, in the limit ε to 0 we obtain formally:

$$i\partial_t\phi_k = H^\perp\phi_k + \sum_{l,m,n}{}^{k} \gamma_{lmnk}\phi_l\overline{\phi_m}\phi_n, \quad k \geq 0, \tag{1.8}$$

where $\sum_{l,m,n}^k$ denotes the sum over all $l, m, n \geq 0$ such that $\mu_n + \mu_l - \mu_m - \mu_k = 0$, and ϕ_m denotes the (weak) limit of ϕ_m^ε as ε tends to zero.

Equations (1.8) are a denumerable system of two-dimensional GPEs, strongly coupled through the cubic nonlinearities. We want to investigate the properties of this coupling. For every fixed k, all triples of the form $(l, m, n) = (l, l, k)$ appear in $\sum_{l,m,n}^{k}$, leading to the contribution $\sum_l \gamma_{llkk}|\phi_l|^2$ to the potential in the ϕ_k-equation. However, by the special form of the eigenvalues of the harmonic oscillator, other coupling terms may also occur, since the condition $\mu_n + \mu_l - \mu_m - \mu_k = 0$ reduces to $n + l - m - k = 0$. For example, in the ϕ_0-equation, the term $\gamma_{0121}\phi_1^2\bar{\phi}_2$ is not of potential type.

If not all states ω_k appear in the spectral decomposition of the initial datum ψ_I, which states will appear in the solution for positive time t? The question can be answered in terms of the following definition.

Definition 1.1. The index set $I \subset \{0, 1, 2, \ldots\}$ is called *closed*, iff $(l, m, n) \in I^3$ and $k = l + n - m \geq 0$ imply $k \in I$. The closure $\bar{I}$ of I is the smallest closed index set containing I.

Now the answer to the above question is: Define $I = \{k \geq 0\colon \phi_k(x, t = 0) \neq 0\}$. Then, for all $t \geq 0$, $\phi_k(x, t) = 0$ for $k \notin \bar{I}$.

It remains to characterize the closed index sets.

Lemma 1.1. *A nonempty index set I is closed iff it has the form $I = \{p + jq\colon j \geq 0\}$ with either $0 \leq p < q$ or $q = 0$.*

Proof. The "if" is obvious. For the proof of "only if", assume that I is closed, $\mathrm{card}(I) > 1$, and that $k_0 = p < k_1 = p + q$ are the two smallest elements of I. If $p \geq q$ would hold, then $k_0 + k_0 - k_1 = p - q \in I$. However, $k_0 + k_0 - k_1 < k_0$ contradicting the assumption that k_0 is the smallest element of I. This proves $p < q$.

Now we shall prove by induction that I has the form stated in the lemma. Assume $k_j = p + jq$, $0 \leq j \leq n$, are the $n + 1$ smallest elements of I. Then $p + (n + 1)q = k_n + k_1 - k_0 \in I$. If there were a $k_{n+1} \in I$ with $k_n < k_{n+1} < p + (n + 1)q$, then $k_n + k_n - k_{n+1} \in I$ and $k_{n-1} < k_n + k_n - k_{n+1} < k_n$, i.e., there were an element of I between k_{n-1} and k_n, contradicting our assumption that $k_0, \ldots, k_n$ are the $n + 1$ smallest elements. □

Closed index sets either have one element or infinitely many. In some cases they can be easily related to symmetries of the wave function. In Ref. 3, the case of $I = \{0\}$ is considered, i.e. initially only the ground state is charged. According to the observation mentioned above in this special case the system (1.8) will consist of only one equation for ϕ_0, the modulation of the ground state. In fact, ϕ_0 is proven to be the approximation of the solution ψ of (1.2) on every bounded time interval.[3] Moreover, ϕ_0 satisfies (1.8) with $k = 0$. Other examples are the sets of even and odd integers, corresponding to wave functions which are, respectively, even and odd in terms of the variable z.

It is a well-known fact that (1.2) conserves mass

$$\int_{\mathbb{R}^3} |\psi^\varepsilon|^2 \, dx \, dz,$$

and energy

$$\frac{1}{\varepsilon^2} \int_{\mathbb{R}^3} \left(|\partial_z \psi^\varepsilon|^2 + |z\psi^\varepsilon|^2 \right) dx \, dz + \int_{\mathbb{R}^3} \left(|\nabla_x \psi^\varepsilon|^2 + |x\psi^\varepsilon|^2 + |\psi^\varepsilon|^4 \right) dx \, dz. \tag{1.9}$$

Mass conservation carries over to the limiting system (1.8) in the obvious way. If we multiply (1.8) by $\overline{\phi_k}$, integrate by parts, take the imaginary part and sum over all k, we obtain

$$\frac{d}{dt} \sum_{k \geq 0} \int_{\mathbb{R}^2} |\phi_k|^2 \, dx = 0.$$

The energy contains two terms of different orders of magnitude. We shall show that limiting versions of both terms are conserved in the limit.

First we multiply Eq. (1.8) by $\overline{\partial_t \phi_k}$, take the real part, integrate with respect to x, and sum over all k. We introduce the abbreviation

$$\sum\nolimits^* := \sum_{k \geq 0} \sum_{l,m,n}^{k},$$

i.e. the sum over all $k, l, m, n \geq 0$ such that $\mu_l + \mu_n - \mu_m - \mu_k = 0$. Taking into account the computation (exchanging m and k)

$$\begin{aligned} 2\Re \sum\nolimits^* \gamma_{nmlk} \phi_l \phi_n \overline{\phi_m (\phi_k)_t} &= \Re \sum\nolimits^* \gamma_{nmlk} \phi_l \phi_n \overline{[(\phi_m)_t \phi_k + \phi_m (\phi_k)_t]} \\ &= \frac{1}{2} \Re \sum\nolimits^* \gamma_{nmlk} \left[\phi_l \phi_n (\overline{\phi_m \phi_k})_t + (\phi_l \phi_n)_t \overline{\phi_m \phi_k} \right] \\ &= \frac{1}{2} \Re \sum\nolimits^* \gamma_{nmlk} (\phi_l \phi_n \overline{\phi_m \phi_k})_t, \end{aligned} \tag{1.10}$$

we obtain

$$0 = \frac{d}{dt} \int_{\mathbb{R}^2} \sum_{k \geq 0} \left(|\nabla \phi_k|^2 + |x\phi_k|^2 + \Re \sum_{l,m,n}^{k} \gamma_{nmlk} \phi_l \phi_n \overline{\phi_m \phi_k} \right) dx.$$

Since, by exchanging (m, k) and (l, n),

$$\begin{aligned} \sum\nolimits^* \gamma_{nmlk} \phi_l \phi_n \overline{\phi_m \phi_k} &= \frac{1}{2} \sum\nolimits^* \gamma_{nmlk} \left[\phi_l \phi_n \overline{\phi_m \phi_k} + \phi_m \phi_k \overline{\phi_l \phi_n} \right] \\ &= \sum\nolimits^* \gamma_{nmlk} \Re (\phi_l \phi_n \overline{\phi_m \phi_k}), \end{aligned}$$

we deduce that $\sum^* \gamma_{nmlk} \phi_l \phi_n \overline{\phi_m \phi_k}$ is real. Therefore the quantity

$$E_1 = \int_{\mathbb{R}^2} \sum_{k \geq 0} \left(|\nabla_x \phi_k|^2 + |x\phi_k|^2 + \sum_{l,m,n}^{k} \gamma_{nmlk} \phi_l \phi_n \overline{\phi_m \phi_k} \right) dx. \tag{1.11}$$

is real and conserved by (1.8). It is clear that the first two terms in E_1 are positive. In order to see the positivity of the exchange term in the energy we take a function $\beta^\varepsilon(t,z)$ with the expansion:

$$\beta^\varepsilon(t,z) = \sum_{k\geq 0} \beta_k e^{-i\mu_k t/\varepsilon^2} \omega_k(z)$$

and compute

$$0 \leq \int_{\mathbb{R}} |\beta^\varepsilon(t,z)|^4 \, dz = \sum_{k,l,m,n\geq 0} \gamma_{nmlk} e^{-i(\mu_l+\mu_n-\mu_m-\mu_k)t/\varepsilon^2} \beta_l \beta_n \overline{\beta_m \beta_k}$$
$$\stackrel{\varepsilon\to 0}{\to} \sum\nolimits^{*} \gamma_{nmlk} \beta_l \beta_n \overline{\beta_m \beta_k}.$$

This shows the non-negativity of E_1, which is a limiting version of the second ($O(1)$-) term in the energy (1.9). The first term in (1.9) formally converges to

$$E_2 = \int_{\mathbb{R}^2} \sum_{k\geq 0} \mu_k |\phi_k|^2 \, dx.$$

For proving conservation of E_2, we multiply Eq. (1.8) by $\mu_k \overline{\phi_k}$, integrate with respect to x, take the imaginary part and sum over all $k \geq 0$. Then we obtain, by appropriately exchanging indices:

$$\begin{aligned}
&\frac{d}{dt} \int_{\mathbb{R}^2} \sum_{k\geq 0} \mu_k |\phi_k|^2 dx \\
&= \Im \sum_{k\geq 0} \int_{\mathbb{R}^2} \mu_k \left[H^\perp \phi_k + \sum_{l,m,n}^{k} \gamma_{lmnk} \phi_l \overline{\phi_m} \phi_n \right] \overline{\phi_k} \, dx \\
&= \Im \int_{\mathbb{R}^2} \sum\nolimits^{*} \gamma_{lmnk} \mu_k \overline{\phi_k \phi_m} \phi_l \phi_n \, dx = \frac{1}{2} \Im \int_{\mathbb{R}^2} \sum\nolimits^{*} \gamma_{lmnk} (\mu_k + \mu_m) \overline{\phi_k \phi_m} \phi_l \phi_n \, dx \\
&= \frac{1}{4} \Im \int_{\mathbb{R}^2} \sum\nolimits^{*} \gamma_{lmnk} \left[(\mu_k + \mu_m) \overline{\phi_k \phi_m} \phi_l \phi_n + (\mu_l + \mu_n) \overline{\phi_l \phi_n} \phi_k \phi_m \right] dx \\
&= \frac{1}{4} \Im \int_{\mathbb{R}^2} \sum\nolimits^{*} \gamma_{lmnk} (\mu_k + \mu_m - \mu_l - \mu_n) \overline{\phi_k \phi_m} \phi_l \phi_n \, dx = 0.
\end{aligned}$$

2. Global Existence for Finite Subsystems

The first step in the numerical approximation of (1.8) is to cutoff the denumerable system at some finite index N. Define $\Phi := (\phi_k(t,x))_{k\leq N}$, where ϕ_k satisfies:

$$i\partial_t \phi_k = H^\perp \phi_k + f_k(\Phi), \tag{2.1}$$
$$\phi_k(0,x) = \phi_k^I(x), \tag{2.2}$$

with $k \leq N$ and

$$f_k(\Phi) = \sum_{\substack{\mu_n+\mu_l-\mu_m-\mu_k=0 \\ n,l,m\leq N}} \gamma_{lmnk} \phi_l \overline{\phi_m} \phi_n. \tag{2.3}$$

The method used to show uniqueness and global existence of the finite system works analogously to the proof for the well-posedness of the NLS in the subcritical case.[8,5,4,6] For the sake of completeness, we present a brief sketch here.

Definition 2.1. Denote by $(L^p)^N$ the following space:

$$(L^p)^N = \left\{ \Phi = (\phi_k)_{k\le N} \colon \phi_k \in L^p(\mathbb{R}^2)\ \forall\, k \le N;\ \max_{k\le N} \|\phi_k\|_{L^p(\mathbb{R}^2)} < \infty \right\}, \tag{2.4}$$

equipped with the maximum norm $|\Phi|_{(L^p)^N} = \max_{k\le N} \|\phi_k\|_{L^p(\mathbb{R}^2)}$. Define by

$$\Sigma := \left\{ \Psi = (\psi_k)_{k\le N} \colon \sum_{k\le N} \|\psi_k\|^2_{H^1(\mathbb{R}^2)} + \sum_{k\le N} \||x|\psi_k\|^2_{L^2(\mathbb{R}^2)} < \infty \right\}. \tag{2.5}$$

First one has to show by a contraction argument uniqueness and existence of the Cauchy problem on a small time interval $I \subset \mathbb{R}$; $|I| < T$ in

$$\mathcal{X}(I) := C(I, (L^4)^N).$$

Note that Σ is continuously embedded in $(L^4)^N$. Since the time interval of existence of a local solution with initial data in Σ depends only on the Σ-norm, one can show global existence if one finds an *a priori* estimate for the Σ-norm of the solution. Notice that the energy is positive. This fact allows then to recover directly estimates for the Σ-norm. In order to prove the conservation laws at a nonformal level one has to introduce a regularization, which can be removed subsequently by a standard limiting argument. Hereafter we sketch the existence result.

Theorem 2.1. *Let $\Phi^I \in \Sigma$. Then the IVP* (2.1), (2.2) *has a unique solution Φ in $\mathcal{X}(\mathbb{R})$. Furthermore $\Phi \in C_b(\mathbb{R}, \Sigma)$ and satisfies the following equalities:*

$$E_1[\Phi^I] = E_1[\Phi(t)], \quad |\Phi^I|_{(L^2)^N} = |\Phi(t)|_{(L^2)^N}, \tag{2.6}$$

with

$$E_1[\Phi(t)] := \frac{1}{2}\left[|\nabla\Phi(t)|^2_{(L^2)^N} + |x|\ \Phi(t)|^2_{(L^2)^N} + \int_{\mathbb{R}^2} \sum_{k\le N} f_k(\Phi(t,x))\overline{\phi_k(t,x)}\, dx \right].$$

For the proof we proceed as in Ref. 8. The following lemmas and the derived conservation laws provide the tools needed in the proof.

Lemma 2.1. *The map $\Phi \mapsto \mathbf{f}(\Phi)$, where $\mathbf{f}(\Phi) = (f_k(\Phi))_{k\le N}$, is continuous from $(L^4)^N$ to $(L^{4/3})^N$ and satisfies the estimate:*

$$|\mathbf{f}(\Phi) - \mathbf{f}(\Psi)|_{(L^{4/3})^N} \le C|\Phi - \Psi|_{(L^4)^N}\left(|\Phi|^2_{(L^4)^N} + |\Psi|^2_{(L^4)^N}\right), \tag{2.7}$$

where C is a generic constant and may depend on N.

Proof. We easily obtain:

$$\begin{aligned}
&\left|\phi_l\overline{\phi_m}\phi_n - \psi_l\overline{\psi_m}\psi_n\right| \\
&\quad\le \left|\phi_l\overline{\phi_m}\phi_n - \psi_l\overline{\phi_m}\phi_n\right| + \left|\psi_l\overline{\phi_m}\phi_n - \psi_l\overline{\psi_m}\phi_n\right| + \left|\psi_l\overline{\psi_m}\phi_n - \psi_l\overline{\psi_m}\psi_n\right| \\
&\quad= |\phi_l - \psi_l||\overline{\phi_m}\phi_n| + |\phi_m - \psi_m||\psi_l\phi_n| + |\phi_n - \psi_n||\overline{\psi_m}\psi_l| \\
&\quad\le \frac{1}{2}\left[|\phi_l - \psi_l|(|\phi_m|^2 + |\phi_n|^2) + |\phi_m - \psi_m|(|\psi_l|^2 + |\phi_n|^2)\right. \\
&\qquad\left. + |\phi_n - \psi_n|(|\psi_m|^2 + |\psi_l|^2)\right],
\end{aligned}$$

such that the nonlinearity can be estimated by:

$$\begin{aligned}
&\|f_k(\Phi) - f_k(\Psi)\|_{L^{4/3}} \\
&\quad\le C \sum_{\substack{\mu_n+\mu_l-\mu_m-\mu_k=0 \\ n,l,m\le N}} \gamma_{lmnk}\Big[\|\phi_l - \psi_l\|_{L^4}(\|\phi_m\|_{L^4}^2 + \|\phi_n\|_{L^4}^2) \\
&\qquad + \|\phi_m - \psi_m\|_{L^4}(\|\psi_l\|_{L^4}^2 + \|\phi_n\|_{L^4}^2) + \|\phi_n - \psi_n\|_{L^4}(\|\psi_m\|_{L^4}^2 + \|\psi_l\|_{L^4}^2)\Big].
\end{aligned}$$

Summing up over all $k \le N$, making use of the symmetry of the indices in the sum over $\mu_l + \mu_n = \mu_k + \mu_m$, we obtain:

$$\begin{aligned}
&\sum_{k\le N} \|f_k(\Phi) - f_k(\Psi)\|_{L^{4/3}} \\
&\quad\le C \sum_{\substack{\mu_n+\mu_l-\mu_m-\mu_k=0 \\ n,l,m\le N}} \gamma_{lmnk}\|\phi_k - \psi_k\|_{L^4} \\
&\qquad\times \left(\|\phi_l\|_{L^4}^2 + \|\phi_m\|_{L^4}^2 + \|\phi_n\|_{L^4}^2 + \|\psi_l\|_{L^4}^2 + \|\psi_m\|_{L^4}^2 + \|\psi_n\|_{L^4}^2\right) \\
&\quad\le C\left(\sum_{k\le N}\|\phi_k - \psi_k\|_{L^4}^2\right)^{1/2} \times \left[\sum_{k\le N}\left(\sum_{\substack{\mu_n+\mu_l-\mu_m-\mu_k=0 \\ n,l,m\le N}} \gamma_{lmnk}\right.\right. \\
&\qquad\left.\left.\times \left(\|\phi_l\|_{L^4}^2 + \|\phi_m\|_{L^4}^2 + \|\phi_n\|_{L^4}^2 + \|\psi_l\|_{L^4}^2 + \|\psi_m\|_{L^4}^2 + \|\psi_n\|_{L^4}^2\right)\right)^2\right]^{1/2} \\
&\quad\le C\left(\sum_{k\le N}\|\phi_k - \psi_k\|_{L^4}^2\right)^{1/2}\left(\sum_{l\le N}(\|\phi_l\|_{L^4}^2 + \|\psi_l\|_{L^4}^2)\right) \\
&\quad\le C|\Phi - \Psi|_{(L^4)^N}(|\Phi|_{(L^4)^N}^2 + |\Psi|_{(L^4)^N}^2).
\end{aligned}$$

□

Corresponding to (2.1) we write the integral equation:

$$\phi_k(t) = U(t)\phi_k^I + [F_k(0,t)\Phi](t), \tag{2.8}$$

with $(U(t))_{t\in\mathbb{R}}$ being the group of isometries generated by $-iH^\perp$ and

$$[F_k(t_1,t_2)\Phi](t) := i\int_{t_1}^{t_2} U(t-\tau)f_k(\Phi(\tau))d\tau.$$

Lemma 2.2. *The map* $(t_1, t_2, \Phi) \mapsto F(t_1, t_2)\Phi$ *is a continuous map from* $I \times I \times \mathcal{X}(I)$ *to* $\mathcal{X}(I)$. *Moreover* F *satisfies:*

$$|F(t_1,t_2)\Phi - F(t_1,t_2)\Psi|_{\mathcal{X}(I)} \leq C|t_1 - t_2|^{1/2}|\Phi - \Psi|_{\mathcal{X}(I)} \left(|\Phi|^2_{\mathcal{X}(I)} + |\Psi|^2_{\mathcal{X}(I)}\right).$$

Proof. As a consequence of Lemma 2.1 we have for any $\Phi \in \mathcal{X}(I)$ continuity of the function $\tau \mapsto f(\Phi(\tau))$. Furthermore we can use information on the operator $U(t)$, which is actually a bounded operator from $L^{4/3}$ to L^4, for t different from zero, such that for $\Theta \in \mathcal{C}(I, (L^{4/3})^N)$ the map $\tau \mapsto U(t-\tau)\Theta(\tau)$ (where we apply the operator componentwise) is continuous from $I \setminus \{t\}$ to $(L^4)^N$. Finally the combination of the two maps provides the desired continuity result and we estimate:

$$\begin{aligned}
&|[F(t_1,t_2)\Phi - F(t_1,t_2)\Psi](t)|_{(L^4)^N} \\
&\quad \leq \sum_{k\leq N} \|[F_k(t_1,t_2)\Phi - F_k(t_1,t_2)\Psi](t)\|_{L^4} \\
&\quad \leq \sum_{k\leq N} \int_{t_1}^{t_2} \|U(t-\tau)[f_k(\Phi(\tau)) - f_k(\Psi(\tau))]\|_{L^4} d\tau \\
&\quad \leq \sum_{k\leq N} \int_{t_1}^{t_2} [|t-\tau|^{-1/2} \|f_k(\Phi(\tau)) - f_k(\Psi(\tau))\|_{L^{4/3}}] d\tau \\
&\quad = \int_{t_1}^{t_2} [|t-\tau|^{-1/2} \sum_{k\leq N} \|f_k(\Phi(\tau)) - f_k(\Psi(\tau))\|_{L^{4/3}}] d\tau \\
&\quad \leq |t_1 - t_2|^{1/2} |f_k(\Phi) - f_k(\Psi)|_{\mathcal{C}(I,(L^{4/3})^N)}.
\end{aligned}$$

The statement is then a consequence of Lemma 2.1. □

3. Numerical Approximation

In this section we describe the method used to numerically solve the asymptotic approximation (1.8) of the GPE with strongly anisotropic potential. We have already seen in the first part of this work that in the limit ε to zero ("infinite" confinement in z-direction) we formally obtain a system of GPEs. To treat the system numerically we truncate the expansion at a finite index N and consider only a finite number of limiting equations (2.1), with $0 \leq k < N$. Moreover, we consider here a spatial dimension reduction from 2D to 1D, for which the theory developed in the previous sections applies just as for the presented case of reduction from 3D to 2D. In other words, we consider the following rescaled GPE:

$$\begin{aligned}
&i\psi_t = H^{\perp}\psi + \tfrac{1}{\varepsilon^2} H\psi + |\psi|^2\psi, \\
&\psi(0,x,z) = \psi^I(x,z), \quad x,z \in \mathbb{R}.
\end{aligned} \tag{3.1}$$

In order to solve the GPE (3.1) (for benchmark tests), we use the time-splitting spectral method (TSSP).[2]

For $N = 1$, we have only one equation in the limiting system:

$$\begin{aligned} i\partial_t\phi_0 &= H^\perp\phi_0 + \gamma_{0000}|\phi_0|^2\phi_0, \\ \phi(0,x) &= \phi_0^I(x), \quad x \in \mathbb{R}, \end{aligned} \tag{3.2}$$

where

$$\gamma_{klmn} = \int_{\mathbb{R}} \omega_k(z)\omega_l(z)\omega_m(z)\omega_n(z)\,dz,$$

(μ_k, ω_k) is the k-eigenpair satisfying

$$\frac{1}{2}(-\partial_{zz} + z^2)\omega_k(z) = \mu_k\omega_k(z),$$

with ω_k normalized to 1 in $L^2(\mathbb{R})$.

For $N = 2$, we have the following limiting coupled system:

$$\begin{aligned} i\partial_t\phi_0 &= H^\perp\phi_0 + \left(\gamma_{0000}|\phi_0|^2 + 2\gamma_{0011}|\phi_1|^2\right)\phi_0, \\ i\partial_t\phi_1 &= H^\perp\phi_1 + \left(2\gamma_{0011}|\phi_0|^2 + \gamma_{1111}|\phi_1|^2\right)\phi_1. \end{aligned} \tag{3.3}$$

It is obvious that for both cases, $N = 1^2$ and $N = 2^1$ respectively, we can use (the Strang-splitting version of) TSSP for discretizing the system in a straightforward way, since both equations are of NLS-type such that the moduli of the wave functions ϕ_0 and ϕ_1 are conserved in the potential-splitting step.

On the other hand, if we consider $N = 3$ we have:

$$\begin{aligned} i\partial_t\phi_0 &= H^\perp\phi_0 + (\gamma_{0000}|\phi_0|^2 + 2\gamma_{0011}|\phi_1|^2 + 2\gamma_{0022}|\phi_2|^2)\phi_0 + \gamma_{0112}\phi_1^2\bar{\phi}_2, \\ i\partial_t\phi_1 &= H^\perp\phi_1 + (2\gamma_{0011}|\phi_0|^2 + \gamma_{1111}|\phi_1|^2 + 2\gamma_{1122}|\phi_2|^2)\phi_1 + 2\gamma_{0112}\phi_0\bar{\phi}_1\phi_2, \\ i\partial_t\phi_2 &= H^\perp\phi_2 + (2\gamma_{0022}|\phi_0|^2 + 2\gamma_{1122}|\phi_1|^2 + \gamma_{2222}|\phi_2|^2)\phi_2 + \gamma_{0112}\bar{\phi}_0\phi_1^2. \end{aligned}$$

For $t \in [t_n, t_{n+1}]$ we discretize this system of three equations by splitting it in three subsystems which we are going to solve in five steps:

Step 1. For the time step of length $\Delta t/2$ we solve:

$$\begin{aligned} i\partial_t\phi_0 &= \left(\frac{x^2}{2} + \gamma_{0000}|\phi_0|^2 + 2\gamma_{0011}|\phi_1|^2 + 2\gamma_{0022}|\phi_2|^2\right)\phi_0, \\ i\partial_t\phi_1 &= \left(\frac{x^2}{2} + 2\gamma_{0011}|\phi_0|^2 + \gamma_{1111}|\phi_1|^2 + 2\gamma_{1122}|\phi_2|^2\right)\phi_1, \\ i\partial_t\phi_2 &= \left(\frac{x^2}{2} + 2\gamma_{0022}|\phi_0|^2 + 2\gamma_{1122}|\phi_1|^2 + \gamma_{2222}|\phi_2|^2\right)\phi_2. \end{aligned}$$

Since for this time step each ODE leaves $|\phi_0|, |\phi_1|$ and $|\phi_2|$ invariant in time, we can integrate each equation (separately) exactly in time, given initial data at t_n.

Step 2. For the time step of length $\Delta t/2$ we solve:

$$\begin{aligned} i\partial_t\phi_0 &= -\frac{1}{2}\Delta_x\phi_0, \\ i\partial_t\phi_1 &= -\frac{1}{2}\Delta_x\phi_1, \\ i\partial_t\phi_2 &= -\frac{1}{2}\Delta_x\phi_2, \end{aligned}$$

by using the Fourier pseudospectral discretization in space and then integrating the ordinary differential system (ODEs) in phase space exactly in time.

Step 3. For the time step of length Δt we solve:

$$\begin{aligned} i\partial_t\phi_0 &= \gamma_{0112}\phi_1^2\bar{\phi}_2, \\ i\partial_t\phi_1 &= 2\gamma_{0112}\phi_0\phi_2\bar{\phi}_1, \\ i\partial_t\phi_2 &= \gamma_{0112}\phi_1^2\bar{\phi}_0. \end{aligned} \tag{3.4}$$

Here we discuss in detail how we implement the discretization of (3.4). We can rewrite this system as:

$$i\partial_t\Phi = \gamma_{0112}A(\Phi)\Phi, \quad \text{where} \quad A(\Phi) := \begin{pmatrix} 0 & \phi_1\bar{\phi}_2 & 0 \\ \phi_2\bar{\phi}_1 & 0 & \phi_0\bar{\phi}_1 \\ 0 & \phi_1\bar{\phi}_0 & 0 \end{pmatrix} \tag{3.5}$$

and $\Phi = (\phi_0, \phi_1, \phi_2)^{\mathrm{T}}$. Integrate (3.5) over the time interval $[t_n, t_{n+1}]$, approximate the integral by the trapezoidal quadrature, we get

$$\begin{aligned} \Phi(t_{n+1}) &= e^{-i\gamma_{0112}\int_{t_n}^{t_{n+1}} A(\Phi(\tau))d\tau} \approx e^{-i\gamma_{0112}\frac{\Delta t}{2}[A(\Phi(t_n))+A(\Phi(t_{n+1}))]} \\ &\approx e^{-i\gamma_{0112}\frac{\Delta t}{2}[A(\Phi^n)+A(\Phi^{(1)})]} := e^{-i\gamma_{0112}\Delta t B(\Phi^n)}, \end{aligned}$$

where $\Phi^n := \Phi(t_n)$ and $\Phi^{(1)}$ is an approximation of $\Phi(t_{n+1})$ and can be computed from the ODEs (3.5) by any explicit method. Here we use the Forward Euler method to compute it as:

$$\begin{aligned} \Phi^{(1)} &= \Phi^n - i\Delta t\gamma_{0112}A(\Phi^n)\Phi^n, \\ B(\Phi^n) &= \frac{1}{2}[A(\Phi^n) + A(\Phi^{(1)})] := \begin{pmatrix} 0 & b_{12} & 0 \\ \bar{b}_{12} & 0 & b_{23} \\ 0 & \bar{b}_{23} & 0 \end{pmatrix}, \end{aligned}$$

where $b_{12} = \frac{1}{2}(\phi_1^n\bar{\phi}_2^n + \phi_1^{(1)}\bar{\phi}_2^{(1)}), b_{23} = \frac{1}{2}(\phi_0^n\bar{\phi}_1^n + \phi_0^{(1)}\bar{\phi}_1^{(1)})$. Since A is Hermitian, i.e. $\bar{A}^{\mathrm{T}} = A$, thus B is also Hermitian. Therefore, we can find explicitly a unitary matrix P with $P^{-1} = \bar{P}^{\mathrm{T}}$ and a real diagonal matrix Λ such that

$$B = P\Lambda P^{-1} = P\Lambda\bar{P}^{\mathrm{T}},$$

where

$$\lambda = \sqrt{|b_{12}|^2 + |b_{23}|^2}, \quad \Lambda = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix}, \quad P = \frac{1}{\lambda\sqrt{2}}\begin{pmatrix} \sqrt{2}b_{23} & b_{12} & -b_{12} \\ 0 & \lambda & \lambda \\ -\sqrt{2}b_{12} & \bar{b}_{23} & -\bar{b}_{23} \end{pmatrix}.$$

Thus we can compute one-step approximation of the ODEs (3.5) as

$$\Phi^{n+1} = Pe^{-i\gamma_{0112}\Delta t\Lambda}\bar{P}^{\mathrm{T}}\Phi^n.$$

Remark 3.1. Since B is Hermitian and thus Λ is a real diagonal matrix, it is then obvious that we have total mass conservation, i.e.

$$\begin{aligned} \|\Phi^{n+1}\|^2 &:= (\bar{\Phi}^{n+1})^{\mathrm{T}}\Phi^{n+1} = (\bar{\Phi}^n)^{\mathrm{T}}Pe^{i\gamma_{0112}\Delta t\Lambda}\bar{P}^{\mathrm{T}}Pe^{-i\gamma_{0112}\Delta t\Lambda}\bar{P}^{\mathrm{T}}\Phi^n \\ &= (\bar{\Phi}^n)^{\mathrm{T}}\Phi^n = \|\Phi^n\|^2. \end{aligned}$$

Step 4. For the time step of length $\Delta t/2$ we solve again:

$$i\partial_t \phi_0 = -\frac{1}{2}\Delta_x \phi_0,$$
$$i\partial_t \phi_1 = -\frac{1}{2}\Delta_x \phi_1,$$
$$i\partial_t \phi_2 = -\frac{1}{2}\Delta_x \phi_2.$$

Step 5. For the time step of length $\Delta t/2$ we solve again:

$$i\partial_t \phi_0 = \left(\frac{x^2}{2} + \gamma_{0000}|\phi_0|^2 + 2\gamma_{0011}|\phi_1|^2 + 2\gamma_{0022}|\phi_2|^2\right)\phi_0,$$
$$i\partial_t \phi_1 = \left(\frac{x^2}{2} + 2\gamma_{0011}|\phi_0|^2 + \gamma_{1111}|\phi_1|^2 + 2\gamma_{1122}|\phi_2|^2\right)\phi_1,$$
$$i\partial_t \phi_2 = \left(\frac{x^2}{2} + 2\gamma_{0022}|\phi_0|^2 + 2\gamma_{1122}|\phi_1|^2 + \gamma_{2222}|\phi_2|^2\right)\phi_2.$$

For $N = 4$ we can use the analogous type of discretization as in the case of $N = 3$. Writing the system for $N = 4$ explicitly we immediately realize that the matrix A is Hermitian.

We remark that the presented time splitting-spectral technique for $N = 1, 2, 3, 4$ is second order in time and of spectral accuracy in space.

4. Numerical Examples

Example 4.1. For $N = 1$, i.e. in the case of one limiting equation, we choose as initial condition for (3.1)

$$\psi^I(x, z) = \omega_0(z)\phi_0^I(x), \tag{4.1}$$

and solve the IVP on $[-8, 8]\times[-a_z, a_z]$ with periodic boundary conditions. Secondly, we solve (3.2) with initial condition

$$\phi_0(0, x) = \phi_0^I(x) = \left(\frac{1}{\pi}\right)^{1/4} e^{-x^2/2}, \tag{4.2}$$

on $[-8, 8]$ with periodic boundary conditions.

N_x denotes the number of grid points in x-direction, N_z denotes the number of grid points in z-direction and Δt the time step. The numerical values for the experiment setup can be seen in Table 1.

Table 1. Values for the parameters used in numerical experiments.

ε	a_z	N_z	N_x	Δt
0.8	6	128	256	10^{-3}
0.4	3	128	256	10^{-3}
0.2	1.5	256	512	10^{-4}
0.1	0.8	256	512	10^{-4}
0.05	0.4	256	512	10^{-5}

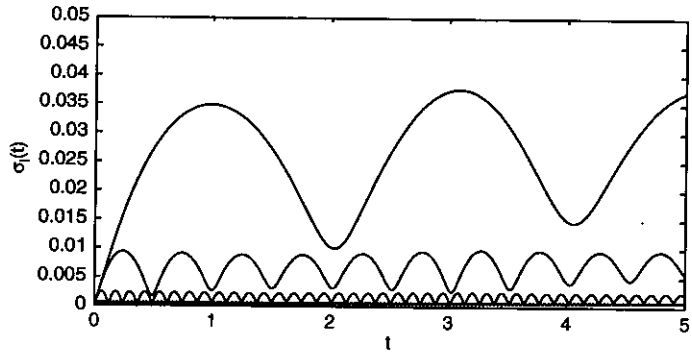

Fig. 1. $\sigma_1^\varepsilon(t)$ with $\varepsilon = 0.8, 0.4, 0.2, 0.1$ and 0.05 (in the order of decreasing peaks).

In Fig. 1, we plot the L^2 norm of the approximation error as function of time, with final time $t = 5$, i.e.

$$\sigma_1^\varepsilon(t) = \|\psi(.,.,t) - \phi_0(.,t)\omega_0(.)e^{-i\mu_0 t/\varepsilon^2}\|_{L^2(\mathbb{R}^2)}, \tag{4.3}$$

for different ε.

From Fig. 1, we can see that when ε decreases by half to $\varepsilon/2$, the error decreases by half too, and the oscillation frequency of the error increases four times.

Example 4.2. For $N = 2$, i.e. in the case of two equations (3.3), we choose initial data as

$$\begin{aligned} \phi_0(0,x) &= \phi_0^I(x) = \left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\pi}\right)^{1/4} e^{-x^2/2}, \\ \phi_1(0,x) &= \phi_1^I(x) = \sqrt{2}x\phi_0^I, \end{aligned} \tag{4.4}$$

and solve the coupled system of GPEs on the x-interval $[-8,8]$ subject to periodic boundary conditions. The initial condition for (3.1) is taken as:

$$\psi^I(x,z) = \omega_0(z)\phi_0^I(x) + \omega_1(z)\phi_1^I(x),$$

with ϕ_0^I and ϕ_1^I as in (4.4). As before we solve the 2D GPE $[-8,8]\times[-a_z,a_z]$ subject to periodic boundary conditions. Furthermore we consider the same experimental setup as before (see detail in Table 1) and plot in Fig. 2 the following quantity for different values of ε:

$$\sigma_2^\varepsilon(t) = \left\|\psi(.,.,t) - \sum_{k=0}^{1}\phi_k(.,t)\omega_k(.)e^{-i\mu_k t/\varepsilon^2}\right\|_{L^2(\mathbb{R}^2)}. \tag{4.5}$$

Example 4.3. For $N = 3$, we proceed analogously for the coupled system (3.4) of three GPEs. We choose initial conditions as

$$\phi_0(0,x) = \phi_0^I(x) = \left(\frac{1}{\sqrt{3}}\right)\left(\frac{1}{\pi}\right)^{1/4} e^{-x^2/2},$$

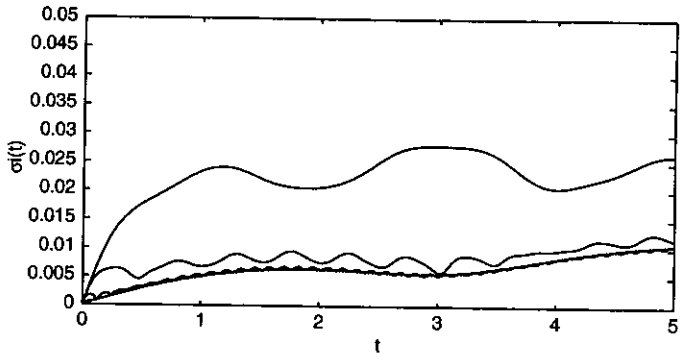

Fig. 2. $\sigma_2^\varepsilon(t)$ with $\varepsilon = 0.8, 0.4, 0.2, 0.1$ and 0.05 (in the order of decreasing peaks).

$$\phi_1(0,x) = \phi_1^I(x) = \sqrt{2}x\phi_0^I, \qquad (4.6)$$
$$\phi_2(0,x) = \phi_2^I(x) = \frac{1}{\sqrt{8}}(4x^2-2)\phi_0^I,$$

and solve on the x-interval $[-8,8]$ subject to periodic boundary conditions. Then we choose initial datum for (3.1) as:

$$\psi^I(x,z) = \omega_0(z)\phi_0^I(x) + \omega_1(z)\phi_1^I(x) + \omega_2(z)\phi_2^I(x), \qquad (4.7)$$

with ϕ_0^I, ϕ_1^I and ϕ_2^I as in (4), and solve as before on $[-8,8] \times [-a_z, a_z]$ subject to periodic boundary conditions. Analogously to $N = 1, 2$ we depict in Fig. 3 the error:

$$\sigma_3^\varepsilon(t) = \left\| \psi(.,.,t) - \sum_{k=0}^{2} \phi_k(.,t)\omega_k(.)e^{-i\mu_k t/\varepsilon^2} \right\|_{L^2(\mathbb{R}^2)}.$$

From Figs. 1–3, we can draw the following conclusions: (i) When $N = 1$, the approximation error clearly "tends to 0" as ε "tends to zero" (cf. Fig. 1). (ii) When $N = 2, 3$, the approximation error decreases when ε decreases and is not too small. When ε is small, it stabilizes at some nonzero values although ε is still decreasing

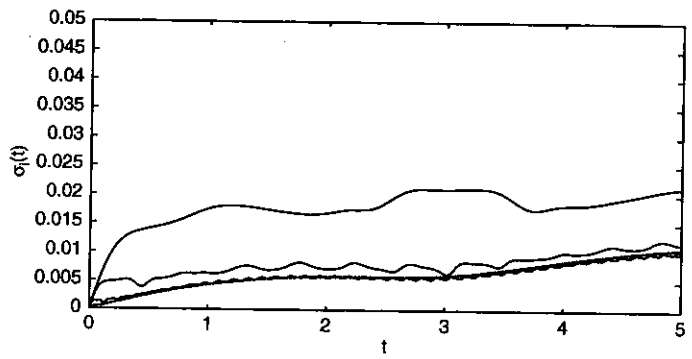

Fig. 3. $\sigma_3^\varepsilon(t)$ with $\varepsilon = 0.8, 0.4, 0.2, 0.1$ and 0.05 (in the order of decreasing peaks).

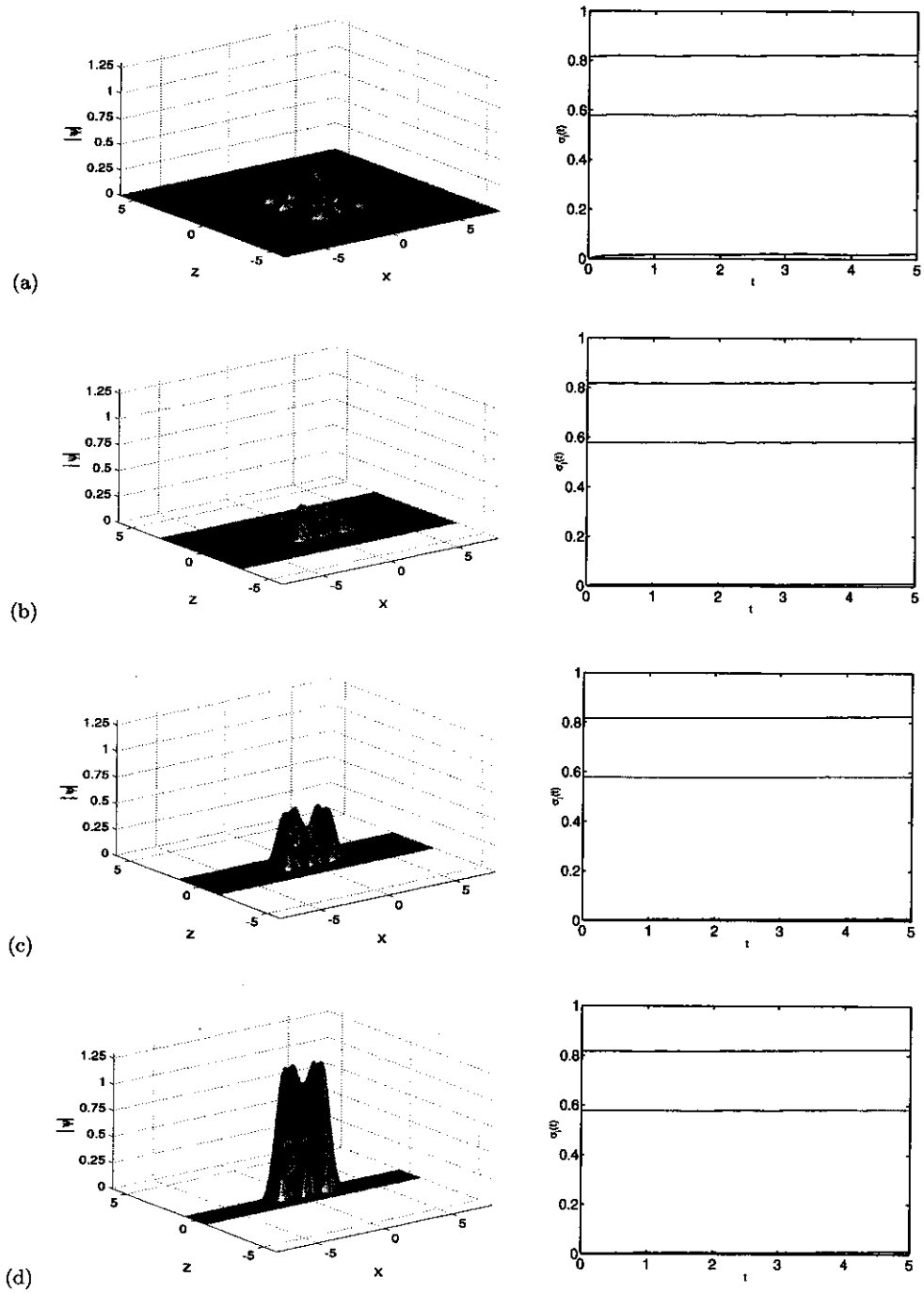

Fig. 4. Surface plots (left column) of the position density $|\psi^\varepsilon(x, t = 5)|^2$ and the approximation errors $\sigma_1^\varepsilon(t)$ (upper), $\sigma_2^\varepsilon(t)$ (middle), $\sigma_3^\varepsilon(t)$ (lower) (right column) for different ε: (a) $\varepsilon = 0.8$; (b) $\varepsilon = 0.4$; (c) $\varepsilon = 0.2$; (d) $\varepsilon = 0.1$.

(cf. Figs. 2 and 3). This is due to the fact that no other Fourier terms are generated for $N = 1$, while all Fourier terms (with indices $k \geq 0$) appear instantaneously for $N = 2, 3$.

Example 4.4. Finally, we compare for fixed values of ε the functions $\sigma_1^\varepsilon(t)$, $\sigma_2^\varepsilon(t)$ and $\sigma_3^\varepsilon(t)$, where $\psi(t)$ is solved with initial data (4.7). Figure 4 shows these functions and a reference GPE-solution $|\psi(t = 5)|^2$ computed with the intial datum (4.7) for different ε.

From Fig. 4, we can observe that: (i) the reference solution concentrates more and more in the z-direction as ε tends to zero; (ii) the more Fourier terms are considered in the approximation, the smaller the approximation error becomes; (iii) when N is fixed, the approximation error does not decrease when ε is decreasing but small, i.e. this implies that expansion error becomes dominant when ε is sufficiently small. In fact, the approximation error consists of two parts: one is from the truncation error, and the other is from the anisotropic confinement.

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References

1. W. Bao, Ground states and dynamics of multi-component Bose–Einstein condensates, *SIAM Multiscale Model Simu.* **2** (2004) 210–236.
2. W. Bao, D. Jaksch and P. A. Markowich, Numerical solution of the Gross–Pitaevskii equation for Bose–Einstein condensation, *J. Comput. Phys.* **187** (2003) 318–342.
3. N. Ben Abdallah, F. Méhats, Ch. Schmeiser and R. M. Weishäupl, The nonlinear Schrödinger equation with a strongly anisotropic harmonic potential, submitted.
4. R. Carles, Remarks on nonlinear Schrödinger equations with harmonic potential, *Ann. Henri Poincaré* **3** (2002) 757–772.
5. T. Cazenave, *An Introduction of Nonlinear Schrödinger Equations*, 3rd edn. (Universidade Federal do Rio de Janeiro, 1996).
6. J. Ginibre and G. Velo, The global Cauchy problem for the nonlinear Schrödinger equation revisited, *Ann. Inst. H. Poincaré, Anal. Nonlinéaire* **2** (1985) 309–327.
7. E. H. Lieb, R. Seiringer and J. Yngvason, One-dimensional behaviour of dilute, trapped Bose gases, *Comm. Math. Phys.* **244** (2004) 347–393.
8. Y. G. Oh, Cauchy problem and Ehrenfest's law of nonlinear Schrödinger equations with potentials, *J. Diff. Eqns.* **81** (1989) 255–274.
9. M. Reed and B. Simon, *Methods of Modern Mathematical Physics* (Academic Press, 1975).