Dynamics and decoherence of two cold bosons in a 1D harmonic trap

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Abstract

We study dynamics of two interacting ultra cold Bose atoms in a harmonic oscillator potential in one spatial dimension. Making use of the exact solution of the eigenvalue problem of a particle in the delta-like potential we study time evolution of initially separable state of two particles. The corresponding time dependent single particle density matrix is obtained and diagonalized and single particle orbitals are found. This allows to study decoherence as well as creation of entanglement during the dynamics. The exact evolution is then compared to the evolution according to the Gross-Pitaevskii equation. We show that if initially the center of mass and relative degrees of freedom are entangled then the Gross-Pitaevskii equation fails to reproduce the exact dynamics and entanglement is produced dynamically.

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Introduction

Hamiltonian separation

All energies are measured in $\hbar\omega$, all lengths in $\sqrt{\hbar/m\omega}$, and all momenta in $\sqrt{\hbar m\omega}$. Hamiltonian of the system of two interacting bosons in the harmonic trap has the form:

$$\mathcal{H} = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}\left(x_1^2 + x_2^2\right) + g\delta(x_1 - x_2) \tag{1}$$

where x_1 and x_2 are positions of atoms interacting via a short range potential modeled by the delta function. In 1D the parameter g is given by $g = -2/a_0$, where a_0 is a scattering length.
To demonstrate entanglement formation we study the evolution of two bosons which initially are in a product quantum state

$$\Psi_0(x_1, x_2) = \Phi_0(x_1)\Phi_0(x_2). \tag{2}$$

Function $\Phi_0(x)$ is a one-particle wave function called the order parameter in the mean field context.
The two particle problem has to be first brought to a single particle one by introducing the center of mass and the relative coordinates:

$$X = \frac{1}{\sqrt{2}}(x_1 + x_2), \qquad \xi = \frac{1}{\sqrt{2}}(x_1 - x_2) \tag{3}$$

In these coordinates Hamiltonian (1) separates into two independent parts – the center of mass part $\mathcal{H}_{\mathrm{CM}}$, and the relative part $\mathcal{H}_{\mathrm{REL}}$:

$$\mathcal{H}_{\mathrm{CM}} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}X^2} + \frac{1}{2}X^2 \tag{4a}$$

$$\mathcal{H}_{\mathrm{REL}} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \frac{1}{2}\xi^2 + \frac{\sqrt{2}}{2}g\,\delta(\xi) \tag{4b}$$

As one can see, the dynamics of the center of mass is described by the standard one dimensional harmonic oscillator Hamiltonian with well known eigenstates. The eigenstates of the Hamiltonian $\mathcal{H}_{\mathrm{REL}}$ are also known and for one dimensional problem have a form

$$\varphi_m(\xi) = \frac{\pi^{-1/4}}{\sqrt{2^m\, m!}}\mathrm{H}_m(\xi)\,\mathrm{e}^{-\xi^2/2}, \qquad m \text{ odd} \tag{5a}$$

$$\varphi_m(\xi) = \mathcal{N}_m\,\mathrm{U}(-\nu_m, \frac{1}{2}, \xi^2)\,\mathrm{e}^{-\xi^2/2}, \qquad m \text{ even} \tag{5b}$$

where $\mathrm{U}(\alpha, \beta, x)$ are confluent hypergeometric functions, and $\mathcal{N}_m$ are normalization coefficients. Since the wave function of identical bosons must be symmetric under exchange of the two particles, therefore the physical wave function is composed from functions with **even *m* only**.

Exact dynamics

The initial wave function can be easily decomposed to the superposition of the eigenstates of the Hamiltonian:

$$\Psi_0(\xi, X) = \sum_{nm}\alpha_{nm}\,\chi_n(X)\varphi_m(\xi) \tag{6}$$

Obviously the evolution of the initial two boson state is given by:

$$\Psi(\xi, X, t) = \sum_{nm}\alpha_{nm}\,\chi_n(X)\varphi_m(\xi)\,\mathrm{e}^{-i(\mathcal{E}_n + E_m)t}. \tag{7}$$

In the original coordinates the wave function reads:

$$\Psi(x_1, x_2, t) = \sum_{nm}\alpha_{nm}\,\chi_n\left(\frac{x_1 + x_2}{\sqrt{2}}\right) \times \varphi_m\left(\frac{x_1 - x_2}{\sqrt{2}}\right)\mathrm{e}^{-i(\mathcal{E}_n + E_m)t}$$

The wave function written in the momentum space of the two atoms is:

$$\psi(k_1, k_2, t) = \int_{-\infty}^{\infty}\mathrm{d}x_1\int_{-\infty}^{\infty}\mathrm{d}x_2 e^{-ik_1x_1}e^{-ik_2x_2}\Psi(x_1, x_2, t). \tag{8}$$

In repeated single particle detections preceded by the ballistic expansion of the system one-particle momentum distribution is monitored:

$$n_{\mathrm{Exact}}(k, t) = \rho(k, k, t), \tag{9}$$

where $\rho(k, k', t)$ is the reduced one particle density matrix in the momentum representation:

$$\rho(k, k', t) = \int_{-\infty}^{\infty}\mathrm{d}k_2\,\psi^*(k, k_2, t)\psi(k', k_2, t) \tag{10}$$

By making its spectral decomposition we can determine the number of orbitals and their relative occupations needed for accurate description of the two bosons dynamics. Time dependence of the eigenvalues of the density matrix is discussed below. Let us mention that the largest eigenvalue is a direct measure of the coherence of the system.

Mean field dynamics

We compare exact dynamics with the approximate one governed by the Gross-Pitaevskii equation. In this approach generation of entanglement between bosons during the evolution is neglected and therefore the quantum state of the system remains separable:

$$\Psi(x_1, x_2, t) = \Phi(x_1, t)\Phi(x_2, t). \tag{11}$$

This assumption leads directly to the Gross-Pitaevskii equation which determines the dynamics of the one-particle wave function $\Phi(x, t)$:

$$i\partial_t\Phi(x, t) = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2 + g|\Phi(x, t)|^2\right)\Phi(x, t). \tag{12}$$

The probability density in momentum space reads:

$$n_{\mathrm{GP}}(k, t) = |\phi(k, t)|^2, \tag{13}$$

where $\phi(k, t)$ is the Fourier transform of the time dependent solution of the GP equation, $\phi(k, t) = \int \mathrm{d}x\, e^{-ikx}\Phi(x, t)$. We compare the exact one-particle momentum distribution (9) with that predicted by the Gross-Pitaevskii approximation (13). Moreover we compare the Gross-Pitaevskii momentum distribution (13) with the momentum distribution of the dominant orbital.

Results

We concentrate on a one particular class of the initial states. We assume that at the beginning each particle is in the state described by the Schrödinger cat like wave function

$$\Phi_0(x) = \mathcal{N}\left[\mathrm{e}^{-(x-L)^2/2} + \mathrm{e}^{-(x+L)^2/2}\right] \tag{14}$$

Parameter L measures the separation between two wave packets moving in the opposite direction in the relative coordinates space. When $L = 0$ then the initial state is very close to the ground state of the system, for large L the initial state is still separable but it is highly delocalized.

Dependence on delocalization

Fig. 1 shows time dependence of the eigenvalues of the one-particle density matrix and momentum distributions for generic interaction strength $g = -0.2$ and $L = 1$, i.e. when the extension of the initial state is equal to the trap length unit. Because one of the eigenvalues is incessantly much larger than the others the system coherence is large and the Gross-Pitaevskii description is quite accurate in this case.
When L is large enough then a few orbitals can play the crucial role in the dynamics and the mean field approximation is no longer valid. Fig. 2a shows the time dependence of the eigenvalues of the density matrix for $L = 3$. As we see, the main orbital initially dominates, but later the other orbital becomes much more important than the first one. The dynamics is obviously much more complicated than it is predicted by the mean field approach. It is clear when we compare the momentum density distribution predicted by the exact and the mean field solutions (Fig. 2b). We see also that Gross-Pitaevskii equation properly describes the dynamics of the first orbital rather then the whole system.

Dependence on interaction strength

Time dependence of the eigenvalues for a moderate interaction strength ($g = -0.2$) was discussed previously. For stronger interactions this picture changes significantly. For strong interaction ($g = -0.4$) and $L = 2$, after a few trap periods, many different orbitals become important. Moreover the orbital which dominates at the beginning becomes unimportant after a very short time. Therefore we do not expect that the Gross-Pitaevskii approximation may give correct predictions in this case. On the other hand when the interaction is very weak we expect that the production of entanglement is very slow even for highly delocalized states. Time dependence of the eigenvalues of the one-particle density matrix in these two situations is presented in fig. 3.

Correlations

Mutual interactions between particles obviously leads to the quantum correlations between particles. To study them we use the correlation measure **K** and von Neumann entropy **S**:

$$\mathbf{K}(\rho) = \left(\sum_i \lambda_i^2\right)^{-1}, \qquad \mathbf{S}(\rho) = -\sum_i \lambda_i \log\lambda_i \tag{15}$$

where λ_i are the eigenvalues of the one-particle density matrix ρ. Measure **K** has very simple interpretation. It gives an effective number of single particle orbitals occupied in the given many body state. In particular when one-particle density matrix has n equal eigenvalues then $\mathbf{K} = n$. Time dependence of this two measures of entanglement in the system for two different regimes of interaction strength are presented in Fig. 4.

Summary

We show that the two particle state, although initially being a product state does not preserve the product form during the evolution. The reason is that the initial state entangles the center of mass and relative coordinates of the two particle system. These two degrees of freedom evolve according to different Hamiltonians. This situation cannot be correctly described by the GP equation.

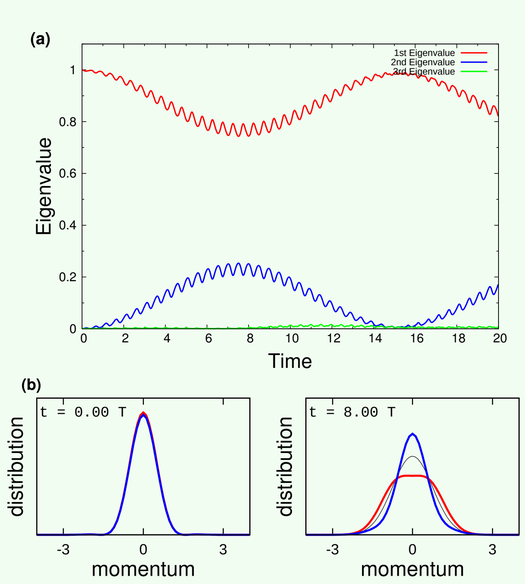

Figure 1: (a) Eigenvalues of the one-particle density matrix (10). Unit of time is equal to the period of the trap. In this situation (parameters: $g = -0.2$, $L = 1$) the initial state is not far from the ground state of the system. One eigenvalue still dominates, therefore system should be quite well described by the mean field approximation. (b) Two plots present the one-particle momentum distributions (in dimensionless units) predicted by the exact (thick solid line) and the Gross-Pitaevskii solutions (dotted line) in two interesting moments. Third (thin solid) line comes from the exact solution and presents the momentum distribution of the first orbital. As was expected all three predictions are almost the same for considered set of parameters.

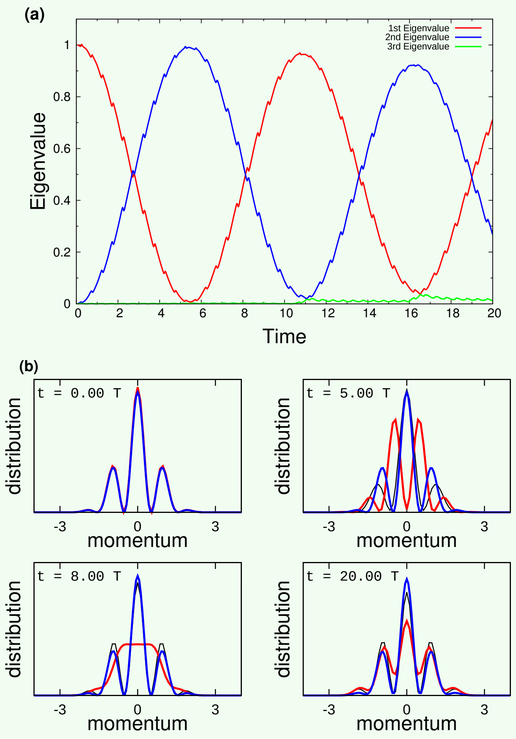

Figure 2: Analogous situation as in Fig. 1 but for $L = 3$. As long as the first eigenvalue dominates the predictions are almost the same. After five periods (the second eigenvalue become the largest) predictions are highly different. Solutions of the exact and GP dynamics become similar when the first eigenvalue starts to dominate again. Notice that third line presenting momentum distribution of first one-particle orbital of an exact solution recovers predictions of the Gross-Pitaevskii equation.

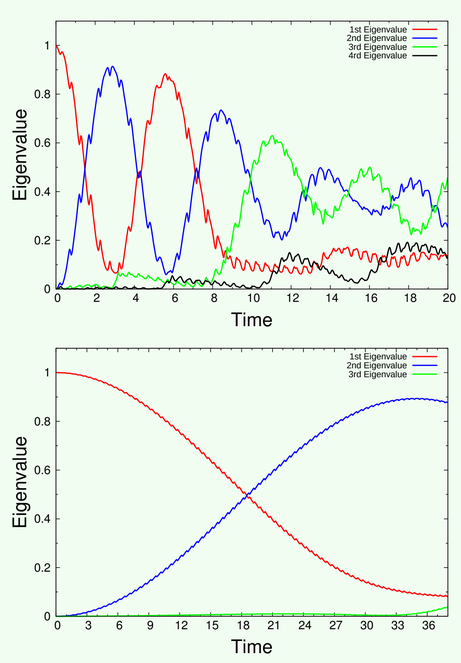

Figure 3: Eigenvalues of the one-particle density matrix as functions of time for highly delocalized initial state with $L = 2$ in two interaction strength regimes: (a) $g = -0.4$ – interaction between bosons is strong; many orbitals play a crucial role during the evolution of the system; the exact dynamics can not be recover by the mean field approximation. (b) $g = -0.04$ – interaction between bosons is very week; during the first eighteen trap periods only one eigenvalue dominates, therefore the dynamics of the system can be quite correctly described by the mean field approximation for a long time. Unit of time is equal to the period of the trap.

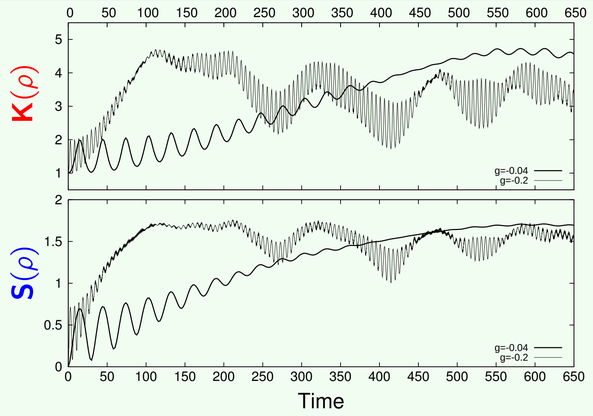

Figure 4: Time dependence of the number of dominant eigenvalues **K** and of the von Neumann entropy **S** for $g = -0.04$ (thick line) and $g = -0.2$ (thin line). Unit of time is equal to the period of the trap. Obviously in the beginning, when the system is in separable state, entanglement and von Neumann entropy are equal to 1 and 0 respectively. We observe that correlation **K** and entropy **S** increase in time and seem to saturate for large time. Even though they have different physical interpretation they behave very similarly which might seem quite surprising. They reach 'stationary regime' faster for stronger interactions. Every minimum observed in correlation function corresponds to the moment when there is a dominant eigenvalue in the Schmidt decomposition of the one-particle density matrix. Long time modulations of correlation functions are related to the quantum nature of the system and discreetness of the energy spectrum. In such cases evolution is always quasi-periodic and due to the interference of amplitudes long time scale oscillations do appear. In our case the number of modes with no zero amplitudes is relatively small and therefore oscillations of correlation functions appear on a time scale of few hundred trap periods.