Second order averaging for the nonlinear Schrödinger equation with strong anisotropic potential

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Abstract

We consider the three dimensional Gross-Pitaevskii equation (GPE) describing a Bose-Einstein Condensate (BEC) which is highly confined in vertical z direction. The confining potential induces high oscillations in time. If the confinement in the z direction is a harmonic trap – an approximation which is widely used in physical experiments – the very special structure of the spectrum of the confinement operator implies that the oscillations are periodic in time. Based on this observation, it can be proved that the GPE can be averaged out with an error of order of ε, which is the typical period of the oscillations. In this article, we construct a more accurate averaged model, which approximates the GPE up to errors of order $\mathcal{O}(\varepsilon^2)$. Then, expansions of this model over the eigenfunctions (modes) of the confining operator $\mathbf{H}_z$ in the z-direction are given in view of numerical applications. Efficient numerical methods are constructed to solve the GPE with cylindrical symmetry in 3D and the approximation model with radial symmetry in 2D, and numerical results are presented for various kinds of initial data.

Key words. Gross-Pitaevskii equation, dimension reduction, second order averaging, Laguerre-Hermite pseudo-spectral method.

1 Introduction

In this paper, we consider the approximation of the Gross-Pitaevskii equation (GPE) modeling the evolution of anisotropic Bose-Einstein Condensates in the space $(x, z) \in \mathbb{R}^2 \times \mathbb{R}$. The wavefunction of the condensate Ψ^ε satisfies the GPE in dimensionless form [6, 25]

$$i\partial_t \Psi^\varepsilon(t,x,z) = \mathbf{H}_x \Psi^\varepsilon(t,x,z) + \frac{1}{\varepsilon}\mathbf{H}_z \Psi^\varepsilon(t,x,z) + \delta|\Psi^\varepsilon|^2\Psi^\varepsilon, \quad (x,z) \in \mathbb{R}^2 \times \mathbb{R}, \tag{1.1}$$

with initial data

$$\Psi^\varepsilon(t=0) = \Psi^{init} \in L^2(\mathbb{R}^2 \times \mathbb{R}), \tag{1.2}$$

where

$$\mathbf{H}_x = \frac{1}{2}\left(-\Delta_x + |x|^2\right), \quad \mathbf{H}_z = \frac{1}{2}\left(-\partial_z^2 + z^2 - 1\right), \quad \delta \in \mathbb{R},$$

and $\varepsilon \in]0,1]$ is a small parameter to describe the strength of the confinement in the z direction compared with that in the x plane. Notice that the singularly perturbed Hamiltonian $\mathbf{H}_z$ is a harmonic oscillator (conveniently shifted here such that it admits integer eigenvalues). For discussions on this scaling, we refer to [2, 3, 8]. When ε goes small, the evolution of the wave function Ψ^ε essentially occurs in the x-plane because of the strong confinement in the z direction. By introducing the filtered unknown

$$\Phi^\varepsilon = e^{it\mathbf{H}_z/\varepsilon}\,\Psi^\varepsilon,$$

we get the equation

$$i\partial_t\Phi^\varepsilon(t,x,z) = \mathbf{H}_x\Phi^\varepsilon(t,x,z) + F\left(\frac{t}{\varepsilon},\Phi^\varepsilon\right), \qquad \Phi^\varepsilon(t=0) = \Psi^{init}, \tag{1.3}$$

where F is equal to

$$F(\tau,\Phi) = \delta\, e^{i\tau\mathbf{H}_z}\left(\left|e^{-i\tau\mathbf{H}_z}\Phi\right|^2 e^{-i\tau\mathbf{H}_z}\,\Phi\right). \tag{1.4}$$

When ε is small, (1.1) (or, equivalently, (1.3)) couples the high oscillations in time generated by the strong confinement operator with a nonlinear dynamics in the x plane, which is the only phenomenon that we want to describe. There are similar dimension reduction problems on the strongly partially confined electron gas, described by a Schrödinger-Poisson system [7,16]. For partially confined BEC (1.1), the early works [3,8] focused on the initial data concentrated on the ground mode of $\mathbf{H}_z$. For general initial data, following the ideas in [19, 28], it is desirable to filter out the oscillations and to derive approximate models for (1.3) by using averaging techniques. Recently, averaging techniques have been used for instance to investigate laser-matter interaction [9, 10, 13, 14], fluid mechanics [24] and geometric optics [23].

In [6], Ben Abdallah et al. have developed an averaging technique and proved that, for general confining potentials in the z direction, the limiting model as ε goes to zero is

$$i\partial_t\Phi = \mathbf{H}_x\Phi + F_{av}\left(\Phi\right), \qquad \Phi(t=0) = \Psi^{init}, \tag{1.5}$$

where the long time average of F is defined by

$$F_{av}(\Phi) = \lim_{T\to+\infty}\frac{1}{T}\int_0^T F(\tau,\Phi)\,d\tau.$$

In the specific case of a harmonic confinement operator, like here, this convergence result can be quantified. The important point is that $\mathbf{H}_z$ admits only integer eigenvalues and the function F is 2π-periodic with respect to the τ variable. Therefore, the expression of F_{av} is not a limit but a simple integral, and we have in fact

$$F_{av}(\Phi) = \frac{1}{2\pi}\int_0^{2\pi} F(\tau,\Phi)\,d\tau. \tag{1.6}$$

On top of that, one can characterize the rate of convergence and prove that Φ is a first order approximation of Φ^ε in ε (see below in Theorem 1.1).

As expected, the limiting equation takes the form of a nonlinear Schrödinger equation in the x variable only. This interesting dimension reduction also minimizes the cost of

numerical simulations, see [3]. However, simulating the averaged equation produces an intrinsic error of order $\mathcal{O}(\varepsilon)$ and, for instance when ε is not very small, it can be desirable to gain precision by seeking the next order approximation of (1.1). The aim of this paper is to go beyond the analysis of [6] and to obtain a second order (in ε) approximate description for the limiting behavior of Ψ^ε as $\varepsilon \to 0$, then to investigate numerical methods at the same order of approximation.

The second order approximation can be constructed by adapting ODE techniques, in the spirit of [6], see e.g. [27]. Since $F(\tau, \Phi)$ is 2π-periodic, the antiderivative of $F(\tau, \Phi) - F_{av}(\Phi)$ is also 2π-periodic. Let us choose the antiderivative with zero average,

$$F^1(\tau, \Phi) = \int_0^\tau \left(F(\sigma, \Phi) - F_{av}(\Phi)\right) d\sigma - \frac{1}{2\pi} \int_0^{2\pi} \int_0^s \left(F(\sigma, \Phi) - F_{av}(\Phi)\right) d\sigma \, ds. \tag{1.7}$$

Then we introduce the derivative of F at u in the direction v

$$D_u F(\tau, u)(v) = \delta e^{i\tau \mathbf{H}_z} \left(\left| e^{-i\tau \mathbf{H}_z} u \right|^2 e^{-i\tau \mathbf{H}_z} v \right) + 2\delta e^{i\tau \mathbf{H}_z} \left(\mathrm{Re} \left(e^{-i\tau \mathbf{H}_z} u e^{i\tau \mathbf{H}_z} \overline{v} \right) e^{-i\tau \mathbf{H}_z} u \right) \tag{1.8}$$

and denote

$$G(\tau, \Phi) = D_\Phi F(\tau, \Phi) \left(F^1(\tau, \Phi) \right), \tag{1.9}$$

which is also a 2π–periodic function of τ. We denote by G_{av} its average

$$G_{av}(\Phi) = \frac{1}{2\pi} \int_0^{2\pi} G(\tau, \Phi) \, d\tau = \frac{1}{2\pi} \int_0^{2\pi} D_\Phi F(\tau, \Phi) \left(F^1(\tau, \Phi) \right) d\tau. \tag{1.10}$$

In order to state our main theorem, we introduce the convenient scale of functional spaces. For all $\ell \in \mathbb{R}_+$, we set

$$B_\ell := \left\{ \psi \in H^\ell(\mathbb{R}^3) \middle| (|x|^2 + z^2)^{\ell/2} \psi \in L^2(\mathbb{R}^3) \right\}$$

endowed with one of the two following equivalent norms:

$$\|u\|_{B_\ell}^2 := \|u\|_{L^2(\mathbb{R}^3)}^2 + \|\mathbf{H}_x^{\ell/2} u\|_{L^2(\mathbb{R}^3)}^2 + \|\mathbf{H}_z^{\ell/2} u\|_{L^2(\mathbb{R}^3)}^2 \tag{1.11}$$

or

$$\|u\|_{B_\ell}^2 := \|u\|_{H^\ell(\mathbb{R}^3)}^2 + \|(|x|^2 + z^2)^{\ell/2} u\|_{L^2(\mathbb{R}^3)}^2. \tag{1.12}$$

The equivalence can be established in view of the early work [11, 21, 22], see e.g. Theorem 2.1 in [6]. Our main theorem is the following.

Theorem 1.1 *For some real number $m > 3/2$, assume that the initial datum Ψ^{init} belongs to B_{m+4}. Let $\Phi^\varepsilon(t, x, z) = e^{-i\tau \mathbf{H}_z/\varepsilon} \Psi^\varepsilon$ be the solution of the filtered equation*

$$i\partial_t \Phi^\varepsilon(t, x, z) = \mathbf{H}_x \Phi^\varepsilon(t, x, z) + F\left(\frac{t}{\varepsilon}, \Phi^\varepsilon\right), \quad \Phi^\varepsilon(t = 0) = \Psi^{init}, \tag{1.13}$$

where

$$F(\tau, \Phi) = \delta \, e^{i\tau \mathbf{H}_z} \left| e^{-i\tau \mathbf{H}_z} \Phi \right|^2 e^{-i\tau \mathbf{H}_z} \Phi \,.$$

Define also $\widetilde{\Phi}$ *as the solution of the averaged problem*

$$i\partial_t\widetilde{\Phi} = \mathbf{H}_x\widetilde{\Phi} + F_{av}\left(\widetilde{\Phi}\right), \qquad \widetilde{\Phi}(t=0) = \Psi^{init}, \tag{1.14}$$

where F_{av} *is defined by* (1.6)*. Lastly, define* $\widetilde{\Phi}^\varepsilon$ *as the solution of*

$$i\partial_t\widetilde{\Phi}^\varepsilon = \mathbf{H}_x\widetilde{\Phi}^\varepsilon + F_{av}(\widetilde{\Phi}^\varepsilon) - i\varepsilon G_{av}(\widetilde{\Phi}^\varepsilon), \tag{1.15}$$

$$\widetilde{\Phi}^\varepsilon(t=0) = \Psi^{init} + i\varepsilon F^1(0,\Psi^{init}), \tag{1.16}$$

where F_{av}*,* F^1*,* G_{av} *are defined by* (1.6)*,* (1.7) *and* (1.10) *separately. Then, we have the following conclusions.*

(i) There is $T_0 > 0$*, depending only on* $\|\Psi^{init}\|_{B_{m+4}}$*, such that* Φ^ε*,* $\widetilde{\Phi}$ *and* $\widetilde{\Phi}^\varepsilon$ *are uniquely defined and are uniformly bounded in the space* $C([0,T_0];B_{m+4})$*, independently of* $\varepsilon \in]0,1]$*.*

(ii) The function $\widetilde{\Phi}$ *is a first order approximation of the solution* Φ^ε *in* $C([0,T_0];B_m)$*, i.e., for some* $C>0$*, we have*

$$\|\Phi^\varepsilon(t) - \widetilde{\Phi}\|_{B_m} \leq C\varepsilon, \quad \forall t\in[0,T_0].$$

(iii) The function

$$\Phi_1^\varepsilon(t) = \widetilde{\Phi}^\varepsilon(t) - i\varepsilon F^1\left(\frac{t}{\varepsilon}, \widetilde{\Phi}^\varepsilon(t)\right)$$

is a second order approximation of the solution Φ^ε *in* $C([0,T_0];B_m)$*, i.e., for some* $C>0$*, we have*

$$\|\Phi^\varepsilon(t) - \Phi_1^\varepsilon(t)\|_{B_m} \leq C\varepsilon^2, \quad \forall t\in[0,T_0].$$

Remark 1.1 *The key property here is the periodicity of* $F(\tau,\Phi)$*, and the result can be generalized to other dimensions* $\mathbb{R}^d = \mathbb{R}^{d-p}\times\mathbb{R}^p$*, more general nonlinearities* $f(|\psi|^2)\psi$ *in (1.1) and other operators* $\mathbf{H}_z$ *such that* $F(\tau,\Phi)$ *defined by* (1.4) *is periodic.*

The paper is organized as follows. In Section 2, we introduce some useful preliminary lemmas. Theorem 1.1 is proved in Section 3, the proofs of items *(i)*, *(ii)* and *(iii)* being respectively done in Subsections 3.1, 3.2 and 3.3. In Section 4, efficient numerical methods are introduced and numerical results are presented. Lastly, some conclusions are drawn in Section 5.

2 Preliminaries

We first recall some useful properties satisfied by the space B_ℓ.

Lemma 2.1 (Proposition 2.5 in [6]) *Take a real number* $\ell > 3/2$*. Define the Sobolev space* B_ℓ *as the completion of the set of smooth functions* $u(x,z)$ *under the norm* (1.11) *or, equivalently, under the norm* (1.12)*. Then,* B_ℓ *is a Hilbert space and we have the*

continuous embedding $B_\ell \subset L^\infty(\mathbb{R}^3)$. *Moreover, for any nonlinear function* $f \in C^\infty(\mathbb{R})$ *(with a possibly unbounded support) satisfying* $f(0) = 0$, *the mapping*

$$u \in B_\ell \longmapsto f(u) \in B_\ell$$

is well-defined and locally Lipschitz continuous. It satisfies the tame estimate

$$\|f(u)\|_{B_\ell} \leq C_f(\|u\|_{L^\infty(\mathbb{R}^3)})\|u\|_{B_\ell}.$$

Here, $C_f(s) > 0$ *depends on* f *and* $s \geq 0$. *It is a locally bounded function of* s.

In particular, B_ℓ is an algebra for $\ell > 3/2$. Now we make two elementary but important remarks for the sequel. First, since the operators $\mathbf{H}_z$ and $\mathbf{H}_x$ commute with the propagators $e^{i\tau\mathbf{H}_z}$ and $e^{i\tau\mathbf{H}_x}$, which are unitary on $L^2(\mathbb{R}^3)$, these two propagators will also be unitary on B_ℓ, endowed with the norm (1.11). Second, for all $u \in L^2(\mathbb{R}^3)$ the function $e^{i\tau\mathbf{H}_z}u$ is 2π-periodic with respect to τ.

From these remarks and from Lemma 2.1, one can deduce the following technical lemma. Its proof is left to the reader and uses repeatedly that B_ℓ is an algebra and that $e^{i\tau\mathbf{H}_z}$ is unitary on B_ℓ and leaves invariant the set of functions in $C(\mathbb{R}; B_\ell)$ which are 2π-periodic with respect to τ.

Lemma 2.2 *For* $\ell > 3/2$, *take* $\Phi(x, z) \in B_\ell$. *Then* $F(\tau, \Phi)$ *defined by* (1.4) *is* 2π*-periodic in* τ, *and the following holds true:*

(i) $F^1(\tau, \Phi)$ *defined by* (1.7) *and* $G(\tau, \Phi)$ *defined by* (1.9) *are both* 2π*-periodic in* τ *and belong to* $C(\mathbb{R}; B_\ell)$.

(ii) F_{av} *and* G_{av} *are locally Lipschitz continuous in* B_ℓ. *Moreover, for any* ℓ' *with* $3/2 < \ell' \leq \ell$, *the following estimates hold,*

$$\|F_{av}(\Phi)\|_{B_\ell} \leq C_{\ell'}(\|\Phi\|_{B_{\ell'}})\|\Phi\|_{B_\ell}, \quad \|G_{av}(\Phi)\|_{B_\ell} \leq C_{\ell'}(\|\Phi\|_{B_{\ell'}})\|\Phi\|_{B_\ell},$$

where $C_{\ell'}(s)$ *only depends on* ℓ' *and* $s \geq 0$.

(iii) The derivative of $F(\tau, u)$ *defined by* (1.8) *satisfies the estimate*

$$\|D_u F(\tau, u)(v)\|_{B_\ell} \leq C_1\left(\|u\|_{B_\ell} + \|v\|_{B_\ell}\right)\|v\|_{B_\ell}, \quad \forall v \in B_\ell,$$

where $C_1(s)$ *only depends on* $s \geq 0$ *and is locally bounded.*

Let us now state our second lemma.

Lemma 2.3 *Take a real number* $m > 3/2$ *and* $T > 0$. *Consider a function* $u^\varepsilon(\tau, t, x, z)$ *defined for* $\varepsilon \in]0, 1]$ *and for* $(\tau, t, x, z) \in \mathbb{R} \times [0, T] \times \mathbb{R}^2 \times \mathbb{R}$ *and satisfying the following assumptions:*

i) $u^\varepsilon \in C(\mathbb{R} \times [0, T]; B_{m+2})$ *and is uniformly bounded with respect to* ε;

ii) u^ε *is differentiable with respect to* t *and* $\partial_t u \in C(\mathbb{R} \times [0, T]; B_m)$ *is uniformly bounded with respect to* ε;

iii) u^ε is 2π-periodic with respect to τ and its average over one period is zero:

$$\int_0^{2\pi} u(\tau,t,x,z)d\tau = 0. \tag{2.1}$$

Then, we have the estimate

$$\sup_{t\in[0,T]} \left\| \int_0^t e^{-i(t-s)\mathbf{H}_x} u^\varepsilon(s/\varepsilon,s,x,z)\,ds \right\|_{B_m} \leq C\varepsilon, \tag{2.2}$$

where $C > 0$ depends on T_0, on $\sup_{\varepsilon\in]0,1]} \|u^\varepsilon\|_{L^\infty(\mathbb{R}\times[0,T];B_{m+2})}$ and on $\sup_{\varepsilon\in]0,1]} \|\partial_t u^\varepsilon\|_{L^\infty(\mathbb{R}\times[0,T];B_m)}$.

Proof. We have to estimate in B_m the function

$$R^\varepsilon = \int_0^t e^{-i(t-s)\mathbf{H}_x} u^\varepsilon(s/\varepsilon,s,x,z)\,ds.$$

Let us introduce the antiderivative of u^ε with respect to its first argument

$$U^\varepsilon(\tau,t,x,z) = \int_0^\tau u^\varepsilon(s,t,x,z)\,ds. \tag{2.3}$$

From assumption *iii)*, we deduce that U^ε is 2π-periodic with respect to τ and that

$$U^\varepsilon(\tau,t,x,z) = \int_0^{2\pi[\frac{\tau}{2\pi}]} u^\varepsilon(s,t,x,z)\,ds + \int_{2\pi[\frac{\tau}{2\pi}]}^\tau u^\varepsilon(s,t,x,z)\,ds = \int_{2\pi[\frac{\tau}{2\pi}]}^\tau u^\varepsilon(s,t,x,z)\,ds. \tag{2.4}$$

Hence, from assumptions *i)* and *ii)*, we obtain, for all $(\tau,t)\in\mathbb{R}\times[0,T]$, the two estimates

$$\|U^\varepsilon(\tau,t,\cdot,\cdot)\|_{B_{m+2}} \leq \int_{2\pi[\frac{\tau}{2\pi}]}^\tau \|u^\varepsilon(s,t,\cdot,\cdot)\|_{B_{m+2}}\,ds \leq 2\pi\|u^\varepsilon\|_{L^\infty(\mathbb{R}\times[0,T];B_{m+2})} \tag{2.5}$$

and

$$\|\partial_t U^\varepsilon(\tau,t,\cdot,\cdot)\|_{B_m} \leq \int_{2\pi[\frac{\tau}{2\pi}]}^\tau \|\partial_t u^\varepsilon(s,t,\cdot,\cdot)\|_{B_m}\,ds \leq 2\pi\|\partial_t u^\varepsilon\|_{L^\infty(\mathbb{R}\times[0,T];B_m)}. \tag{2.6}$$

Now, an integration by parts yields

$$\begin{aligned} R^\varepsilon &= \int_0^t e^{-i(t-s)\mathbf{H}_x}\left(\varepsilon\frac{d}{ds}\left(U^\varepsilon(s/\varepsilon,s,x,z)\right) - \varepsilon\partial_t U^\varepsilon(s/\varepsilon,s,x,z)\right)ds \\ &= \varepsilon U^\varepsilon(t/\varepsilon,t,x,z) - i\varepsilon\int_0^t e^{-i(t-s)\mathbf{H}_x}\mathbf{H}_x U^\varepsilon(s/\varepsilon,s,x,z)\,ds \\ &\quad -\varepsilon\int_0^t e^{-i(t-\tau)\mathbf{H}_x}\partial_t U^\varepsilon(s/\varepsilon,s,x,z)\,ds. \end{aligned}$$

Hence, using that $e^{-is\mathbf{H}_x}$ is unitary on every B_ℓ (endowed with the norm (1.11)), we get

$$\begin{aligned}\|R^\varepsilon\|_{B_m} &\leq \varepsilon\|U^\varepsilon(t/\varepsilon,t,\cdot,\cdot)\|_{L^\infty(\mathbb{R}\times[0,T];B_m)} + \varepsilon\int_0^t \|\mathbf{H}_x U^\varepsilon(s/\varepsilon,s,\cdot,\cdot)\|_{B_m}\,ds \\ &\quad +\varepsilon\int_0^t \|\partial_t U^\varepsilon(s/\varepsilon,s,\cdot,\cdot)\|_{B_m}\,ds \\ &\leq C\varepsilon\left(\|U^\varepsilon(\tau,t,\cdot,\cdot)\|_{L^\infty(\mathbb{R}\times[0,T];B_{m+2})} + \|\partial_t U^\varepsilon(\tau,t,\cdot,\cdot)\|_{L^\infty(\mathbb{R}\times[0,T];B_m)}\right).\end{aligned}$$

Together with (2.5) and (2.6), this gives (2.2). The proof of the lemma is complete. □

3 Proof of the main theorem

In this section, we prove Theorem 1.1. Items *(i)*, *(ii)* and *(iii)* in this theorem are respectively proved in Subsections 3.1, 3.2, 3.3.

3.1 The Cauchy problems

In this subsection, we focus on the three Cauchy problems, the initial problem (1.13), the averaged problem (1.14) and the second order approximation (1.15). More precisely, we prove item *(i)* of Theorem 1.1.

In [6], it is already proved that there is $T_0 > 0$ depending only on $\|\Psi^{init}\|_{B_{m+4}}$ such that Φ^ε and $\widetilde{\Phi}$ are uniquely defined as solutions of (1.13) and (1.14) and are uniformly bounded in the space $C([0,T_0];B_{m+4})$, independently of ε. Let us adapt this proof to show the same result for $\widetilde{\Phi}^\varepsilon$ (up to a possible change of T_0).

First, rewrite the differential equation in its integral form

$$\begin{aligned}\widetilde{\Phi}^\varepsilon(t,x,z) &= e^{-it\mathbf{H}_x}\widetilde{\Phi}^\varepsilon(0,x,z) \\ &\quad -i\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(F_{av}(\widetilde{\Phi}^\varepsilon(s,x,z)) - i\varepsilon G_{av}(\widetilde{\Phi}^\varepsilon(s,x,z))\right)ds. \qquad (3.1)\end{aligned}$$

From Lemma 2.2, one gets the following Lipschitz estimate

$$\begin{aligned}&\left|\left|\int_0^t e^{-i(t-s)\mathbf{H}_x}[F_{av}(u(s,x,z)) - i\varepsilon G_{av}(u(s,x,z)) - F_{av}(v(s,x,z)) + i\varepsilon G_{av}(v(s,x,z))]\,ds\right|\right|_{B_{m+4}} \\ &\leq t\sup_{s\in[0,t]}\left|\left|F_{av}(u(s,x,z)) - i\varepsilon G_{av}(u(s,x,z)) - F_{av}(v(s,x,z)) + i\varepsilon G_{av}(v(s,x,z))\right|\right|_{B_{m+4}} \\ &\leq t\,C_L(\|u\|_{C([0,t];B_{m+4})},\|v\|_{C([0,t];B_{m+4})})\|u-v\|_{C([0,t];B_{m+4})},\end{aligned}$$

where $u,v\in C([0,t];B_{m+4})$. The function $C_L(.,.)$ is independent of $\varepsilon\in]0,1]$ and is non-decreasing with respect to its arguments. Hence, for any given $\varepsilon>0$, it is easy to prove by a fixed-point argument, see e.g. [15], that there exists a maximal time $T_\varepsilon\in]0,+\infty]$, such that the integral equation (3.1) admits a unique solution $\widetilde{\Phi}^\varepsilon(t,x,z)$ in the space $C([0,T_\varepsilon];B_{m+4})$. Moreover, if $T_\varepsilon<+\infty$ then $\|\widetilde{\Phi}^\varepsilon(t,\cdot)\|_{B_m}\to+\infty$ as $t\nearrow T_\varepsilon$.

Next, we want to show T_ε has a lower bound T_0 as $\varepsilon \to 0$. First, taking the scalar product of both sides of the equation with $\widetilde{\Phi}^\varepsilon$, we get

$$\begin{aligned}\partial_t \left(\|\widetilde{\Phi^\varepsilon}(t,x,z)\|^2_{L^2(\mathbb{R}^3)} \right) &= 2\mathcal{I}m \left(F_{av}(\widetilde{\Phi}^\varepsilon(\tau,x,z)) - i\varepsilon G_{av}(\widetilde{\Phi}^\varepsilon(\tau,x,z)), \widetilde{\Phi}^\varepsilon \right)_{L^2} \\ &\leq 2(\|F_{av}(\widetilde{\Phi}^\varepsilon)\|_{L^2} + \varepsilon \|G_{av}(\widetilde{\Phi}^\varepsilon)\|_{L^2}) \|\widetilde{\Phi}^\varepsilon\|_{L^2} \\ &\leq C_1(\|\widetilde{\Phi}^\varepsilon\|_{B_m}) \|\widetilde{\Phi}^\varepsilon\|^2_{B_{m+4}}\end{aligned}$$

where $C_1(u)$ is a locally bounded, non-decreasing function of u. Second, multiplying both sides of (1.15) by $\mathbf{H}_x^{m+4}\overline{\widetilde{\Phi}^\varepsilon} + \mathbf{H}_z^{m+4}\overline{\widetilde{\Phi}^\varepsilon}$ and noticing that the self-adjoint operators $\mathbf{H}_x$ and $\mathbf{H}_z$ commute, we get

$$\begin{aligned}&\partial_t \left(\|\mathbf{H}_x^{(m+2)/2}\widetilde{\Phi}^\varepsilon(t,x,z)\|^2_{L^2(\mathbb{R}^3)} + \|\mathbf{H}_z^{(m+2)/2}\widetilde{\Phi}^\varepsilon(t,x,z)\|^2_{L^2(\mathbb{R}^3)} \right) \\ = \;& 2\mathcal{I}m \left([\mathbf{H}_x^{(m+2)/2} + \mathbf{H}_z^{(m+2)/2}][F_{av}(\widetilde{\Phi}^\varepsilon(\tau,x,z)) - i\varepsilon G_{av}(\widetilde{\Phi}^\varepsilon(\tau,x,z))], [\mathbf{H}_x^{(m+2)/2} + \mathbf{H}_z^{(m+2)/2}]\widetilde{\Phi}^\varepsilon \right)_{L^2} \\ \leq \;& \|F_{av}(\widetilde{\Phi}^\varepsilon) - i\varepsilon G_{av}(\widetilde{\Phi}^\varepsilon)\|_{B_{m+4}} \|\widetilde{\Phi^\varepsilon}\|_{B_{m+4}} \leq C_2(\|\widetilde{\Phi}^\varepsilon\|_{B_m}) \|\widetilde{\Phi^\varepsilon}\|^2_{B_{m+4}}\end{aligned}$$

where $C_2(s)$ is a locally bounded, non-decreasing function of $s \geq 0$. For the above two steps, we have applied Lemma 2.2. Finally, we have

$$\partial_t \left(\|\widetilde{\Phi}^\varepsilon(t,x,z)\|^2_{B_{m+4}} \right) \leq C(\|\widetilde{\Phi}^\varepsilon\|_{B_m}) \|\widetilde{\Phi}^\varepsilon\|^2_{B_{m+4}},$$

for possibly large value of $C(\cdot)$. Noticing that the initial datum (1.16) satisfies

$$\|\widetilde{\Phi}^\varepsilon(0,x,z)\|_{B_{m+4}} \leq C\left(\|\Psi^{init}\|_{B_{m+4}} \right),$$

by the Gronwall lemma, we obtain the existence of a common $T_0 > 0$ such that $\widetilde{\Phi}^\varepsilon$ remains bounded on $[0, T_0]$ for $\varepsilon \in]0, 1]$. The proof of item *(i)* of the main Theorem 1.1 is complete.

3.2 First order approximation

In this subsection, we prove item *(ii)* of the main Theorem 1.1, i.e. we show that the error between the solution Φ^ε of the initial equation (1.13) and the solution $\widetilde{\Phi}$ of the averaged equation (1.14) (defined on a common interval $[0, T_0]$) is of order $\mathcal{O}(\varepsilon)$. It is already proved in [6] that this error goes to zero as $\varepsilon \to 0$. Here, we simply revisit this proof in our special case where $\mathbf{H}_z$ admits only integer eigenvalues. In such a case the proof is significantly simpler and is quantitative. Here, C will denote a generic constant (independent of ε) that may change from line to line.

Let us first recall the available estimates on Φ^ε and $\widetilde{\Phi}$. From the previous step (Subsection 3.1), we already know that

$$\|\Phi^\varepsilon\|_{L^\infty([0,T_0];B_{m+4})} + \|\widetilde{\Phi}\|_{L^\infty([0,T_0];B_{m+4})} \leq C, \tag{3.2}$$

and, using directly Eq. (1.13), (1.14),

$$\|\partial_t \Phi^\varepsilon\|_{L^\infty([0,T_0];B_{m+2})} + \|\partial_t \widetilde{\Phi}\|_{L^\infty([0,T_0];B_{m+2})} \leq C. \tag{3.3}$$

Now, the difference $\Delta^\varepsilon(t) := \Phi^\varepsilon(t) - \widetilde{\Phi}(t)$, satisfies the equation

$$i\partial_t \Delta^\varepsilon(t) = \mathbf{H}_x \Delta^\varepsilon(t) + F\left(t/\varepsilon, \Phi^\varepsilon(t)\right) - F_{av}(\widetilde{\Phi}(t)), \quad t \in [0, T_0],$$

with initial value $\Delta^\varepsilon(0) = 0$. The integral representation of this equation is

$$\begin{aligned}
\Delta^\varepsilon(t) &= e^{-it\mathbf{H}_x}\Delta^\varepsilon(0) - i\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(F\left(s/\varepsilon, \Phi^\varepsilon(s)\right) - F_{av}(\widetilde{\Phi}(s))\right) ds \\
&= -i\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(F\left(s/\varepsilon, \Phi^\varepsilon(s)\right) - F\left(s/\varepsilon, \widetilde{\Phi}(s)\right)\right) ds \\
&\quad -i\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(F\left(s/\varepsilon, \widetilde{\Phi}(s)\right) - F_{av}(\widetilde{\Phi}(s))\right) ds.
\end{aligned}$$

Noticing that $F(\tau, \Phi)$ is locally Lipschitz continuous in B_m, with a Lipschitz constant independent of τ, and denoting

$$I^\varepsilon = \int_0^t e^{-i(t-s)\mathbf{H}_x}\left(F\left(s/\varepsilon, \widetilde{\Phi}(s)\right) - F_{av}(\widetilde{\Phi}(s))\right) ds,$$

we deduce that

$$\|\Delta^\varepsilon(t)\|_{B_m} \leq C_L \int_0^t \|\Delta^\varepsilon(s)\|_{B_m}\, ds + \|I^\varepsilon\|_{B_m}, \qquad t \in [0, T_0], \tag{3.4}$$

where C_L depends on $\|\widetilde{\Phi}\|_{C([0,T];B_m)}$. Now we claim that

$$\sup_{t\in[0,T_0]} \|I^\varepsilon\|_{B_m} \leq C\varepsilon. \tag{3.5}$$

From (3.4), from the claim (3.5) and from the Gronwall lemma, one deduces that

$$\|\Phi^\varepsilon(t) - \widetilde{\Phi}\|_{L^\infty([0,T_0];B_m)} = \|\Delta^\varepsilon\|_{L^\infty([0,T_0];B_m)} \leq C\varepsilon$$

which proves item *(ii)* of Theorem 1.1.

It remains to prove the claim (3.5). To this aim, we use Lemma 2.3 with

$$u^\varepsilon(\tau, t, x, z) = F\left(\tau, \widetilde{\Phi}(t, x, z)\right) - F_{av}(\widetilde{\Phi}(t, x, z)).$$

Let us prove that this function satisfies the assumptions of Lemma 2.3. Notice that u^ε does not depend on ε here. Properties *i)* and *ii)* stem from (3.2) and (3.3), from the regularity properties of F and F_{av} and from Lemmas 2.1 and 2.2. Property *iii)* stems from the definition of F_{av} and from the fact that F is 2π-periodic with respect to τ. Therefore, one can apply the average Lemma 2.3 to this function u^ε and the claim (3.5) is proved.

3.3 Second order approximation

End of the proof of Theorem 1.1. Here we prove item *(iii)* of Theorem 1.1. Consider the difference

$$\delta^\varepsilon(t) := \Phi^\varepsilon(t) - \widetilde{\Phi}^\varepsilon(t) + i\varepsilon F^1(t/\varepsilon, \widetilde{\Phi}^\varepsilon(t)), \quad t \in [0, T_0].$$

Our aim is to prove that $\|\delta^\varepsilon\|_{B_m} = \mathcal{O}(\varepsilon^2)$, uniformly in time on $[0, T_0]$. We have

$$\partial_t F^1(t/\varepsilon, \widetilde{\Phi}^\varepsilon(t)) = \varepsilon^{-1}\left(F(t/\varepsilon, \widetilde{\Phi}^\varepsilon(t)) - F_{av}(\widetilde{\Phi}^\varepsilon(t))\right) + D_\Phi F^1(t/\varepsilon, \widetilde{\Phi}^\varepsilon(t))\left(\partial_t \widetilde{\Phi}^\varepsilon(t)\right),$$

thus, combining with (1.13) and (1.15), we see that $\delta^\varepsilon(t)$ satisfies

$$\begin{aligned} i\partial_t \delta^\varepsilon(t) &= \mathbf{H}_x \delta^\varepsilon(t) + F(t/\varepsilon, \Phi^\varepsilon(t)) - F(t/\varepsilon, \widetilde{\Phi}^\varepsilon(t)) + i\varepsilon G_{av}(\widetilde{\Phi}^\varepsilon(t)) \\ &\quad -\varepsilon D_\Phi F^1(t/\varepsilon, \widetilde{\Phi}^\varepsilon(t)) \cdot \partial_t \widetilde{\Phi}^\varepsilon(t) - i\varepsilon \mathbf{H}_x F^1(t/\varepsilon, \widetilde{\Phi}^\varepsilon(t)), \end{aligned} \tag{3.6}$$

with $\delta^\varepsilon(0) = 0$. Recall that we have introduced the function

$$\Phi_1^\varepsilon = \widetilde{\Phi}^\varepsilon(t) - i\varepsilon F^1(t/\varepsilon, \widetilde{\Phi}^\varepsilon(t)).$$

The integral representation of (3.6) reads

$$\begin{aligned} \delta^\varepsilon(t) &= -i\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(F\left(s/\varepsilon, \Phi^\varepsilon(s)\right) - F\left(s/\varepsilon, \Phi_1^\varepsilon(s)\right)\right) ds \\ &\quad -i\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(F\left(s/\varepsilon, \Phi_1^\varepsilon(s)\right) - F(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s)) + i\varepsilon G(t/\varepsilon, \widetilde{\Phi}^\varepsilon(s))\right) ds \\ &\quad -\varepsilon\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(G(t/\varepsilon, \widetilde{\Phi}^\varepsilon(s)) - G_{av}(\widetilde{\Phi}^\varepsilon(s))\right) ds \\ &\quad +i\varepsilon\int_0^t e^{-i(t-s)\mathbf{H}_x}(D_\Phi F^1(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s))\left(\partial_t \widetilde{\Phi}^\varepsilon(s)\right) + i\mathbf{H}_x F^1(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s)))ds. \end{aligned} \tag{3.7}$$

By the first step of Theorem 1.1, already proved in Subsection 3.1, Φ^ε and $\widetilde{\Phi}^\varepsilon$ are uniformly bounded in $C([0, T_0]; B_{m+4})$ and $\partial_t \Phi^\varepsilon$ and $\partial_t \widetilde{\Phi}^\varepsilon$ are uniformly bounded in $C([0, T_0]; B_{m+2})$. Moreover, $F(\tau, \Phi)$ and $F^1(\tau, \Phi)$ are locally Lipschitz continuous with respect to Φ, with constants uniform in ε, so Φ_1^ε is also uniformly bounded in $C([0, T_0]; B_{m+4})$, and

$$\|F\left(s/\varepsilon, \Phi^\varepsilon(s)\right) - F\left(s/\varepsilon, \Phi_1^\varepsilon(s)\right)\|_{B_m} \leq C\|\Phi^\varepsilon(s) - \Phi_1^\varepsilon(s)\|_{B_m} = C\|\delta^\varepsilon(s)\|_{B_m}. \tag{3.8}$$

Next, we claim the four following estimates, for $t \in [0, T_0]$:

$$\|\int_0^t e^{-i(t-s)\mathbf{H}_x}\mathbf{H}_x F^1(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s))\, ds\|_{B_m} \leq C\varepsilon, \tag{3.9}$$

$$\|\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(D_\Phi F^1(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s))\left(\partial_t \widetilde{\Phi}^\varepsilon(s)\right)\right) ds\|_{B_m} \leq C\varepsilon, \tag{3.10}$$

$$\|\int_0^t e^{-i(t-s)\mathbf{H}_x}\left(G(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s)) - G_{av}(\widetilde{\Phi}^\varepsilon(s))\right) ds\|_{B_m} \leq C\varepsilon, \tag{3.11}$$

$$\|F(s/\varepsilon, \Phi_1^\varepsilon(s)) - F(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s)) + i\varepsilon G(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s))\|_{B_m} \leq C\varepsilon^2, \tag{3.12}$$

where the generic constant C only depends on $\|\Psi^{init}\|_{B_{m+4}}$. Assuming all these properties are true, and using Eq. (3.7), we deduce that, for $t \in [0, T_0]$,

$$\|\delta^\varepsilon(t)\|_{B_m} \leq C_1 \int_0^t \|\delta^\varepsilon(s)\|_{B_m} ds + \mathcal{O}(\varepsilon^2)$$

and the Gronwall lemma yields

$$\sup_{t\in[0,T_0]} \|\delta^\varepsilon(t)\|_{B_m} \leq C\varepsilon^2. \tag{3.13}$$

This is the desired conclusion.

Now, it remains to prove the claims (3.9)–(3.12) by repeated applications of the averaging Lemma 2.3.

Proof of (3.9). Set $u^\varepsilon(\tau,t,x,z) = \mathbf{H}_x F^1(\tau, \widetilde{\Phi}^\varepsilon(t,x,z))$. From the definition (1.7) of F^1, u^ε is 2π-periodic function with respect to τ, with zero average. Moreover, we have

$$\|u^\varepsilon(\tau,t,\cdot)\|_{B_{m+2}} \leq \|F^1(\tau,\widetilde{\Phi}^\varepsilon(t,\cdot))\|_{B_{m+4}} \quad \text{and} \quad \|\partial_t u^\varepsilon(\tau,t,\cdot)\|_{B_m} \leq \|\partial_t F^1(\tau,\widetilde{\Phi}^\varepsilon(t,\cdot))\|_{B_{m+2}}$$

so it can be deduced from the regularity of $\widetilde{\Phi}^\varepsilon$ that u^ε satisfies the assumptions of Lemma 2.3. Hence the conclusion of this lemma gives (3.9).

Proof of (3.10). Denote

$$R_1^\varepsilon = \int_0^t e^{-i(t-s)\mathbf{H}_x} \left(D_\Phi F^1(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s)) \left(\partial_t \widetilde{\Phi}^\varepsilon(s) \right) \right) ds. \tag{3.14}$$

Using Eq. (1.15), we get

$$R_1^\varepsilon = -i \int_0^t e^{-i(t-s)\mathbf{H}_x} D_\Phi F^1(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s)) \left(\mathbf{H}_x \widetilde{\Phi}^\varepsilon(s) + F_{av}(\widetilde{\Phi}^\varepsilon(s)) - i\varepsilon G_{av}(\widetilde{\Phi}^\varepsilon(s)) \right) ds.$$

Now we set

$$u^\varepsilon(\tau,t,x,z) = D_\Phi F^1(\tau, \widetilde{\Phi}^\varepsilon(t,x,z)) \left(\mathbf{H}_x \widetilde{\Phi}^\varepsilon(t,x,z) + F_{av}(\widetilde{\Phi}^\varepsilon(t,x,z)) - i\varepsilon G_{av}(\widetilde{\Phi}^\varepsilon(t,x,z)) \right).$$

Like $F^1(\tau,\Phi)$, the function $D_\Phi F^1(\tau,\Phi)$ is a 2π-periodic function with respect to τ, with zero average. Moreover, by using Lemma 2.1, Lemma 2.2 and the definitions (1.7), (1.8), (1.9) and (1.10), we deduce from the B_{m+4} regularity of $\widetilde{\Phi}^\varepsilon$ and the B_{m+2} regularity of $\partial_t \widetilde{\Phi}^\varepsilon$ that u^ε satisfies assumptions *i)* and *ii)* of Lemma 2.3. This enables to deduce from this lemma that $\|R_1^\varepsilon\| \leq C\varepsilon$ for all $t \in [0,T_0]$, which gives (3.10).

Proof of (3.11). Since F and F^1 are 2π-periodic with respect to τ, by (1.9) the function $G(\tau,\Phi) - G_{av}(\Phi)$ is also 2π-periodic. Moreover, by definition of G_{av}, its average vanishes. Furthermore, it is again straightforward to deduce from the regularity of $\widetilde{\Phi}^\varepsilon$ that

$$u^\varepsilon(\tau,t,x,z) = G(\tau/\varepsilon, \widetilde{\Phi}^\varepsilon(\tau)) - G_{av}(\widetilde{\Phi}^\varepsilon(\tau))$$

satisfies assumptions *i)* and *ii)* of Lemma 2.3. Application of this lemma gives (3.11).

Proof of (3.12). For $\Phi_1, \Phi_2 \in B_m$, denote

$$Y = F(\tau, \Phi_1 + \Phi_2) - F(\tau,\Phi_1) - D_u F(\tau,\Phi_1)\Phi_2. \tag{3.15}$$

After a simple calculation,

$$Y = \delta e^{i\tau\mathbf{H}_z} \left(2e^{-i\tau\mathbf{H}_z}\Phi_1 e^{i\tau\mathbf{H}_z}\overline{\Phi_2} + e^{i\tau\mathbf{H}_z}\overline{\Phi_1}e^{-i\tau\mathbf{H}_z}\Phi_2 + |e^{-i\tau\mathbf{H}_z}\Phi_2|^2 \right) e^{-i\tau\mathbf{H}_z}\Phi_2.$$

Thus, by using Lemma 2.1 and the fact that $e^{-i\tau \mathbf{H}_z}$ is an isometry on B_m, we get

$$\|Y\|_{B_m} \leq C\|\Phi_2\|^2_{B_m}$$

where C depends on $\|\Phi_1\|_{B_m} + \|\Phi_2\|_{B_m}$. Let $\Phi_1 = \widetilde{\Phi}^\varepsilon(s)$ and $\Phi_2 = -i\varepsilon F^1(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s))$. We have

$$\begin{aligned} Y(s) &= F(s/\varepsilon, \Phi_1 + \Phi_2) - F(s/\varepsilon, \Phi_1) - D_u F(s/\varepsilon, \Phi_1)\Phi_2 \\ &= F(s/\varepsilon, \Phi_1^\varepsilon(s)) - F(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s)) + i\varepsilon G(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s)) \end{aligned}$$

and

$$\|Y(s)\|_{B_m} \leq C\varepsilon^2 \|F^1(s/\varepsilon, \widetilde{\Phi}^\varepsilon(s))\|_{B_m} \leq C\varepsilon^2$$

for $s \in [0, T_0]$. This proves (3.12). The proof of Theorem 1.1 is complete. □

4 Numerical experiments

We have constructed a second order approximation (1.15) to the full 3D model (1.1). In practice, an efficient way to implement this approximate model Eq. (1.15) is needed. One possible and natural approach consists in expanding the functions F_{av}, F^1, G_{av} defined by (1.6), (1.7) and (1.10) separately, on the eigenfunctions of the operator $\mathbf{H}_z$.

4.1 Mode expansion

4.1.1 Expansion of the functions F_{av}, F^1 and G_{av}

We start with the expansion of $F(\tau, \Phi)$ defined by (1.4). Recall that the eigenvalues of $\mathbf{H}_z$ are the nonnegative integers. Let $\chi_p(z)$ be the normalized eigenfunction associated to the eigenvalue $p \in \mathbb{N}$:

$$\mathbf{H}_z \chi_p = p\chi_p\,, \qquad \int \chi_p^2\, dz = 1.$$

Note that χ_p is the generalized Hermite function

$$\chi_p(z) = e^{-z^2/2} H_p(z)/\sqrt{2^p p!}\pi^{1/4}, \quad z \in \mathbb{R}, \tag{4.1}$$

where $H_p(z)$ $(p = 0, 1, \ldots.)$ are the Hermite polynomials satisfying

$$H_p''(z) - 2zH_p'(z) + 2pH_p(z) = 0, \quad z \in \mathbb{R}, \quad p \geq 0, \tag{4.2}$$

$$\int_{-\infty}^{\infty} H_p(z)H_n(z)e^{-z^2} dz = \sqrt{\pi}2^p p!\delta_{pn}, \quad p, n \geq 0. \tag{4.3}$$

Consider a function $\Phi \in B_m$ expanded on this basis as

$$\Phi(x, z) = \sum_{p=0}^{+\infty} \varphi_p(x)\chi_p(z)\,.$$

Then we have

$$F(\tau,\Phi) = \delta \sum_{p_1,p_2,p_3,p_4} a_{p_1p_2p_3p_4}\, e^{i\tau\Omega_{p_1p_2p_3p_4}}\, \varphi_{p_2}(x)\varphi_{p_3}(x)\overline{\varphi_{p_4}}(x)\, \chi_{p_1}(z), \tag{4.4}$$

where we define the coefficients

$$\Omega_{pqrs} = p + s - q - r, \quad a_{pqrs} = \langle \chi_p \chi_q \chi_r \chi_s \rangle.$$

Here and in the sequel, $\langle\cdot\rangle$ denotes the integration over the z variable. We write the expansion (4.4) shortly as

$$F(\tau,\Phi) = \delta \sum_{p_1,p_2,p_3,p_4} a_{1234}\, e^{i\tau\Omega_{1234}}\, \varphi_{p_2}\varphi_{p_3}\overline{\varphi_{p_4}} \otimes \chi_{p_1}\,. \tag{4.5}$$

In the above sums, and in the sequel, a_{1234} and Ω_{1234} stand respectively for $a_{p_1p_2p_3p_4}$ and $\Omega_{p_1p_2p_3p_4}$.

The expansion of F_{av} (1.6) is obtained by averaging $F(\tau,\Phi)$ over time. Noticing that the average of $e^{i\tau\Omega_{1234}}$ vanishes if $\Omega_{1234} \neq 0$, let us define the following index set, whose information is preserved after averaging $F(\tau,\Phi)$ given by (4.5), for any $p \in \mathbb{N}^*$,

$$\Lambda(p) = \{(q,r,s),\ \text{such that } p+s = q+r\}. \tag{4.6}$$

Then we have

$$F_{av}(\Phi) = \delta \sum_{p_1=0}^{\infty} \sum_{(p_2,p_3,p_4)\in\Lambda(p_1)} a_{1234}\, \varphi_{p_2}\varphi_{p_3}\overline{\varphi_{p_4}} \otimes \chi_{p_1}. \tag{4.7}$$

Recalling the definition (1.7) of $F^1(\tau,\Phi)$, only terms with $\Omega_{1234} \neq 0$ in the expansion (4.5) of $F(\tau,\Phi)$ contribute to F^1 so, denoting the complement of $\Lambda(p)$ in $\mathbb{N}^3$ by

$$\Lambda^c(p) = \{(q,r,s),\ \text{such that } p+s \neq q+r\}, \tag{4.8}$$

it is easy to obtain

$$F^1(\tau,\Phi) = -i\delta \sum_{p_1=0}^{\infty} \sum_{(p_2,p_3,p_4)\in\Lambda^c(p_1)} \frac{a_{1234}}{\Omega_{1234}}\, e^{i\tau\Omega_{1234}}\, \varphi_{p_2}\varphi_{p_3}\overline{\varphi_{p_4}} \otimes \chi_{p_1}\,. \tag{4.9}$$

To compute $G(\tau,\Phi)$ and $G_{av}(\Phi)$, let us first compute the derivative of F with respect to Φ in a direction $U = \sum_p u_p \otimes \chi_p$. By evaluating $\frac{d}{ds}F(\tau,\Phi+sU)|_{s=0}$, we get

$$D_\Phi F(\tau,\Phi)\cdot U = \delta \sum_{p_1,p_2,p_3,p_4} a_{1234}\, e^{i\tau\Omega_{1234}}\, (2u_{p_2}\varphi_{p_3}\overline{\varphi_{p_4}} + \varphi_{p_2}\varphi_{p_3}\overline{u_{p_4}}) \otimes \chi_{p_1}.$$

By substituting the expansion of F^1 instead of U, we get, after renumbering,

$$\begin{aligned} G(\tau,\Phi) = \quad & -2i\delta^2 \sum_{p_1,p_2,p_5,p_7} \sum_{\substack{(p_4,\,p_3,\,p_6)\\ \in\,\Lambda^c(p_7)}} \frac{a_{7125}\, a_{7346}}{\Omega_{7346}}\, e^{i\tau(\Omega_{1725}+\Omega_{7346})}\, (\varphi_{p_2}\varphi_{p_3}\varphi_{p_4}\overline{\varphi_{p_5}\varphi_{p_6}}) \otimes \chi_{p_1} \\ & +i\delta^2 \sum_{p_1,p_2,p_3,p_7} \sum_{\substack{(p_6\,,\,p_5\,,\,p_4)\\ \in\,\Lambda^c(p_7)}} \frac{a_{7123}\, a_{7456}}{\Omega_{7564}}\, e^{i\tau(\Omega_{1237}-\Omega_{7564})}\, (\varphi_{p_2}\varphi_{p_3}\varphi_{p_4}\overline{\varphi_{p_5}\varphi_{p_6}}) \otimes \chi_{p_1}\,. \end{aligned}$$

Finally, in order to average out this function $G(\tau,\Phi)$ over one period, let us introduce the index set and coefficients

$$\Xi(p_1)=\{(p_2,p_3,p_4,p_5,p_6) \text{ such that } p_1+p_5+p_6=p_2+p_3+p_4\},$$

$$b_{123456}=2\sum_{\substack{p_7 \text{ such that}\\ \Omega_{7346}\neq 0}}\frac{a_{7125}\,a_{7346}}{\Omega_{7346}}-\sum_{\substack{p_7 \text{ such that}\\ \Omega_{7564}\neq 0}}\frac{a_{7123}\,a_{7456}}{\Omega_{7564}}\,.$$

Straightforward calculations lead to

$$G_{av}(\Phi)=-i\delta^2\sum_{p_1}\sum_{\substack{p_2,p_3,p_4,p_5,p_6\\ \in\Xi(p_1)}} b_{123456}\ (\varphi_{p_2}\varphi_{p_3}\varphi_{p_4}\overline{\varphi_{p_5}\varphi_{p_6}})\otimes\chi_{p_1}\,. \tag{4.10}$$

4.1.2 Initial data polarized on a single mode

The solution of (1.13) is written as $\Phi^\varepsilon(t,x,z)=\sum_{p=0}^{\infty}\varphi_p^\varepsilon(t,x)\chi_p(z)$ and the solution of (1.14) is written as $\Phi(t,x,z)=\sum_{p=0}^{\infty}\varphi_p(t,x)\chi_p(z)$. In this subsection, we assume that the initial data is polarized on a single mode of the confinement Hamiltonian, i.e. for a given $p_0\in\mathbb{N}$ we have

$$\forall p\in\mathbb{N}\setminus\{p_0\},\qquad \varphi_p^\varepsilon(t=0)=0\quad\text{and}\quad\varphi_{p_0}^\varepsilon(t=0)=\varphi^{init}.$$

In this case, the averaged system (1.14) reads

$$i\partial_t\varphi_{p_1}=\mathbf{H}_x\varphi_{p_1}+\delta\sum_{(p_2,p_3,p_4)\in\Lambda(p_1)}a_{1234}\,\varphi_{p_2}\varphi_{p_3}\overline{\varphi_{p_4}},\qquad\varphi_{p_1}(t=0)=\delta_{p_0,p_1}\,\varphi^{init}.$$

It is readily seen from this expression that $\varphi_p(t)=0$ for all t as soon as $p\neq p_0$: the wave-function remains polarized on the mode p_0 for all time. Then the first order approximation result gives that

$$\forall p\in\mathbb{N}\setminus\{p_0\}\qquad\varphi_p^\varepsilon(t)=\mathcal{O}(\varepsilon). \tag{4.11}$$

Consider now the second order approximation. To simplify notations, we also denote the solution of the second order approximation model (1.15) by

$$\Phi(t,x,z)=\sum_{p=0}^{\infty}\varphi_p(t,x)\chi_p(z).$$

By taking (4.11) into account, it is possible to write another second order approximation of the initial model, by keeping in the system only the terms of order zero and one in ε. By neglecting the products $\varphi_{p_2}\varphi_{p_3}\overline{\varphi_{p_4}}$ as soon as at least two indices differ from p_0, we obtain

$$F^1(\tau,\Phi)=-i\delta\sum_{p=1}^{\infty}\frac{a_{000\mathrm{p}}}{p}\ e^{i\tau(E_p-E_0)}\,|\varphi_{p_0}|^2\varphi_{p_0}\otimes\chi_p+\mathcal{O}(\varepsilon)\,,$$

$$F_{av}(\Phi) = \delta\, a_{0000}\,|\varphi_{p_0}|^2\varphi_{p_0}\otimes\chi_{p_0} + 2\delta\sum_{p_1\neq p_0} a_{0011}\,|\varphi_{p_0}|^2\varphi_{p_1}\otimes\chi_{p_1}$$
$$+\delta\sum_{p_1\neq p_0}\sum_{p_2=2p_0-p_1} a_{0012}\,(\varphi_{p_0})^2\overline{\varphi_{p_2}}\otimes\chi_{p_1} + \mathcal{O}(\varepsilon^2),$$
$$G_{av}(\Phi) = -i\delta^{\,2}\, b_{000000}\,|\varphi_{p_0}|^4\varphi_{p_0}\otimes\chi_{p_0} + \mathcal{O}(\varepsilon)\,.$$

Initial data on the ground state. If $p_0 = 0$, then the last term in F_{av} is always zero and the whole system can be written as an autonomous equation for the first mode (denoted here φ instead of φ_0), and a system of linear equations for the excited modes. The solution Ψ^ε of the initial equation (1.1) can be written as

$$\Psi^\varepsilon = \varphi\otimes\chi_0 + \varepsilon\delta\sum_{p=1}^{\infty}\widetilde{a_p}\left(\varphi_p\, e^{-itp/\varepsilon} - |\varphi|^2\varphi\right)\otimes\chi_p + \mathcal{O}(\varepsilon^2), \tag{4.12}$$

where φ solves the equation

$$i\partial_t\varphi = \mathbf{H}_x\varphi + \delta a_0|\varphi|^2\varphi - \varepsilon\delta^2\, b_0\,|\varphi|^4\varphi\,, \qquad \varphi(t=0) = \varphi^{init} \tag{4.13}$$

and, for $p \geq 1$, φ_p solves the equation

$$i\partial_t\varphi_p = \mathbf{H}_x\varphi_p + 2\delta a_p|\varphi|^2\varphi_p\,, \qquad \varphi_p(t=0) = |\varphi^{init}|^2\varphi^{init}\,. \tag{4.14}$$

Notice that φ_p (for $p \geq 1$) has been rescaled here, its equation (4.14) being linear. The coefficients in these equations are defined by

$$a_p = \langle(\chi_0)^2(\chi_p)^2\rangle, \qquad b_0 = \sum_{p=1}^{\infty}\frac{\langle(\chi_0)^3\chi_p\rangle^2}{p}, \qquad \widetilde{a}_p = \frac{\langle(\chi_0)^3\chi_p\rangle}{p}. \tag{4.15}$$

Remark that b_0 is positive, so the quintic term in (4.13) for φ is focusing. Remark also that only Eq. (4.13) for the first mode can be kept if the only useful quantities are quadratic observables integrated over the z variable, since the contributions of the excited modes are $\mathcal{O}(\varepsilon^2)$. For instance the surface density satisfies:

$$\langle|\Psi|^2\rangle = |\varphi|^2 + \mathcal{O}(\varepsilon^2).$$

Initial data on the first excited state. If $p_0 = 1$, then the solution of the second-order approximate system reads

$$\Psi^\varepsilon = \varphi_1\, e^{-itE_1/\varepsilon}\otimes\chi_1 + \varepsilon\delta\sum_{p\neq 1}^{\infty}\hat{a}_p\left(\varphi_p\, e^{-itp/\varepsilon} - |\varphi|^2\varphi\, e^{-it/\varepsilon}\right)\otimes\chi_p + \mathcal{O}(\varepsilon^2). \tag{4.16}$$

The term of order zero φ_1 satisfies the equation

$$i\partial_t\varphi_1 = \mathbf{H}_x\varphi_1 + \delta a_1^1|\varphi_1|^2\varphi_1 - \varepsilon\delta^2\, b_1\,|\varphi_1|^4\varphi_1\,, \qquad \varphi_1(t=0) = \varphi^{init}. \tag{4.17}$$

The modes $p = 0$ and $p = 2$ are coupled since for φ_0 and φ_2 we have

$$i\partial_t\varphi_0 = \mathbf{H}_x\varphi_0 + 2\delta a_0^1|\varphi_1|^2\varphi_0 + a\delta\varphi_1^2\overline{\varphi_2}, \qquad \varphi_0(t=0) = |\varphi^{init}|^2\varphi^{init}, \tag{4.18}$$

$$i\partial_t\varphi_2 = \mathbf{H}_x\varphi_2 + 2\delta a_2^1|\varphi_1|^2\varphi_2 + a\delta\varphi_1^2\overline{\varphi_0}, \qquad \varphi_2(t=0) = |\varphi^{init}|^2\varphi^{init}. \tag{4.19}$$

For $p \geq 3$, we have a system of decoupled equations

$$i\partial_t\varphi_p = \mathbf{H}_x\varphi_p + 2\delta a_p^1|\varphi|^2\varphi_p\,, \qquad \varphi_p(t=0) = |\varphi^{init}|^2\varphi^{init}\,. \tag{4.20}$$

In these equations, the coefficients are defined by

$$a_p^1 = \langle(\chi_p)^2(\chi_1)^2\rangle, \quad b_1 = \sum_{p\neq 1}^{\infty}\frac{\langle(\chi_1)^3\chi_p\rangle}{p-1}, \quad \hat{a}_p = \frac{\langle(\chi_1)^3\chi_p\rangle}{p-1}, \quad a = \langle(\chi_1)^2\chi_0\chi_2\rangle. \tag{4.21}$$

4.1.3 The general case

We also deal with cases where the initial data are polarized on several modes of the confinement Hamiltonian. In particular, we simulate data polarized on two modes $p_0, p_1 \in \mathbb{N}$, i.e.

$$\forall p \in \mathbb{N} \qquad \varphi_p^\varepsilon(t=0) = 0, \qquad \text{if } p \notin \{p_0,\, p_1\}.$$

As noticed in [6], infinitely many modes may be activated. For instance, if $p_0 = 0$ and $p_1 = 1$, all the modes $p \in \mathbb{N}$ are involved.

The second order approximation reads

$$\Psi^\varepsilon = e^{-i\frac{t}{\varepsilon}\mathbf{H}_z}\left(\Phi - F^1\left(\frac{t}{\varepsilon}, \Phi\right)\right) + \mathcal{O}(\varepsilon^2) \tag{4.22}$$

where Φ solves the equation

$$\begin{cases} i\partial_t\Phi = \mathbf{H}_x\Phi + F_{av}(\Phi) - i\varepsilon G_{av}(\Phi), \\ \Phi(t=0) = \Psi^{init} + i\varepsilon F^1(0, \Psi^{init}). \end{cases} \tag{4.23}$$

4.2 The numerical methods

There have been various efficient and accurate numerical methods proposed for solving the nonlinear Schrödinger equation, such as the time-splitting pseudospectral method [2, 20, 26, 30], finite difference method [1], and Runge-Kutta or Crank-Nicolson pseudospectral method [12, 17]. In our case, we adopt a Laguerre-Hermite pseudospectral method [4, 5]. In detail, we assume that the initial data Ψ^{init} has a cylindrical symmetry: it is radially symmetric in the (x_1, x_2) plane. Thus the solution $\Psi^\varepsilon(t, x, z)$ of Eq. (1.1) can be written as

$$\Psi^\varepsilon(t, x_1, x_2, z) = \Psi^\varepsilon(t, r, z), \qquad r = |x|.$$

Notice that in this cylindrical symmetric case,

$$\mathbf{H}_x = -\frac{1}{2}\Delta_x + \frac{1}{2}|x|^2 = -\frac{1}{2r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{r^2}{2}, \tag{4.24}$$

where the eigenfunctions of $-\frac{1}{2r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)+\frac{r^2}{2}$ are the generalized Laguerre functions L_m $(m=0,1,\ldots,M)$ defined by [18]

$$L_m(r)=\sqrt{\frac{1}{\pi}}e^{-r^2/2}\hat{L}_m(r^2),\quad 0\le r<\infty. \tag{4.25}$$

Here $\hat{L}_m(r)$ is the Laguerre polynomial of degree m which satisfies

$$r\hat{L}_m''(r)+(1-r)\hat{L}_m'(r)+m\hat{L}_m(r)=0,\quad m=0,1,\ldots, \tag{4.26}$$

$$\int_0^\infty e^{-r}\hat{L}_m(r)\hat{L}_n(r)\,dr=\delta_{mn},\qquad m,n=0,1,\ldots. \tag{4.27}$$

Laguerre functions L_m $(m=0,1,\ldots,M)$ are eigenfunctions of $\mathbf{H}_x$ with eigenvalue $2m+1$, i.e.,

$$\mathbf{H}_xL_m(r)=-\frac{1}{2r}\frac{\partial}{\partial r}\left(r\frac{\partial L_m(r)}{\partial r}\right)+\frac{r^2}{2}L_m(r)=E_m^rL_m(r),\ E_m^r=2m+1,\ m\ge 0,$$

$$2\pi\int_0^\infty L_m(r)L_n(r)dr=\int_0^\infty e^{-r}\hat{L}_m(r)\hat{L}_n(r)\,dr=\delta_{mn},\quad m,n\ge 0.$$

Recall that generalized Hermite functions (4.1) are eigenfunctions of $\mathbf{H}_z$. Thus, with an initial data Ψ^{init} with cylindrical symmetry, we can use time-splitting Laguerre-Hermite pseudospectral method [4] to simulate the full model (1.1), which reduces the 3D problem to a 2D problem and saves computation time. To compute the approximation (1.15), we implement the time-splitting Laguerre pseudospectral method [4].

4.2.1 Single mode initial data

Initial data on the ground state. In order to solve (4.13), (4.14), we apply the second order time-splitting Laguerre pseudospectral method with radial symmetry. We split the equations into two parts, for the ground mode

$$i\partial_t\varphi=A\varphi\quad\text{and}\quad i\partial_t\varphi=B\varphi,$$

and for other modes,

$$i\partial_t\varphi_p=A\varphi_p\quad\text{and}\quad i\partial_t\varphi_p=\widetilde{B}\varphi_p,\quad p\ge 0,$$

where $A=\mathbf{H}_x$ and the operators B and $\widetilde{B}$ are given by

$$B\varphi=\delta a_0|\varphi|^2\varphi-\varepsilon\delta^2\,b_0\,|\varphi|^4\varphi, \tag{4.28}$$

and

$$\widetilde{B}\varphi_p=2\delta a_p|\varphi|^2\varphi_p\,. \tag{4.29}$$

Choose time step $t_n=n\Delta t$, $n=0,1,\ldots$, and let $\{\hat{r}_j\}_{j=0}^M$ be the Laguerre-Gauss-Radau points (see [29]) which are the $M+1$ roots of the polynomial $r\hat{L}_M'(r)$. For a general function U, we define the transform $\mathcal{F}_L$ by

$$\mathcal{F}_L(U)_j=\sum_{\ell=0}^M e^{-iE_\ell^r\Delta t/2}\hat{U}_\ell L_\ell(r_j),\quad \hat{U}_\ell=\sum_{j=0}^M\omega_j^rU(r_j)L_\ell(r_j), \tag{4.30}$$

where r_j and ω_j^r are the Laguerre-Gauss-Radau points and weights, which are given by

$$\omega_j^r = \pi \hat{\omega}_j^r e^{\hat{r}_j}, \qquad r_j = \sqrt{\hat{r}_j}, \qquad j = 0, 1, \ldots, M, \tag{4.31}$$

and where $\{\hat{\omega}_j^r\}_{j=0}^M$ are the weights for the Laguerre-Gauss quadrature [29] satisfying

$$\sum_{j=0}^{M} \hat{\omega}_j^r \hat{L}_m(\hat{r}_j)\hat{L}_n(\hat{r}_j) = \delta_{nm}, \quad n, m = 0, 1, \ldots, M. \tag{4.32}$$

Let φ_j^n, $\varphi_j^{p,n}$ be the approximations for $\varphi(r_j, t_n)$ and $\varphi_p(r_j, t_n)$ respectively, and φ^n, $\varphi^{p,n}$ be the solution vectors with the corresponding components φ_j^n, $\varphi_j^{p,n}$. The second order time-splitting Laguerre pseudospectral method for solving (4.13), (4.14) can be written as

$$\begin{aligned}
&\varphi_j^{(1)} = \mathcal{F}_L(\varphi^n)_j, \quad \varphi_j^{(2)} = e^{-i\Delta t(\delta a_0 |\varphi_j^{(1)}|^2 \varphi_j^{(1)} - \varepsilon\delta^2 b_0 |\varphi_j^{(1)}|^4)} \varphi_j^{(1)}, \quad \varphi_j^{n+1} = \mathcal{F}_L(\varphi^{(2)})_j, \\
&\varphi_j^{p,(1)} = \mathcal{F}_L(\varphi^{p,n})_j, \quad \varphi_j^{p,(2)} = e^{-i\delta a_p \Delta t(|\varphi_j^n|^2 + |\varphi_j^{n+1}|^2)} \varphi_j^{p,(1)}, \quad \varphi_j^{p,n+1} = \mathcal{F}_L(\varphi^{p,(2)})_j.
\end{aligned}$$

Initial data on the first excited mode. Eq. (4.17) and (4.20) are solved by the same method as described above for the ground mode case. We only need to describe our numerical method for the two coupled equations (4.18) and (4.19). After splitting, we get

$$i\partial_t \varphi_0 = \mathbf{H}_x \varphi_0, \quad i\partial_t \varphi_0 = 2\delta a_0^1 |\varphi_1|^2 \varphi_0 + a\delta \varphi_1^2 \overline{\varphi_2}, \tag{4.33}$$

$$i\partial_t \varphi_2 = \mathbf{H}_x \varphi_2, \quad i\partial_t \varphi_2 = 2\delta a_2^0 |\varphi_1|^2 \varphi_2 + a\delta \varphi_1^2 \overline{\varphi_0}, \tag{4.34}$$

which should be solved simultaneously. The $\mathbf{H}_x$ part is easy to deal with, and for the other part, we adopt the modified Euler method.

4.2.2 Initial data on multiple modes

Considering initial data on multiples modes, we use the splitting method to solve equation (4.23), where the whole system is split into two parts,

$$i\partial_t \Phi = A\Phi, \qquad i\partial_t \Phi = B\Phi, \tag{4.35}$$

with

$$A\Phi = \mathbf{H}_x \Phi, \qquad \text{and } B\Phi = F_{av}(\Phi) - i\varepsilon G_{av}(\Phi).$$

We truncate the problem into finite modes, i.e.,

$$\Phi(x, z, t) = \sum_{p=0}^{N} \phi_p(x, t)\chi_p(z),$$

and also truncate the projection of (4.23) over the eigenbasis. Let $\phi_p(r_j, t_n)$ be the numerical approximation of $\phi_p(r, t)$ $(p = 0, 1, 2, \ldots, N)$ at position r_j, time t_n, and Φ^n denotes the corresponding numerical approximation for Φ. To solve the part $B\Phi = F_{av}(\Phi) - i\varepsilon G_{av}(\Phi)$, the following fourth order Runge-Kutta method is used,

$$\Phi^{n+1} = \Phi^n + \frac{1}{6}\left(\Phi_1 + 2\Phi_2 + 2\Phi_3 + \Phi_4\right), \quad t_{n+1} = t_n + \Delta t,$$

where

$$\Phi_1 = \Delta t B \Phi^n, \quad \Phi_2 = \Delta t B(\Phi^n + \frac{\Delta t}{2}\Phi_1),$$
$$\Phi_3 = \Delta t B(\Phi^n + \frac{\Delta t}{2}\Phi_2), \quad \Phi_4 = \Delta t B(\Phi^n + \Delta t \Phi_3).$$

The explicit formula of F_{av} and G_{av} are given in equation (4.7) and (4.10), where the coefficients a_{pqrs} and $b_{p_1p_2p_3P_4p_5p_6}$ have to be computed. For first order approximation, only coefficients a_{pqrs} are needed.

4.3 Numerical results

For the numerical experiments conducted in this section, initial data is always normalized such that the solution Ψ^ε of 3D GPE (1.1) satisfies $\|\Psi^\varepsilon(t)\|_{L^2} = 1$ $(t \geq 0)$. For the numerical tests, we report the absolute L^2 error of the first order approximation, which is equivalent to the relative L^2 error. For the second order approximation, we also show the corresponding absolute L^2 error (equivalent to the relative error).

Example 1. We take initial data polarized on the ground mode of $\mathbf{H}_z$, i.e.,

$$\Psi^{init}(x,z) = \varphi^{init}(x)\chi_0(z), \quad \chi_0(z) = \frac{1}{\pi^{1/4}} e^{-\frac{z^2}{2}}. \tag{4.36}$$

where φ^{init} is given by

$$\varphi^{init}(x) = \phi(|x|) = \frac{1}{\sqrt{\pi}} e^{-\frac{|x|^2}{2}}.$$

Figure 1 shows both the first and second order approximation of GPE (1.1) for large ε. The results show that the second order description (4.13), (4.14) provides a better approximation. Figure 2 illustrates the second order convergence of approximation (4.13), (4.14) when ε is small. In the simulation for the second order model, since the coefficients $\tilde{a}_p$ (4.15) essentially determine the accuracy of the truncation in practical computations, we list a table (Table 1, second column) to show the first value of $\tilde{a}_p$. Note that in this special case, only the even indices are useful since $\tilde{a}_{2p-1} = 0$ for $p \geq 1$. From Table 1, we can see that the coefficients decrease fast as p increases. Thus in practical computations, there is no need to use many modes. In our case, we use 17 modes as a typical choice. Extensive numerical results (not shown here for brevity) have shown the truncation is accurate enough.

Example 2. We take initial data polarized on the first excited mode of $\mathbf{H}_z$, i.e.,

$$\Psi^{init}(x,z) = \varphi^{init}(x)\chi_1(z), \quad \chi_1(z) = \frac{\sqrt{2}z}{\pi^{1/4}} e^{-\frac{z^2}{2}}. \tag{4.37}$$

where φ^{init} is given by

$$\varphi^{init}(x) = \phi(|x|) = \frac{1}{\sqrt{\pi}} e^{-\frac{|x|^2}{2}}.$$

Similar observations as for the previous example can be seen in Figures 3 and 4. Here, the coefficients $\hat{a}_p$ (4.21) essentially determine the accuracy of the truncation in practical

p	$\tilde{a}_{2p}$	$\hat{a}_{2p+1}$
1	-7.0523698E-2	-3.0537657E-2
2	1.5268828E-2	-8.5355346E-3
3	-4.6461566E-3	9.2194311E-3
4	1.6297806E-3	-6.1116771E-3
5	-6.1845824E-4	3.5895894E-3
6	2.4672028E-4	-2.0015159E-3
7	-1.0189098E-4	1.0852107E-3
8	4.3161788E-5	-5.7837198E-4
9	-1.8642541E-5	3.0472858E-4
10	8.1767258E-6	-1.5924948E-4

Table 1: Value for $\tilde{a}_{2p}$ (4.15) and $\hat{a}_{2p+1}$ (4.21) for different $p \geq 1$.

computation, we list a table (Table 1, third column) to show the value of these coefficients. Note that we have $\hat{a}_{2p-2} = 0$ for $p \geq 1$. Again, we can see that the coefficients decrease fast. In the corresponding numerical tests, we use both 17 modes.

Example 3. We take a multiple modes initial data,

$$\Psi^{init} = \frac{1}{\sqrt{2\pi}} e^{-\frac{|x|^2}{2}} (\chi_0(z) + \chi_1(z)). \tag{4.38}$$

In this case, we use 9 modes to perform the simulation for the second order model, and there are 65520 useful $b_{p_1p_2p_3p_4p_5p_6}$ coefficients, which causes huge time costs. In our test, only those whose absolute value is ≥ 0.01 (1217 coefficients) are considered. Figures 5 and 6 show that the second order approximation indeed performs better in short time simulation, and fail for longer times because of the ignored parts.

In the case of **Example 1**, Table 2 shows the time costs of the full 3D model (1.1), the first order approximation (1.5) and second order approximation (1.15). Independent of the parameter δ and ε, the computational time mainly depends on the time step, the number of grid point (for both 3 models) and the number of modes involved (for the second order approximation (1.15)).

It is worth noticing that, in the full 3D GPE, we need to take a small time step Δt to resolve the oscillation induced by the small parameter $\varepsilon > 0$. For the reduced models (1.5) and (1.15), since there is no such oscillation, we could use larger time step and save computation time. Table 3 shows the L^2 difference of the numerical solution of 3D GPE with different time steps, in the setup of **Example 1** and $\varepsilon = 0.01$, $\delta = 50$. We also show the L^2 error between the first order model (1.5) and the second order model (1.15). It is clearly seen that to correctly compute the solution to the full GPE, time step Δt should be small, basically of order $\mathcal{O}(\varepsilon)$. For the first order and second order approximation, we see that we can use a larger time step, while the approximation errors barely change.

	$\Delta t = 0.1$	$\Delta t = 0.01$	$\Delta t = 0.001$	$\Delta t = 0.0001$
3D model	2.5min	24.4 min	4.05 hour	40.6 hour
1st order	3.2s	4s	13s	1.7 min
2nd order	5.1s	23s	3.51 min	34.8 min

Table 2: CPU time for simulating the three models with $\delta = 50$ and $\varepsilon = 0.1$, 300×300 grid points in $r \times z$ direction, for different time steps in time interval $[0, 4]$. 21 modes are involved in the second order approximation.

		$\Delta t = 0.02$	$\Delta t = 0.01$	$\Delta t = 0.001$	$\Delta t = 0.0001$
$t = 1$	3D model	2.28E-2	1.15E-2	4.37E-5	
	1st order	1.06E-2	1.05E-2	1.05E-2	1.05E-2
	2nd order	5.59E-3	5.42E-3	5.37E-3	5.36E-3
$t = 3.5$	3D model	4.67E-2	2.06E-2	1.21E-4	
	1st order	2.50E-2	2.45E-2	2.45E-2	2.44E-2
	2nd order	1.63E-2	1.58E-2	1.57E-2	1.56E-2

Table 3: L^2 difference of the numerical solution compared with the 'true solution' (3D model using $\Delta t = 0.0001$) for the three models with $\delta = 50$ and $\varepsilon = 0.01$, at time $t = 1$ and $t = 3.5$. 21 modes are involved in the second order approximation.

5 Conclusion

We have considered the 3D GPE highly confined in the vertical z direction by a harmonic potential, represented by $\mathbf{H}_z/\varepsilon$. After reviewing the first order approximation [6], the second order approximation (1.15) was investigated, by noticing that the special structure of the spectrum of $\mathbf{H}_z$ induces periodic oscillations in time. To implement numerically this result, expansion over the modes of $\mathbf{H}_z$ was carried out. For numerical examples, we have considered two kinds of initial data, namely the single mode case and the multiple modes case. Furthermore, efficient numerical methods were carried out for cylindrically symmetric initial data. We compared the first order approximation and second order approximation, and found that the second order approximation indeed performed better, at least for initial data on a single mode. For initial data on multiple modes, the computational complexity increases very fast (almost like N^6) with respect to the number N of the modes. This causes great time cost in simulating the reduced system in 2D and. In such a case, simulating the second order approximation does not improve significantly the computational cost, compared to the first order approximation.

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Figure 1: For **Example 1**, comparison between L^2 error of the first order approximation

Figure 2: For **Example 1**, L^2 error of the second order approximation with $\delta = 1$ (left), Log-log plot of the maximum error in time interval $[0, 0.4]$ (right).

Figure 3: For **Example 2**, comparison between L^2 error of the first order approximation (left column) and that of the second order approximation (right column), with different δ, from top to bottom, $\delta = 0.1, 1, 10, 50$.

Figure 4: For **Example 2**, L^2 error of the second order approximation with $\delta = 1$ (left), Log-log plot of the maximum error in time interval $[0, 0.3]$ (right).

Figure 5: For **Example 3**, L^2 error of the first order approximation with $\delta = 10$ (left) and $\delta = 50$ (right), 17 modes are involved in the simulation.

Figure 6: For **Example 3**, L^2 error of the second order approximation with $\delta = 10$ (left) and $\delta = 50$ (right), 9 modes are involved in the simulation.