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On the Stability of a Quantum Dynamics of a Bose-Einstein Condensate Trapped in a One-Dimensional Toroidal Geometry

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Abstract We rigorously analyze the stability of the "quasi-classical" dynamics of a Bose-Einstein condensate with repulsive and attractive interactions, trapped in an effective 1D toroidal geometry. The "classical" dynamics, which corresponds to the Gross-Pitaevskii mean field theory, is stable in the case of repulsive interaction, and unstable (under some conditions) in the case of attractive interaction. The corresponding quantum dynamics for observables is described by using a closed system of linear partial differential equations. In both cases of stable and unstable quasi-classical dynamics the quantum effects represent a singular perturbation to the quasi-classical solutions, and are described by the terms in these equations which consist of a small quasi-classical parameter which multiplies high-order

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"spatial" derivatives. We demonstrate that as a result of the quantum singularity for observables a convergence of quantum solutions to the corresponding classical solutions exists only for limited times, and estimate the characteristic time-scales of the convergence.

Keywords Gross-Pitaevskii equation · Repulsive interaction · Attractive interaction · Singular perturbation

1 Introduction

Bose-Einstein condensates (BECs) represent unique systems which, among other things, allow one to study theoretically and experimentally different properties of quantum dynamics in the quasi-classical region of parameters. Note that for BECs the "classical" region of parameters corresponds to the mean field theory which is described by the Gross-Pitaevskii (GP) equation. In particular, in the example considered below, the GP limit corresponds to $N \to \infty$, $a \to 0$ and $aN \to$ constant, where N is the number of atoms in the condensate and a is the scattering length.

Usually the quasi-classical parameter is defined as $\varepsilon = \hbar/J$, where $\hbar$ is a Planck constant, and J is a characteristic action of the system. As the atoms in the BEC are in a collective state, one can approximately use $J \sim \hbar N$. Then, for the BEC systems the quasi-classical parameter can be reduced to $\varepsilon = 1/N$. (Generally, the quasi-classical parameter which appears in the BEC systems has more complicated structure, see below.) Because $N \sim 10^3$–10^6, the quasi-classical parameter is small, $\varepsilon \sim 10^{-3}$–$10^{-6} \ll 1$. These BEC systems can be considered as "mesoscopic" systems, as the parameter ε is small, but not too small. This means that one can study a quasi-classical dynamics in these systems, and even the quantum dynamics "close" to the classical one. At the same time, one cannot really study experimentally a transition from the quantum dynamics to the pure classical (GP) dynamics, as this "thermodynamic limit" corresponds to $N \to \infty$ (see below).

The stability of the BEC systems with repulsive and attractive interactions, including quantum effects, was studied theoretically and experimentally in many papers, see [4, 7–10, 13, 14, 18–20], and also references therein.

In this paper we consider theoretically stability of the quantum dynamics of the BEC trapped in an effective 1D toroidal geometry, see Fig. 1. Our approach is based on the closed system of linear partial differential equations for time-dependent quantum observable values (observables). Initially this approach was developed in [1–3, 5, 6, 17]. In application to the BEC system considered below, our mathematical approach is close to one described in [2, 5] for the quantum Fermi-Pasta-Ulam problem.

The main attention is paid to the properties of convergence of the quantum dynamics to the corresponding classical limit described by the GP equation, for both repulsive and attractive interactions. We show that for stable GP dynamics (with repulsive and attractive interactions) the process of convergence takes place on a time-scale which is significantly larger than in the case of an unstable GP dynamics. We present the explicit estimates for the parameters of convergence (uniformly in the time domain) in the quasi-classical region of parameters.

How can one measure to what extent the classical solution $F_{\rm cl}(\tau, x)$ is still suitable to approximate the quasi-classical solution $F(\tau, x, \varepsilon)$ for small values of the quasi-classical parameter ε? The classical method of successive approximations readily gives $F(\tau, x, \varepsilon)$ as an asymptotic series in powers of $|\varepsilon|$. This series actually converges to $F_{\rm cl}(\tau, x)$ at each point $(\tau, x) \in [0, \infty) \times [0, \infty)$, when $\varepsilon \to 0$. Hence $F(\tau, x, \varepsilon)$ is pointwise close to $F_{\rm cl}(\tau, x)$, if $|\varepsilon|$ is small enough. In order to evaluate the closeness, it was suggested in [2] to study

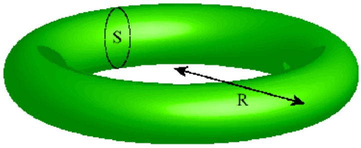

Fig. 1 A one-dimensional toroidal geometry

whether the convergence is uniform in parameters τ, x and ε. Another way of stating this is to say that for a given $|\varepsilon| \ll 1$ the classical solution approximates well partial sums of the asymptotic series for all $\tau \in [0, T]$ and $x \in [0, R]$. It is clear that the larger are intervals $[0, T]$ and $[0, R]$ the less $|\varepsilon|$ required. On the other hand, given any $|\varepsilon| \ll 1$, we can take higher order partial sums of the asymptotic series to guarantee the same precision in the same region of parameters τ and x.

Our analysis demonstrates rather strikingly that whether or not the classical solution is stable in the sense of Lyapunov is of crucial importance. When stable, the classical solution is much better suited to approximate the quasi-classical one. The characteristic times at which the approximation has accuracy $|\varepsilon|$ behave like $1/\sqrt{|\varepsilon|}$ in the stable case and like $\log(1/|\varepsilon|)$ in the unstable one.

2 Quasi-Classical Equations for Observables

We assume that the many-body dynamics of the system is described by the quantum field equation

$$\imath \frac{\partial \hat{\Psi}}{\partial \tau} = \left(-\frac{\partial^2}{\partial \theta^2} + 2\pi \varepsilon \hat{\Psi}^\dagger \hat{\Psi} \right) \hat{\Psi} \tag{2.1}$$

(see [4, 11] and references therein).

In (2.1)

$$\varepsilon = 4a\frac{R}{S}, \qquad \tau = \frac{\hbar}{2mR^2} t,$$

where R and S are the radius of the torus and the area of the cross-section of the torus, correspondingly; τ is a dimensionless time; a is the interatomic scattering length with $a > 0$ for a repulsive interaction, and $a < 0$ for an attractive interaction.

The operator function $\hat{\Psi}(\tau, \theta)$ has the form

$$\hat{\Psi}(\tau, \theta) = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} \hat{a}_j(\tau) e^{\imath j\theta}. \tag{2.2}$$

In (2.2)

$$[\hat{a}_j(\tau), \hat{a}^\dagger_{j'}(\tau)] = \delta_{j,j'},$$

$\hat{a}_j(\tau)$ and $\hat{a}^\dagger_{j'}$ being, correspondingly, the annihilation and the creation bosonic operators, $\hat{\Psi}(\tau, \theta)$ is periodic in θ with period 2π, i.e., $\hat{\Psi}(\tau, \theta + 2\pi) = \hat{\Psi}(\tau, \theta)$, and

$$\int_0^{2\pi} \hat{\Psi}^\dagger(\tau, \theta) \hat{\Psi}(\tau, \theta) d\theta = \sum_{j=-\infty}^{\infty} \hat{n}_j \equiv \hat{N},$$

where $\hat{n}_j$ is the operator of the number of particles in the mode with momentum j, and $\hat{N}$ is the operator of the total number of particles in the condensate.

From (2.1) and (2.2) we obtain the system of equations for the operators $\hat{a}_j(\tau)$

$$\imath\,\dot{\hat{a}}_j = j^2\hat{a}_j + \varepsilon \sum_{k_1,k_2,k_3=-\infty}^{\infty} \hat{a}^\dagger_{k_1}\hat{a}_{k_2}\hat{a}_{k_3}\delta_{j+k_1-k_2-k_3,0}, \tag{2.3}$$

where "dot" stands for $\partial/\partial\tau$.

To treat the system (2.3) we use the techniques of projection onto the basis of coherent states, cf. [2–4, 17]. (Different approaches for analyzing the stability of the bosonic systems can be found in [15, 16] and also references therein.) Assume that at $\tau = 0$ each mode of the bosonic field can be represented by a coherent state described by a complex number α_j. We denote

$$\alpha_j(\tau) = \langle\vec{\alpha}|\hat{a}_j(\tau)|\vec{\alpha}\rangle = \alpha_j(\tau,\vec{\alpha},\vec{\alpha}^*),$$

where

$$|\vec{\alpha}\rangle = \prod_{j=-\infty}^{\infty}|\alpha_j\rangle$$

is the vector of states of the bosonic field at $\tau = 0$. From (2.3) it follows that the operator $\hat{a}_j(\tau)$ satisfies the Heisenberg equation

$$\imath\,\dot{\hat{a}}_j = [\hat{a}_j(\tau), \hat{H}_{\text{eff}}], \tag{2.4}$$

with the effective Hamiltonian

$$\hat{H}_{\text{eff}} = \sum_{k=-\infty}^{\infty} k^2\hat{a}^\dagger_k\hat{a}_k + \frac{1}{2}\varepsilon \sum_{k_1,k_2,k_3,k_4=-\infty}^{\infty} \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\hat{a}_{k_3}\hat{a}_{k_4}\delta_{k_1+k_2-k_3-k_4,0}.$$

Applying the projection thus yields

$$\begin{aligned} &\imath\,\dot{\alpha}_j(\tau) = \hat{T}\alpha_j(\tau),\\ &\alpha_j(0) = \alpha_j, \end{aligned} \tag{2.5}$$

where

$$\begin{aligned} \hat{T} = &\sum_{k=-\infty}^{\infty} k^2\left(\alpha_k\frac{\partial}{\partial\alpha_k} - C.C.\right)\\ &+ \varepsilon \sum_{k_1,k_2,k_3,k_4=-\infty}^{\infty}\left(\alpha_{k_1}\alpha_{k_2}\alpha^*_{k_3}\frac{\partial}{\partial\alpha_{k_4}} - C.C.\right)\delta_{k_1+k_2-k_3-k_4,0}\\ &+ \frac{1}{2}\varepsilon \sum_{k_1,k_2,k_3,k_4=-\infty}^{\infty}\left(\alpha_{k_1}\alpha_{k_2}\frac{\partial}{\partial\alpha_{k_3}}\frac{\partial}{\partial\alpha_{k_4}} - C.C.\right)\delta_{k_1+k_2-k_3-k_4,0}, \end{aligned}$$

the $C.C.$ meaning complex conjugated terms (cf. [2, 4] for more details).

Equation (2.5) is easily checked to possess a solution with the form of a finite amplitude periodic wave

$$\begin{aligned} &\alpha_j(\tau) = \exp(-\imath\, j^2\tau - (1-\exp(-\imath\,\varepsilon\tau))|\alpha_j|^2)\alpha_j,\\ &\alpha_{j'}(\tau) = 0, \quad \text{if } j' \neq j. \end{aligned} \tag{2.6}$$

Note that the solution (2.6) formally turns into the Gross-Pitaevskii (GP) solution (which we also will call a "classical" solution)

$$\alpha_{\mathrm{cl},j}(\tau)=\exp(-\imath(j^2+\varepsilon|\alpha_j|^2)\tau)\alpha_{\mathrm{cl},j}, \tag{2.7}$$

when $|\varepsilon|\to 0$, $|\alpha_j|\to\infty$, and $|\varepsilon||\alpha_j|^2\to$ const.

The quantum solution (2.6) and the characteristic time-scales for the validity of the "classical" solution (2.7), $\tau_\hbar$, and of quantum revivals, τ_r,

$$\tau_\hbar=\frac{\sqrt{2}}{|\alpha_j||\varepsilon|},$$
$$\tau_r=\frac{2\pi}{|\varepsilon|},$$

were first discussed in [3] (see also [12, 13]). Below we shall show that the time-scale $\tau_\hbar$ is different from the characteristic time-scales of the stability of the quantum solution (2.6) for both repulsive and attractive interactions.

We now derive the system of equations for studying the stability of the solution (2.6) relative to the decay in neighboring modes $2k\mapsto(k-\ell)+(k+\ell)$. Assume that at the initial instant the amplitudes of the modes $j\neq k$ are small, i.e., $|\alpha_j|\ll|\alpha_k|$. In this case one can seek a solution $\alpha_{k+\ell}$ of (2.6) in the form of an expansion in α_j,

$$\begin{aligned}\alpha_{k+\ell}(\tau,\vec{\alpha},\vec{\alpha}^*)&=c_{\ell,0}(\tau,\alpha_k,\alpha_k^*)\\&\quad+\sum_{j\neq 0}\left(c_{\ell,j}^{(1,0)}(\tau,\alpha_k,\alpha_k^*)\alpha_{k+j}+c_{\ell,j}^{(0,1)}(\tau,\alpha_k,\alpha_k^*)\alpha_{k+j}^*\right)\\&\quad+\dots,\end{aligned}\tag{2.8}$$

the dots meaning the terms containing the products $\alpha_{k+j_1}\alpha_{k+j_2}$, $\alpha_{k+j_1}^*\alpha_{k+j_2}$, $\alpha_{k+j_1}^*\alpha_{k+j_2}^*$, etc. From the initial condition $\alpha_{k+\ell}(0,\vec{\alpha},\vec{\alpha}^*)=\alpha_{k+\ell}$ we readily deduce that

$$\begin{aligned}c_{0,0}(0,\alpha_k,\alpha_k^*)&=\alpha_k, &\qquad c_{\ell,0}(0,\alpha_k,\alpha_k^*)&=0;\\c_{\ell,j}^{(1,0)}(0,\alpha_k,\alpha_k^*)&=\delta_{\ell,j}, &\qquad c_{\ell,j}^{(0,1)}(0,\alpha_k,\alpha_k^*)&=0\end{aligned}\tag{2.9}$$

for $\ell\neq 0$. In (2.8) α_{k+j} and α_{k+j}^* are the initial amplitudes of "small" waves, and α_k the initial amplitude of a "large" wave. The coefficients $c_{\ell,0}$, $c_{\ell,j}^{(1,0)}$ and $c_{\ell,j}^{(0,1)}$, etc. do not explicitly contain smallness related to the amplitudes α_{k+j} with $j\neq 0$.

Below, we will study the dynamics of functions $c_{\ell,0}$, $c_{\ell,j}^{(1,0)}$ and $c_{\ell,j}^{(0,1)}$, for they determine the evolution of small perturbations with amplitudes α_{k+j}. Substituting (2.8) into (2.5) and gatherings the coefficients of the same powers of α_{k+j}, we arrive at a system of equations for the coefficients which is not closed in general, i.e., the equations for $c_{\ell,0}$, $c_{\ell,j}^{(1,0)}$ and $c_{\ell,j}^{(0,1)}$ also include higher order coefficients. However, one can show that higher order coefficients describe the influence of small waves on each other and on the large wave. Hence they do not contribute essentially to the dynamics of the system at the initial stage. A quasi-classical asymptotic of the contribution of higher order coefficients is discussed in [2].

On account of the above remark, we cut off the expansion (2.8) at the linear terms. In this way we get the following closed system of differential equations

$$\begin{aligned}
&\imath\, \dot{c}_{\ell,0} = \hat{M} c_{\ell,0},\\
&\imath\, \dot{c}^{(1,0)}_{\ell,j} = \hat{M} c^{(1,0)}_{\ell,j} + ((k+j)^2 + 2\varepsilon|\alpha_k|^2) c^{(1,0)}_{\ell,j} + 2\varepsilon\alpha_k \frac{\partial}{\partial\alpha_k} c^{(1,0)}_{\ell,j} - \varepsilon\alpha_k^{*2} c^{(0,1)}_{\ell,-j},\\
&\imath\, \dot{c}^{(0,1)}_{\ell,-j} = \hat{M} c^{(0,1)}_{\ell,-j} - ((k-j)^2 + 2\varepsilon|\alpha_k|^2) c^{(0,1)}_{\ell,-j} - 2\varepsilon\alpha_k \frac{\partial}{\partial\alpha_k} c^{(0,1)}_{\ell,-j} + \varepsilon\alpha_k^2 c^{(1,0)}_{\ell,j},
\end{aligned}\tag{2.10}$$

cf. [2], where

$$\hat{M} = (k^2 + \varepsilon|\alpha_k|^2)\alpha_k \frac{\partial}{\partial\alpha_k} + \frac{1}{2}\varepsilon\alpha_k^2 \frac{\partial^2}{\partial\alpha_k^2} - C.C.,$$

and the $C.C.$ stand for complex conjugated terms.

The solution of the first equation (2.10) for $c_{0,0}(\tau)$ has the form (2.6) and describes the dynamics of a "large" wave at first approximation. The remaining system of equations can be further simplified. For this purpose we conclude from (2.9) and the linearity of (2.10) that only two relevant summands in (2.8) are different from zero, namely $c^{(1,0)}_{\ell,\ell}$ and $c^{(0,1)}_{\ell,-\ell}$.

We write $\alpha_k = |\alpha_k| e^{\imath\theta_k}$ and expand the functions $c^{(1,0)}_{\ell,\ell}$ and $c^{(0,1)}_{\ell,-\ell}$ as

$$c^{(1,0)}_{\ell,\ell}(\tau) = \sum_{n=-\infty}^{\infty} f_{\ell,n}(\tau, |\alpha_k|^2) e^{\imath n\theta_k},$$

$$c^{(1,0)}_{\ell,-\ell}(\tau) = \sum_{n=-\infty}^{\infty} g_{\ell,n}(\tau, |\alpha_k|^2) e^{\imath n\theta_k}.$$

It is easy to verify that

$$\alpha_k \frac{\partial}{\partial\alpha_k} = |\alpha_k|^2 \frac{\partial}{\partial|\alpha_k|^2} - \frac{1}{2}\imath \frac{\partial}{\partial\theta_k},$$

$$\alpha_k \frac{\partial}{\partial\alpha_k} - C.C. = -\imath \frac{\partial}{\partial\theta_k},$$

$$|\alpha_k|^2\alpha_k \frac{\partial}{\partial\alpha_k} + \frac{1}{2}\alpha_k^2 \frac{\partial^2}{\partial\alpha_k^2} - C.C. = -\imath|\alpha_k|^2 \frac{\partial}{\partial\theta_k} - \imath|\alpha_k|^2 \frac{\partial^2}{\partial\theta_k \partial|\alpha_k|^2} + \frac{1}{2}\imath \frac{\partial}{\partial\theta_k}.$$

Taking into account that $c^{(1,0)}_{\ell,\ell}(0) = 1$ and $c^{(0,1)}_{\ell,-\ell}(0) = 0$, we deduce the initial conditions for functions $f_{\ell,n}(\tau, |\alpha_k|^2)$ and $g_{\ell,n}(\tau, |\alpha_k|^2)$, namely

$$\begin{aligned}
&f_{\ell,n}(0, |\alpha_k|^2) = \delta_{n,0},\\
&g_{\ell,n}(0, |\alpha_k|^2) = 0.
\end{aligned}\tag{2.11}$$

From (2.10) and (2.11) we derive a closed system of equations for functions $f_{\ell,0}(\tau, |\alpha_k|^2)$ and $g_{\ell,2}(\tau, |\alpha_k|^2)$. Namely,

$$\begin{aligned}
&\imath\, \dot{f}_{\ell,0} = (k+\ell)^2 f_{\ell,0} + 2\varepsilon|\alpha_k|^2 \left(\frac{\partial}{\partial|\alpha_k|^2} + 1\right) f_{\ell,0} - \varepsilon|\alpha_k|^2 g_{\ell,2},\\
&\imath\, \dot{g}_{\ell,2} = \varepsilon|\alpha_k|^2 f_{\ell,0} + (-(k-\ell)^2 + 2k^2) g_{\ell,2} + \varepsilon g_{\ell,2}
\end{aligned}\tag{2.12}$$

under the initial conditions

$$f_{\ell,0}(0,|\alpha_k|^2)=1,\qquad g_{\ell,2}(0,|\alpha_k|^2)=0. \tag{2.13}$$

3 Classical (GP) Solution

By introducing a new variable $x=|\varepsilon||\alpha_k|^2$ in the interval $[0,\infty)$ and new functions $f(\tau,x)$ and $g(\tau,x)$

$$f_{\ell,0}(\tau,|\alpha_k|^2)=e^{-\imath(-(k-\ell)^2+2k^2+\varepsilon)\tau}f(\tau,x),$$
$$g_{\ell,2}(\tau,|\alpha_k|^2)=e^{-\imath(-(k-\ell)^2+2k^2+\varepsilon)\tau}g(\tau,x),$$

the system of equations (2.12) takes the form

$$\imath\dot f=2\Big(x+(\operatorname{sign}\varepsilon)\ell^2-\frac{1}{2}|\varepsilon|\Big)f+2|\varepsilon|x\frac{\partial f}{\partial x}-xg,\qquad \imath\dot g=xf \tag{3.1}$$

under the initial conditions

$$f(0,x)=1,\qquad g(0,x)=0. \tag{3.2}$$

The limit problem for $\varepsilon\to0$ corresponds to the Gross-Pitaevskii equation. This problem depends on the domain of ε from which the limit is taken. For a repulsive interaction ε is positive, and $\operatorname{sign}\varepsilon\to1$ as $\varepsilon\to0+$. For an attractive interaction ε is negative, and $\operatorname{sign}\varepsilon\to-1$ as $\varepsilon\to0-$. Hence, the limit system is

$$\begin{pmatrix}\dot f\\ \dot g\end{pmatrix}=A(x)\begin{pmatrix}f\\ g\end{pmatrix}, \tag{3.3}$$

where

$$A(x)=\begin{pmatrix}-2\imath(x+(\operatorname{sign}\varepsilon)\ell^2-\frac{|\varepsilon|}{2}) & \imath x\\ -\imath x & 0\end{pmatrix}.$$

The matrix $A(x)$ depends on the parameter $x\in[0,\infty)$, and its eigenvalues are

$$\lambda_+(x)=-\imath\Big(x+(\operatorname{sign}\varepsilon)\ell^2-\frac{|\varepsilon|}{2}\Big)+\imath\sqrt{\ell^2-\frac{\varepsilon}{2}}\sqrt{\ell^2-\frac{\varepsilon}{2}+2(\operatorname{sign}\varepsilon)x},$$
$$\lambda_-(x)=-\imath\Big(x+(\operatorname{sign}\varepsilon)\ell^2-\frac{|\varepsilon|}{2}\Big)-\imath\sqrt{\ell^2-\frac{\varepsilon}{2}}\sqrt{\ell^2-\frac{\varepsilon}{2}+2(\operatorname{sign}\varepsilon)x}.$$

Lemma 3.1 *The solution of* (3.3) *under the initial condition* (3.2) *is given by*

$$\begin{pmatrix}f_{\mathrm{cl}}(\tau,x,\varepsilon)\\ g_{\mathrm{cl}}(\tau,x,\varepsilon)\end{pmatrix}=\frac{1}{\lambda_+(x)-\lambda_-(x)}\begin{pmatrix}\lambda_+(x)e^{\tau\lambda_+(x)}-\lambda_-(x)e^{\tau\lambda_-(x)}\\ -\sqrt{\lambda_+(x)\lambda_-(x)}(e^{\tau\lambda_+(x)}-e^{\tau\lambda_-(x)})\end{pmatrix}.$$

Proof Since the characteristic equation of $A(x)$ is $\lambda^2 - \operatorname{tr} A\lambda + \det A = 0$, where

$$\operatorname{tr} A = -2\imath \left(x + (\operatorname{sign} \varepsilon)\ell^2 - \frac{|\varepsilon|}{2} \right),$$
$$\det A = -x^2,$$

the Viète formulas yield

$$\lambda_+ + \lambda_- = \operatorname{tr} A,$$
$$\lambda_+ \lambda_- = \det A.$$

It follows that

$$A(x) = \begin{pmatrix} \lambda_+ + \lambda_- & \sqrt{\lambda_+\lambda_-} \\ -\sqrt{\lambda_+\lambda_-} & 0 \end{pmatrix},$$

which gives the desired assertion by an easy computation. □

We still call the pair

$$F_{\text{cl}}(\tau, x, \varepsilon) = \begin{pmatrix} f_{\text{cl}}(\tau, x, \varepsilon) \\ g_{\text{cl}}(\tau, x, \varepsilon) \end{pmatrix}$$

the classical solution, for it corresponds to a bounded perturbation of the Gross-Pitaevskii equation. It is explicit that $F_{\text{cl}}(\tau, x, \varepsilon)$ converges for $\varepsilon \to 0$ to the genuine classical solution $F_{\text{cl}}(\tau, x, 0)$. It will cause no confusion if we sometimes suppress the parameter ε of $F_{\text{cl}}(\tau, x, \varepsilon)$ and therefore use the same letter to designate both $F_{\text{cl}}(\tau, x, \varepsilon)$ and $F_{\text{cl}}(\tau, x, 0)$.

For a repulsive interaction the classical solution $F_{\text{cl}}(\tau, x, \varepsilon)$ proves to be stable in the sense of Lyapunov for all $x \geq 0$. For an attractive interaction the classical solution is stable in the sense of Lyapunov for all $x \leq \ell^2/2 - \varepsilon/4$, and unstable otherwise. Those $x \geq 0$ for which the classical solution is stable can be precisely described by $\ell^2 - \varepsilon/2 + 2(\operatorname{sign} \varepsilon)x \geq 0$ whatever interaction is considered.

The quantum effects in (3.1) are described in terms which include a small parameter, ε. Below, we consider the properties of convergence of quantum solutions to the corresponding Gross-Pitaevskii solutions for both repulsive and attractive interaction.

The case of unstable classical solutions is actually studied in [5] for the quantum Fermi-Pasta-Ulam problem. Hence we restrict our attention to the domain of $x \geq 0$ for which the classical solution is stable.

4 Quantum Dynamics for Repulsive Interaction

The principal symbol of (3.1) is given by the matrix

$$\begin{pmatrix} -\tau - 2\imath\, |\varepsilon| x\xi & 0 \\ 0 & -\tau \end{pmatrix}$$

with determinant $\tau(\tau + 2\imath\, |\varepsilon| x\xi)$. It follows that (3.1) is a mixed type system with hyperbolic degeneracy on the line $x = 0$. The real characteristics of this system are the lines $x = \text{const}$, hence the Cauchy problem (3.1), (3.2) is noncharacteristic.

The system (3.1) has normal form with respect to the time variable τ, and the coefficients of the system and the Cauchy data (3.2) are entire functions of τ, x and ε. Therefore, it fulfills the conditions of the Cauchy-Kovalevskaya theorem, which implies that the problem (3.1), (3.2) possesses a real analytic solution

$$F(\tau, x, \varepsilon) = \begin{pmatrix} f(\tau, x, \varepsilon) \\ g(\tau, x, \varepsilon) \end{pmatrix}$$

in some neighborhood of the hyperplane $\{\tau = 0\}$ in $\mathbb{R}^3$. The solution is unique in the class of real analytic functions. Moreover, the solution is unique in the class of continuously differentiable functions, which is due to Holmgren's uniqueness theorem.

To analyze the solution $F(\tau, x, \varepsilon)$, we now consider (3.1) as small perturbations of (3.3).

Lemma 4.1 *The Cauchy matrix* $\exp(\tau A(x))$ *of* (3.3) *is given by*

$$\Phi(\tau, x) = T(x) \begin{pmatrix} e^{\tau\lambda_+(x)} & 0 \\ 0 & e^{\tau\lambda_-(x)} \end{pmatrix} T^{-1}(x),$$

where

$$T(x) = \begin{pmatrix} -\sqrt{\lambda_+(x)\lambda_-(x)} & -\sqrt{\lambda_+(x)\lambda_-(x)} \\ \lambda_-(x) & \lambda_+(x) \end{pmatrix},$$

$$T^{-1}(x) = \frac{1}{\lambda_+(x) - \lambda_-(x)} \begin{pmatrix} -\sqrt{\lambda_+(x)/\lambda_-(x)} & -1 \\ \sqrt{\lambda_-(x)/\lambda_+(x)} & 1 \end{pmatrix}.$$

Proof The eigenvector of A corresponding to the eigenvalue $\lambda_\pm$ is easily verified to be

$$v_\pm = \begin{pmatrix} -\sqrt{\lambda_+\lambda_-} \\ \lambda_\mp \end{pmatrix}.$$

Hence the lemma follows by the standard computation of the matrix exponential function. □

In particular, the classical solution is given by $F_{\rm cl}(\tau, x) = \Phi(\tau, x)F_{\rm cl}(0, x)$, where $F_{\rm cl}(0, x)$ is the column with entries 1 and 0.

Using the Cauchy matrix for (3.3), one can write the solution to (3.1) under the initial conditions (3.2) in the form (which is actually a perturbed Green formula)

$$F(\tau, x, \varepsilon) = \Phi(\tau, x)F(0, x, \varepsilon) - \imath|\varepsilon| \int_0^\tau \Phi(\tau - \tau', x)D(x, \partial_x)F(\tau', x, \varepsilon)d\tau' \qquad (4.1)$$

for all $\tau \geq 0$, where $D(x, \partial_x) = \begin{pmatrix} 2x\partial_x & 0 \\ 0 & 0 \end{pmatrix}$.

The first equation in (4.1) includes the only unknown function $f(\tau, x, \varepsilon)$ and it reads

$$f(\tau, x, \varepsilon) = f_{\rm cl}(\tau, x) - 2\imath|\varepsilon|x \int_0^\tau f_{\rm cl}(\tau - \tau', x)\frac{\partial f}{\partial x}(\tau', x, \varepsilon)d\tau' \qquad (4.2)$$

for $\tau \geq 0$.

Having given $f(\tau, x, \varepsilon)$ we obtain the second unknown function $g(\tau, x, \varepsilon)$ by the formula

$$g(\tau, x, \varepsilon) = g_{\rm cl}(\tau, x) - 2\imath|\varepsilon|x \int_0^\tau g_{\rm cl}(\tau - \tau', x)\frac{\partial f}{\partial x}(\tau', x, \varepsilon)d\tau'.$$

5 Asymptotic Expansion

Analysis similar to that in [5] shows that the classical solution $F_{\mathrm{cl}}(\tau, x)$ is the pointwise limit of the quantum solution $F(\tau, x, \varepsilon)$ if $\varepsilon \to 0$, for all $\tau \geq 0$ and $x \geq 0$. Given any small $\varepsilon > 0$, the question arises of the range of times τ for which the classical limit $F_{\mathrm{cl}}(\tau, x)$ still satisfactorily describes the dynamics of quantum decay locally in x, i.e., for x in intervals $[0, X]$ with $X > 0$. To this end we invoke (4.2).

We have been able to develop a satisfactory analytic perturbation theory for holomorphic semigroups only for relatively bounded perturbations. In applications, however, we have often to deal with unbounded perturbations. Naturally, then, we have to content ourselves with obtaining weaker results than the analytic dependence of the semigroup on the parameter ε. In this way we are led to consider asymptotic series in powers of ε which are valid for $\varepsilon \to 0$.

To study the problem we make use of the geometric series to get an asymptotic expansion of $F(\tau, x, \varepsilon)$ in ε. Starting with the integral equation (4.2) of Volterra type, we introduce

$$\mathcal{O} f(\tau, x) = -2\imath\, x \int_0^\tau f_{\mathrm{cl}}(\tau - \tau', x) \frac{\partial f}{\partial x}(\tau', x) d\tau'.$$

Then (4.2) can be written in the form

$$(I - |\varepsilon| \mathcal{O}) f = f_{\mathrm{cl}}$$

whence

$$\begin{aligned} f(\tau, x, \varepsilon) &= (I - |\varepsilon| \mathcal{O})^{-1} f_{\mathrm{cl}}(\tau, x) \\ &= \sum_{k=0}^{\infty} |\varepsilon|^k \mathcal{O}^k f_{\mathrm{cl}}(\tau, x). \end{aligned} \tag{5.1}$$

One verifies by induction that

$$\mathcal{O}^k f_{\mathrm{cl}}(\tau, x) = (-2\imath)^k x \left(\left(\sum_{j=0}^{2k} q_{k,j}^{(+)}(x) \tau^j \right) e^{\tau \lambda_+} + \left(\sum_{j=0}^{2k} q_{k,j}^{(-)}(x) \tau^j \right) e^{\tau \lambda_-} \right)$$

for $k = 1, 2, \dots$, where $q_{k,j}^{(\pm)}(x)$ are irrational functions having the only singularity at the point

$$x = \frac{|\varepsilon|}{4} - \frac{1}{2} (\operatorname{sign} \varepsilon) \ell^2.$$

Since f_{cl} is an entire function, the iterations $\mathcal{O}^k f_{\mathrm{cl}}$ are also entire functions of τ and x.

Note that (5.1) is a regular asymptotic series in powers of the small parameter. In order to investigate the convergence of this series, it will be necessary to obtain sharp estimates for the iterates $\mathcal{O}^k f_{\mathrm{cl}}$. Denote by $\mathcal{X}$ the interval of those $x \geq 0$ for which the classical solution is stable in the sense of Lyapunov. Recall that $\mathcal{X}$ is precisely described by the inequality $\ell^2 - \varepsilon/2 + 2(\operatorname{sign} \varepsilon) x \geq 0$, see Sect. 3.

Theorem 5.1 *There is a continuous function $b(x) > 0$ of $x \in \mathcal{X}$ with the property that*

$$|\mathcal{O}^k f_{\mathrm{cl}}(\tau, x)| \leq C\, (a_k(x) \tau + b(x))^{2k}$$

holds for all $\tau \geq 0$, $x \in \mathcal{X}$ *and* $k = 1, 2, \ldots$ *with* C *a constant independent of* τ, x *and* k, *where*

$$a_k(x) = \begin{cases} \sqrt{\frac{e}{k}}\sqrt{2x}, & \text{if } x < 2\ell^2, \\ \sqrt{\frac{1}{\ell}\frac{e}{k}(\frac{x}{2})^{\frac{3}{4}+\frac{1}{4k}}}, & \text{if } x \geq 2\ell^2. \end{cases}$$

It is clear that the choice of the division point $2\ell^2$ is not essential. We may take it to be $2^5\ell^2$ to make $a_k(x)$ continuous.

Proof An easy computation shows that

$$\mathcal{O}^k f_{\mathrm{cl}}(\tau, x) = \left((-\imath\, x)^k \left(\frac{\lambda_+}{\lambda_+ - \lambda_-}\right)^{k+1} \left(\frac{\partial \lambda_+}{\partial x}\right)^k \frac{\tau^{2k}}{k!} + \ldots\right) e^{\tau\lambda_+}$$
$$+ \left((-\imath\, x)^k \left(\frac{\lambda_-}{\lambda_- - \lambda_+}\right)^{k+1} \left(\frac{\partial \lambda_-}{\partial x}\right)^k \frac{\tau^{2k}}{k!} + \ldots\right) e^{\tau\lambda_-},$$

where the dots stand for the monomials of lower order in τ. Since the eigenvalues $\lambda_\pm(x)$ are purely imaginary, we readily deduce that $|e^{\tau\lambda_\pm(x)}| = 1$ for all $x \in \mathcal{X}$. Hence

$$|\mathcal{O}^k f_{\mathrm{cl}}(\tau, x)| \leq x^k \left(\left|\frac{\lambda_+}{\lambda_+ - \lambda_-}\right|^{k+1} \left|\frac{\partial \lambda_+}{\partial x}\right|^k + \left|\frac{\lambda_-}{\lambda_- - \lambda_+}\right|^{k+1} \left|\frac{\partial \lambda_-}{\partial x}\right|^k \right) \frac{\tau^{2k}}{k!} + \ldots$$

holds whenever $\tau \geq 0$ and $x \in \mathcal{X}$. Our next goal is to evaluate the principal term for x large enough.

It is easily seen that

$$\left|\frac{\lambda_\pm}{\lambda_\pm - \lambda_\mp}\right| \sim \frac{1}{2\ell}\sqrt{\frac{x}{2}},$$
$$\left|\frac{\partial \lambda_\pm}{\partial x}\right| \sim 1$$

for sufficiently large x. Using Stirling's formula, we estimate the principal term by

$$c \left(\frac{1}{\ell}\right)^{k+1} \left(\frac{e}{k}\right)^k \left(\frac{x}{2}\right)^{\frac{3k+1}{2}} \tau^{2k}$$

for large $x > 0$, where the constant c does not depend on x.

In a similar way we estimate the principal term by

$$c \left(\frac{e}{k}\right)^k (2x)^k \tau^{2k}$$

for $x \ll 1$, with c a constant independent of x.

From this the theorem follows by a cumbersome but straightforward analysis of the terms in $\mathcal{O}^k f_{\mathrm{cl}}$. □

Theorem 5.1 implies that (5.1) is an asymptotic series in the powers of ε for the solution of (3.1), (3.2) on bounded subsets of $[0, \infty) \times \mathcal{X}$, provided that ε is small enough. Let us express T as function of ε and x from the inequality $|\varepsilon|^k|\mathcal{O}^k f_{\mathrm{cl}}| < 1$ suggested by the theorem. This will enable us to evaluate the characteristic times of applicability of the classical approximation corresponding to $\varepsilon = 0$.

Corollary 5.2 *The classical solution F_{cl} approximates $F(t,x,\varepsilon)$ at step k for small ε uniformly in $t < T$ with*

$$T \sim \frac{1}{a_k(x)} \frac{1}{\sqrt{|\varepsilon|}}.$$

Proof The series (5.1) majorises by a convergent geometric series for all $t \le T$, provided that

$$\sqrt{|\varepsilon|}(a_k(x)T + b(x)) < 1.$$

This yields

$$\begin{aligned} T &< \frac{1}{a_k(x)} \left(\frac{1}{\sqrt{|\varepsilon|}} - b(x) \right) \\ &\sim \frac{1}{a_k(x)} \frac{1}{\sqrt{|\varepsilon|}} \end{aligned}$$

for $\varepsilon \to 0$, as desired. □

6 Quantum Dynamics for Attractive Interaction

The case of unstable classical solutions is studied in detail in [5]. In this case we may simplify the manual evaluations of Theorem 5.1 by using the Cauchy inequalities for the derivative of a holomorphic function, since we no longer need to guarantee that $|\exp(\tau\lambda_\pm(x))| \le 1$ for all τ and x. For a thorough treatment we refer the reader to [5].

Assume that $\varepsilon < 0$. Then for $x > \ell^2/2$ the eigenvalues of the matrix $A(x)$ are no longer purely imaginary. More precisely,

$$\begin{aligned} \lambda_+(x) &= -\imath\left(x - \ell^2 - \frac{|\varepsilon|}{2}\right) - \sqrt{\ell^2 + \frac{|\varepsilon|}{2}} \sqrt{2x - \left(\ell^2 + \frac{|\varepsilon|}{2}\right)}, \\ \lambda_-(x) &= -\imath\left(x - \ell^2 - \frac{|\varepsilon|}{2}\right) + \sqrt{\ell^2 + \frac{|\varepsilon|}{2}} \sqrt{2x - \left(\ell^2 + \frac{|\varepsilon|}{2}\right)}. \end{aligned}$$

Theorem 6.1 *The series (5.1) converges uniformly in τ, x and ε on compact sets of the form*

$$[0,T] \times \{x \in \mathbb{C} : |x| \le R\} \times \left\{\varepsilon \in \mathbb{R} : |\varepsilon| \le \frac{1}{2Te^{3TR}}\right\},$$

T and R being arbitrary positive numbers.

Proof From the Cauchy formula it follows that if $f(x)$ is an entire function of $x \in \mathbb{C}$ then

$$\sup_{|z| \le r'R} \left|\frac{\partial f}{\partial z}\right| \le \frac{1}{(r - r')R} \sup_{|z| \le rR} |f(z)| \tag{6.1}$$

for all $R > 0$ and $0 < r' < r$.

Analysis similar to that in the proof of Lemma 5.1 in [5] shows that

$$\sup_{|z|\le rR} |f_{\rm cl}(\tau,z)| \le e^{(3rR+2\ell^2)\tau}$$

for any $r > 0$. We next show by induction that for all $k = 1, 2, \ldots$ the following estimate holds:

$$\sup_{|z|\le R/k+1} |\mathcal{O}^k f_{\rm cl}(\tau,z)| \le (2\tau)^k e^{(3R+2\ell^2)\tau}. \tag{6.2}$$

For $k = 1$ we get, by (6.1),

$$\begin{aligned}
&\sup_{|z|\le R/2} |\mathcal{O} f_{\rm cl}(\tau,z)| \\
&\quad\le \sup_{|z|\le R/2} |-2\imath z| \int_0^\tau |f_{\rm cl}(\tau-\tau',z)| \left|\frac{\partial}{\partial z} f_{\rm cl}(\tau',z)\right| d\tau' \\
&\quad\le R\int_0^\tau \exp\left(\left(3\frac{R}{2}+2\ell^2\right)(\tau-\tau')\right)\frac{2}{R}\exp\big((3R+2\ell^2)\tau'\big)d\tau' \\
&\quad= 2\exp\left(\left(3\frac{R}{2}+2\ell^2\right)\tau\right)\int_0^\tau \exp\left(3\frac{R}{2}\tau'\right)d\tau' \\
&\quad\le 2\tau\exp\big((3R+2\ell^2)\tau\big),
\end{aligned}$$

as desired. Having given the inequalities (6.2) up to the number k, we derive, by (6.1),

$$\begin{aligned}
&\sup_{|z|\le R/k+2} |\mathcal{O}^{k+1} f_{\rm cl}(\tau,z)| \\
&\quad\le \frac{2R}{k+2}\int_0^\tau \exp\left(\left(3\frac{R}{k+2}+2\ell^2\right)(\tau-\tau')\right)\frac{(k+1)(k+2)}{R}\sup_{|z|\le R/k+1}|\mathcal{O}^k f_{\rm cl}(\tau',z)|d\tau' \\
&\quad\le 2(k+1)\exp\left(\left(3\frac{R}{k+2}+2\ell^2\right)\tau\right)\int_0^\tau (2\tau')^k\exp\left(3\frac{k+1}{k+2}R\tau'\right)d\tau' \\
&\quad\le 2(k+1)\exp\big((3R+2\ell^2)\tau\big)\int_0^\tau (2\tau')^k d\tau' \\
&\quad\le (2\tau)^{k+1}\exp\big((3R+2\ell^2)\tau\big),
\end{aligned}$$

thus completing the induction step.

Since R is actually arbitrary in (6.2) we easily deduce from this inequality that

$$\sup_{|z|\le R} |\mathcal{O}^k f_{\rm cl}(\tau,z)| \le e^{(3R+2\ell^2)\tau}\left(2\tau e^{3R\tau}\right)^k$$

for all $\tau \ge 0$. Hence it follows that the series (5.1) converges uniformly in τ, x and ε on each set

$$[0,T]\times\{x\in\mathbb{C} : |x|\le R\}\times\{\varepsilon\in\mathbb{R} : |\varepsilon| < (2Te^{3TR})^{-1}\},$$

for

$$|f(\tau,x,\varepsilon)| \le e^{(3R+2\ell^2)\tau}\sum_{k=0}^{\infty}\left(2|\varepsilon|\tau e^{3R\tau}\right)^k$$
$$\le \frac{e^{(3R+2\ell^2)\tau}}{1-2|\varepsilon|\tau e^{3R\tau}},$$

showing the theorem. □

Theorem 6.1 allows one to evaluate the characteristic times of applicability of the classical approximation also in the unstable case of the attractive iteration.

Corollary 6.2 *Let $x/\varepsilon \gg 1$. Then F_{cl} approximates $F(\tau,x,\varepsilon)$ for small $|\varepsilon|$ uniformly in $t\in[0,T]$ with*

$$T \sim \frac{1}{6x}\log\frac{x}{|\varepsilon|}.$$

Proof Rewrite the inequality $|\varepsilon| < (2Te^{3xT})^{-1}$ in the form

$$2|\varepsilon|Te^{3xT} < 1. \tag{6.3}$$

Since the left-hand side is an increasing function of $T\ge 0$, the set of all T satisfying (6.3) is an interval $[0,T_0)$, where $T_0 = T_0(x,\varepsilon)$ is the root of the equation $2\varepsilon Te^{3xT}=1$.

Let us evaluate T_0. From $e^{3xT} > 1+3xT$ it follows that $T < (e^{3xT}-1)/3x$ for all $T\ge 0$. Hence $T_1 < T_0 < T_2$ where T_1 and T_2 are the unique positive solutions of the equations

$$2|\varepsilon|\frac{e^{3xT_1}-1}{3x}e^{3xT_1} = 1,$$
$$2|\varepsilon|T_2(1+3xT_2) = 1,$$

respectively. The solutions of these equations can be explicitly found, more precisely,

$$T_1 = \frac{1}{3x}\log\frac{1}{2}\left(1+\sqrt{1+6\frac{x}{|\varepsilon|}}\right),$$
$$T_2 = \frac{1}{6x}\left(-1+\sqrt{1+6\frac{x}{|\varepsilon|}}\right).$$

The asymptotic of T_1 in the domain of quasi-classical approach $x/|\varepsilon|\gg 1$ is actually

$$T_1 \sim \frac{1}{6x}\log\frac{x}{|\varepsilon|},$$

as is easy to check. □

Using the Laplace transform in the variable $\tau > 0$, which is as usual denoted by

$$\hat{f}(\tau^*) = \int_0^{\infty} e^{-\imath\tau^*\tau} f(\tau)d\tau$$

and is an analytic function of τ^* in the lower half-plane $\Im\tau^* < -\gamma$, one can show an explicit formula for the difference $f - f_{\mathrm{cl}}$. Namely,

$$\hat{f}(\tau^*, x, \varepsilon) = \hat{f}_{\mathrm{cl}}(\tau^*, x, \varepsilon) - \int_0^x \left(\frac{x}{y}\right)^{-\frac{1}{|\varepsilon|}\frac{\tau^*+2(\operatorname{sign}\varepsilon)\ell^2-|\varepsilon|}{2}} \times e^{-\frac{1}{|\varepsilon|}((x-y)+\frac{x^2-y^2}{4\tau^*})} \frac{\partial}{\partial y}\hat{f}(\tau^*, y, \varepsilon)dy, \tag{6.4}$$

where

$$\frac{\partial}{\partial y}\hat{f}(\tau^*, y, \varepsilon) = \frac{2\imath\,\tau^*(\tau^* + y)}{((\tau^* + y)^2 + \tau^*(2(\operatorname{sign}\varepsilon)\ell^2 - |\varepsilon|))^2}.$$

It is possible that an asymptotic expansion of the integral (6.4) in powers of $|\varepsilon|$ may be derived by the saddle-point method but we will not develop this point here.

7 Conclusion

The problem of the stability of the quantum solution (2.6) is analyzed here using the projection method onto the basis of coherent states. The quantum dynamics is described by the system of linear partial differential equations for observables with two independent variables (i) the dimensionless time, τ, and (ii) the dimensionless "coordinate", $x = \varepsilon|\alpha_k|^2$, where $|\alpha_k| = \sqrt{N}$ is the initial amplitude of the BEC prepared in a coherent state. The "classical" Gross-Pitaevskii (GP) limit corresponds to $\varepsilon \to 0$, $N \to \infty$, and $x = \varepsilon N \to$ finite value. The main results obtained in this paper are the following. For repulsive interaction, the GP solution approximates the quantum solution for small ε uniformly in time for $\tau < T$, with $T \sim 1/|\alpha_k|\sqrt{\varepsilon}$. (Note that $T/\tau_\hbar \sim \sqrt{\varepsilon} \ll 1$, where $\tau_\hbar$ is defined in Sect. 2.) For attractive interaction and under the condition, $x/\varepsilon \gg 1$ ($N \gg 1$), the GP solution approximates the quantum solution uniformly in time for $\tau < T$ with $T \sim (1/6x)\log(x/|\varepsilon|)$.

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