

Exact dynamics of two cold bosons in a harmonic trap

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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 a time evolution of some particularly chosen initial states, all being a two-fold product of identical states of both particles. The corresponding time dependent single particle density matrix is obtained and diagonalized and single particle orbitals are found. The evolution of the orbital corresponding to the largest eigenvalue is then compared to the evolution given by 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. We stress that predictions of our study can be verified experimentally in an optical lattice in the low-tunneling limit when two atoms occupy each lattice site.

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I. INTRODUCTION

Theoretical description of a Bose-Einstein condensate of trapped weakly interacting atomic system is traditionally based on a mean field approximation [1]. By assuming that many-body wave function can be written in a form of N-fold product state, i.e. that all atoms occupy the same single particle orbital, the stationary Gross-Pitaevskii (GP) equation for the order parameter is found. Assuming further that the N-fold product approximation holds also in dynamical situations one arrives at the time dependent Gross-Pitaevskii equation. Under most of experimental conditions there are no strong correlations in the system and the GP equation turned-out to be extremely fruitful in predicting and describing a variety of features of those systems. Soon it occurred that also high energy solutions of the GP equation can be useful in studying Bose systems at finite temperatures. The GP equation has become a work horse of the theory of weakly interacting ultra cold bosons.

On the other hand examples when the mean field description does not reproduce the real dynamics have been studied. For instance direct comparison of the mean field and many body theory of vortex nucleation showed that the GP equation fails to describe this phenomenon [2–4]. Similarly a mean field description of attractive Bose systems encounters difficulties [5–7]. Due to permanent progress in experimental techniques the physics of ultra cold atomic gases started to penetrate areas traditionally associated with condensed matter physics where correlations play a crucial role. Evidently, in such situations simple mean field description based on the GP equation becomes insufficient. The Mott insulator-superfluid transition [8] or the Tonks gas [9] are some examples.

In this paper we study low energy collisions of two Bose atoms in a harmonic trap. At energies considered here the range of van der Waals interactions is smaller than

the s-wave scattering length. Therefore, the interaction potential can be approximated by a contact pseudo potential. This approximation occurred to be in excellent agreement with experimental results [10] where binding energy of molecular system have been measured. The molecules were created from atoms in an optical lattice in the limit of small tunneling. This experimental arrangement is perfectly suited for a study of exact dynamics of two trapped atoms. We consider a realistic case of two atoms per lattice site deep in the Mott insulator phase. By applying a Bragg pulses [11] one creates a state in which each atom is in a superposition of two counter propagating wave packets. It is very interesting to check whether the exact dynamics differs significantly from the mean field description based on the GP equation in a case when the correlations are present in the initial state.

II. TWO BOSONS IN A HARMONIC TRAP

We are going to study dynamics of the simplest non-trivial system – two atoms confined in a one dimensional harmonic potential. In fact generalization of our results to two or three spatial dimensions is straightforward. We limit our analysis to the 1D case as this situation captures all features of the dynamics. For simplicity we are using harmonic-oscillator units. It means that all energies are measured in $\hbar\omega$ and all lengths in $\sqrt{\hbar/(m\omega)}$ which is a size of the trapping potential ground state wave function. Hamiltonian of the system of two interacting bosons in the harmonic trap has the form:

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

where x_1 and x_2 are positions of atoms interacting via a short range potential modeled by the delta function. This form of the short range interaction is justified in

the limit of vanishing relative velocity of colliding atoms, where atomic de Broglie wavelength is much larger than a range of two body potential. In 2D and 3D the corresponding Hamiltonian is not a self adjoint operator. To correct for this fact a regularization is required. In contrast to many dimensions, the regularization of the delta function is not necessary in one dimensional case [12]. In 1D the parameter g is given by $g = -2/a_0$, where a_0 is a scattering length [13]. To demonstrate differences and similarities between exact dynamics and a dynamics predicted by the mean field approximation we will study the evolution of two bosons which initially are in a product quantum state

$$\Psi_0(x_1, x_2) = \Phi_0(x_1)\Phi_0(x_2). \quad (2)$$

Function $\Phi_0(x)$ is a one-particle wave function called the order parameter in the mean field context.

The exact dynamics of the two interacting bosons in the harmonic trap can be found because all eigenstates of the full two-body Hamiltonian (1) are known. They are found in [14]. The two particle problem has to be first brought to a single particle one by introducing the center of mass and the relative coordinates:

$$X = \frac{1}{\sqrt{2}}(x_1 + x_2) \quad (3a)$$

$$\xi = \frac{1}{\sqrt{2}}(x_1 - x_2) \quad (3b)$$

In these coordinates Hamiltonian (1) separates into two independent parts – center of mass part, and relative part:

$$\mathcal{H}_{\text{CM}} = -\frac{1}{2} \frac{d^2}{dX^2} + \frac{1}{2} X^2 \quad (4a)$$

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

As one can see the dynamics of the center of mass is described by the standard one dimensional harmonic oscillator Hamiltonian (4a). Its eigenstates are well known and have a standard form

$$\chi_n(X) = \frac{\pi^{-1/4}}{\sqrt{2^n n!}} H_n(X) \cdot e^{-X^2/2}, \quad (5a)$$

where $H_n(x)$ are Hermite polynomials. The energy of n -th eigenstate in our units is obviously given by

$$\mathcal{E}_n = n + \frac{1}{2} \quad (5b)$$

The eigenstates of the Hamiltonian (4b) describing relative dynamics of two particles are given in [14] and for one dimensional problem have a form

$$\varphi_m(\xi) = \frac{\pi^{-1/4}}{\sqrt{2^m m!}} H_m(\xi) \cdot e^{-\xi^2/2}, \quad m \text{ odd} \quad (6a)$$

$$\varphi_m(\xi) = \mathcal{N}_m U(-\nu_m, \frac{1}{2}, \xi^2) \cdot e^{-\xi^2/2}, \quad m \text{ even} \quad (6b)$$

where $U(\alpha, \beta, x)$ are confluent hypergeometric functions, and \mathcal{N}_m are normalization coefficients. Since the wave function of identical bosons must be symmetric under the exchange of the two particles, therefore the physical wave function is composed from functions with even m only. The energies E_m of these even states are given by a sequence of zeros of the function:

$$f(E) = \frac{\Gamma(-E/2 + 3/4)}{\Gamma(-E/2 + 1/4)} - \frac{1}{a_0} \quad (7)$$

and quantum number $\nu_m = (2E_m - 1)/4$. The initial wave function can be easily decomposed to the superposition of the eigenstates of the Hamiltonian:

$$\Psi_0(\xi, X) = \sum_{nm} \alpha_{nm} \chi_n(X) \varphi_m(\xi) \quad (8)$$

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

$$\Psi(\xi, X, t) = \sum_{nm} \alpha_{nm} \chi_n(X) \varphi_m(\xi) e^{-i(\mathcal{E}_n + E_m)t}. \quad (9)$$

The last step is to return to the original coordinates by using relations (3):

$$\begin{aligned} \Psi(x_1, x_2, t) = & \sum_{nm} \alpha_{nm} \chi_n \left(\frac{x_1 + x_2}{\sqrt{2}} \right) \\ & \times \varphi_m \left(\frac{x_1 - x_2}{\sqrt{2}} \right) e^{-i(\mathcal{E}_n + E_m)t} \end{aligned} \quad (10)$$

Standard method of detection of ultra cold trapped atomic systems are destructive. The optical lattice potential is turned off and the system is allowed to expand ballistically. Only after expansion a size of the system exceeds a resolution of a CCD camera. The picture of the CCD camera gives therefore direct insight into the initial momentum distribution of atoms. The wave function Eq.(10) written in the momentum space of the two atoms is:

$$\psi(k_1, k_2, t) = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 e^{-ik_1 x_1} e^{-ik_2 x_2} \Psi(x_1, x_2, t). \quad (11)$$

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

$$n_{\text{Exact}}(k, t) = \rho_1(k, k, t), \quad (12)$$

where $\rho_1(k, k', t)$ is the reduced one particle density matrix in the momentum representation:

$$\rho_1(k, k', t) = \int_{-\infty}^{\infty} dk_2 \psi^*(k, k_2, t) \psi(k', k_2, t) \quad (13)$$

By making its spectral decomposition we can determine the number of orbitals needed for accurate description

of the two bosons dynamics. Time dependence of the eigenvalues of the density matrix is discussed below.

We shall compare this exact dynamics with the approximate one governed by the Gross-Pitaevskii equation. The main idea leading to the mean field approximation relies on the assumption that generation of entanglement between bosons during the evolution is negligible and therefore the quantum state of the system remains separable. In other words all correlations between bosons are neglected and the same wave functions of every particle is assumed during evolution:

$$\Psi(x_1, x_2, t) = \Phi(x_1, t)\Phi(x_2, t). \quad (14)$$

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

$$i\partial_t\Phi(x, t) = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2 + g|\Phi(x, t)|^2 \right) \Phi(x, t). \quad (15)$$

The probability density in momentum space reads:

$$n_{\text{GP}}(k, t) = |\phi(k, t)|^2, \quad (16)$$

where $\phi(k, t)$ is the Fourier transform of the time dependent solution of the GP equation, $\phi(k, t) = \int dx e^{-ikx}\Phi(x, t)$. We compare the exact one-particle momentum distribution with that predicted by the Gross-Pitaevskii approximation. (16) (Fig. 2, 4, 8). In the situation when many eigenvalues are of the same order we can also compare the Gross-Pitaevskii momentum distribution (16) with the momentum distribution of the dominant orbital obtained from diagonalization of the exact one-particle density matrix in the momentum space.

A. Results

To make the detailed comparison 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

$$\Phi_0(x) = \mathcal{N} \left[e^{-(x-L)^2/2} + e^{-(x+L)^2/2} \right] \quad (17)$$

Parameter L measures the separation between two wavepackets moving in the opposite direction in the relative coordinates space. It gives the delocalization of the initial state in the relative coordinates space as compared to the spatial extension of the center of mass wave function. In our case the center of mass wave function corresponds to the trap ground state. Such a choice is motivated by the preparation procedure described above, i.e. we assume that Bragg pulses bringing the atoms into the superposition of wave packets moving in opposite directions are applied. When $L = 0$ then the initial state is very close to the ground state of the system so we expect that the exact dynamics is almost indistinguishable from

the dynamics in the mean field approximation. When L is large then the initial state is still separable but it is highly delocalized. In particular its spatial extension exceeds the center of mass extension. Relative and center of mass degrees of freedom are entangled in the initial state. They evolve in a different way, therefore we expect that the exact dynamics could be dramatically different than the dynamics predicted by a simple mean field approach.

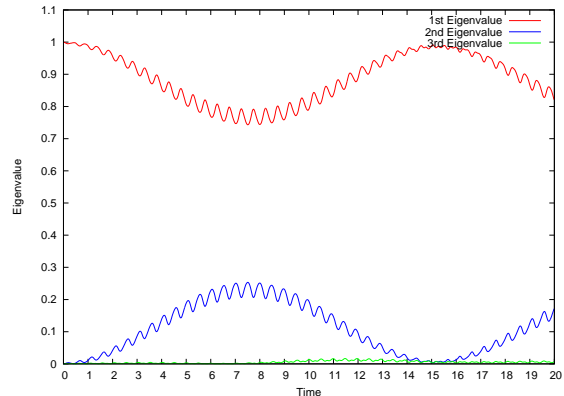


FIG. 1: Eigenvalues of the one-particle density matrix (13). Unit of time is equal to the period of the trap. Parameter L measures the relative extension of the initial state. In this situation (parameters: $a_0 = 10$, $L = 1$) the initial state is not far from the ground state of the system. One eigenvalue still dominates, therefore system should be quite well described by the mean field approximation.

When L is non zero, the situation becomes interesting. For example when $L = 1$ (i.e. when the extension of the initial state is equal to the trap length unit) we observe that the single particle density matrix obtained from the exact dynamics develops more than one large eigenvalue, i.e. many one particle orbitals are involved. Fig. 1 shows time dependence of the eigenvalues of the one-particle density matrix (13). Because one of the eigenvalues is still much larger than the others one can expect that the system should be quite well described by the Gross-Pitaevskii equation. Comparison of the time dependence of the momentum distributions is shown in Fig. 2. It confirms this prediction.

Situation changes dramatically when we increase the delocalization parameter. 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. 3 shows the time dependence of the eigenvalues of the density matrix for $L = 3$. As we see, the main orbital (its eigenvalue is represented by a red line) initially dominates. But after a few periods of the trap oscillations the other orbital becomes much more important than the first one. However after some additional time, the third orbital is the most populated. 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. 4).

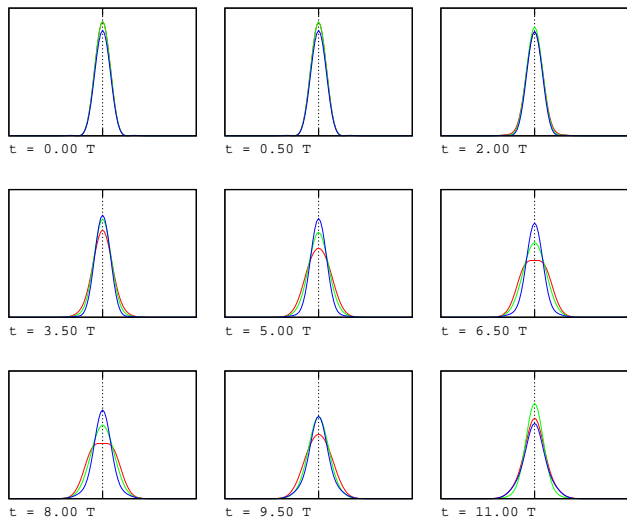


FIG. 2: (Parameters: $a_0 = 10$, $L = 1$) This picture corresponds to the dynamics of the eigenvalues presented in Fig. 1. It presents the time dependence of the one-particle momentum distributions predicted by the exact (red line) and the Gross-Pitaevskii solutions (blue line). Third (green) line comes 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.

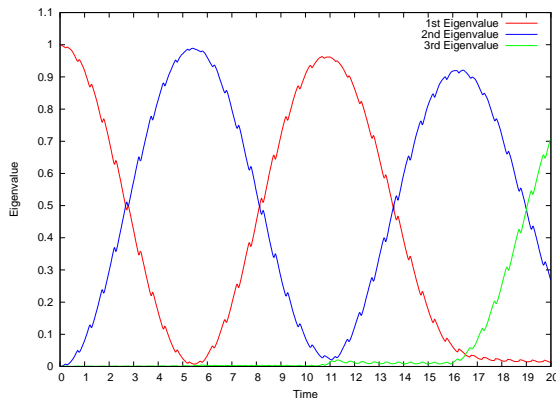


FIG. 3: Eigenvalues of the one-particle density matrix (13). Unit of time is equal to the period of the trap. Parameter L measures the a distance between the two initial wavepackets moving in the opposite direction. In this situation (parameters: $a_0 = 10$, $L = 3$) the initial state is a product of highly delocalized one-particle wave functions. There is no one dominant eigenvalue during the evolution and therefore the Gross-Pitaevskii equation will not predict dynamics correctly.

In this situation we can also check if the Gross-Pitaevskii equation describes correctly the dynamics of the first orbital. Figures 4 and 5 show the evolution of the one-particle momentum distribution. We see that evidently Gross-Pitaevskii equation properly describes the dynamics of the first orbital rather than the whole system. It is the reason why the Gross-Pitaevskii equation

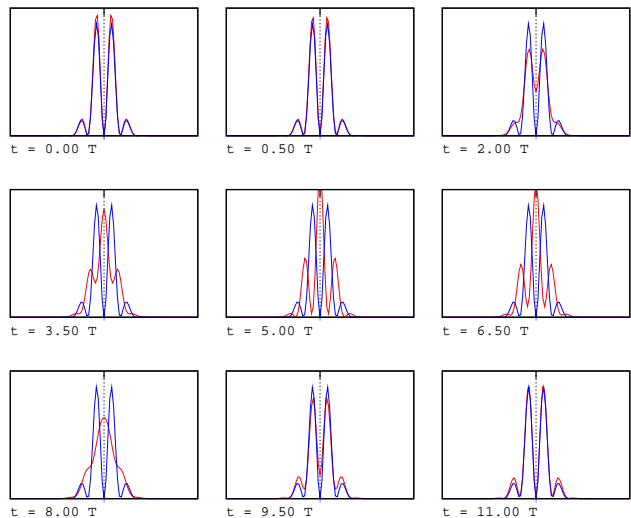


FIG. 4: (Parameters: $a_0 = 10$, $L = 3$) This picture corresponds to the dynamics of eigenvalues presented in Fig. 3. It presents the time dependence of the one-particle momentum distribution predicted by the exact (red line) and Gross-Pitaevskii solutions (blue line). As long as the first eigenvalue dominates during the time evolution the predictions are almost the same. After three periods of the trap the second eigenvalue is the largest one and therefore the predictions are highly different. Predictions of the exact and GP approaches become similar after nine trap periods when the first eigenvalue starts to dominate again.

gives good predictions when only one eigenvalue of the one particle matrix dominates during the entire evolution.

Now we want to show that correctness of the mean field approximation significantly depends on the interaction strength parameter g . It is quite obvious that in the situation when the interaction is switched off, the two particles initially in the state which is not entangled (product state) will stay in such a state during the whole evolution even for a highly delocalized state. In this case the mean field approximation naturally leads to the same solution as the exact solution. It is the interparticle interaction which can produce entangled two body states during the evolution.

Time dependence of the eigenvalues for a moderate interaction strength ($a_0 = 10$) is presented in Fig. 1 and 3. In those situations only two eigenvalues (i.e. two orbitals) are important for many trap periods. For stronger interactions this picture changes significantly. Time dependence for strong interaction ($a_0 = 5$) but for the same initial quantum state as in Fig. 3 is shown in Fig. 6. After a few trap periods many different orbitals becomes important. Moreover the orbital which dominates at the beginning becomes unimportant after a very short time. Therefore it cannot be expected that the Gross-Pitaevskii approximation may give correct predictions in this case.

On the other hand when the interaction is very weak

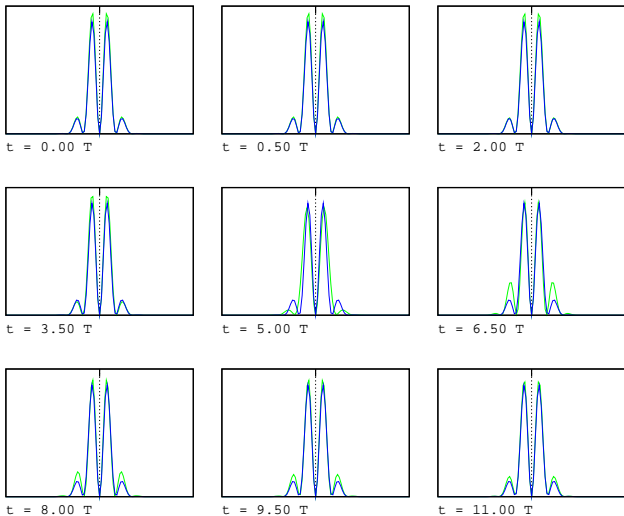


FIG. 5: This figure is made for the same parameters as Fig. 4 and shows the one-particle momentum distribution predicted by the Gross-Pitaevskii solution (blue line) and an exact solution for the 1st orbital (green line). As we see these predictions are very similar during the whole evolution. It suggests that Gross-Pitaevskii equation properly describes the dynamics of the first orbital only rather than the dynamics of the whole system.

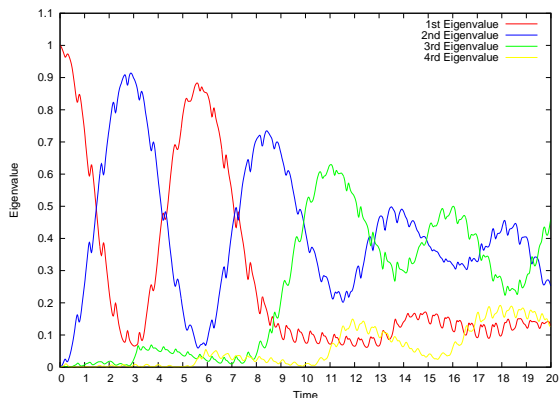


FIG. 6: (parameters: $a_0 = 5$, $L = 2$) The interaction between bosons is strong and the initial state of one particle is highly delocalized. In such a situation many orbitals play a crucial role during the evolution of the system. Therefore the exact dynamics is much more complicated than the dynamics predicted by the mean field approximation.

we can expect that the production of entanglement will be very slow even for highly delocalized states and therefore the mean field approximation may be correct for a long evolution time. Time dependence of the eigenvalues of the one-particle density matrix when the interaction is weak but the initial state is highly delocalized is presented in fig. 7.

In the end we study similarities and differences between prediction of the mean field approach and exact

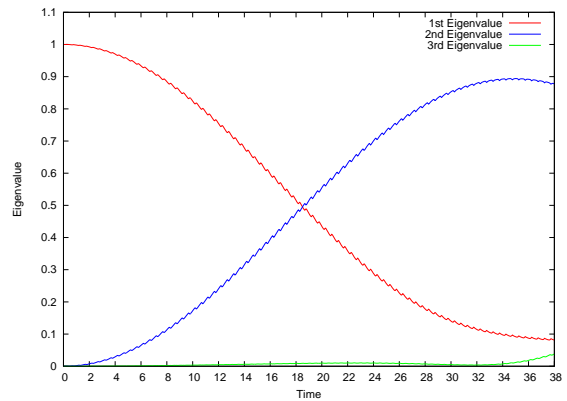


FIG. 7: (parameters: $a_0 = 50$, $L = 2$) In this situation the interaction between bosons is very weak but the initial state is far from the ground state of the system. Since for first eighteen trap periods only one eigenvalue dominates, therefore the dynamics of the system can be quite correctly described by the mean field approximation for a long time. Notice that time scale is two times larger than in the previous situations.

solution in the situation when the initial state of each particle is antisymmetric in position space, i.e. is described by the wave function of the form

$$\Phi_0(x) = \mathcal{N} \left[e^{-(x-L)^2/2} - e^{-(x+L)^2/2} \right]. \quad (18)$$

This function is antisymmetric. Because the Gross-Pitaevskii Hamiltonian is invariant under reflection $x \rightarrow -x$ the symmetry of the initial state will be preserved. As we observe, it is not true for the exact two body dynamics. The evolution preserves only the symmetry of each orbital separately, but not the symmetry of the whole system. It is clearly demonstrated in Fig. 8 and 9 where we compare the momentum distribution predicted by mean field approach with the single particle density obtained from the exact dynamics.

III. SUMMARY

In this paper we study the exact dynamics of two particles trapped in a harmonic trap and interacting by a contact potential. We assumed that initially each particle is transferred by the Bragg pulses to the state being the superposition of two wave packets moving in opposite directions. 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. As a result the single particle reduced matrix develops many eigenvalues during the evolution. This situation cannot be correctly described by the GP equation. Our predictions can be verified in the experiment with deep optical

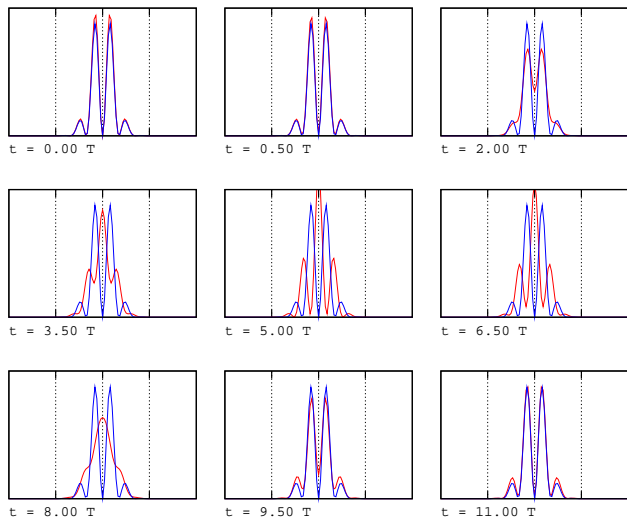


FIG. 8: Time dependence of the one-particle momentum distribution for the antisymmetric initial state $\Phi_0(x) = \mathcal{N} [e^{-(x-L)^2/2} - e^{-(x+L)^2/2}]$ with $L = 3$. Red line represents the density predicted by an exact solution, while blue one the density coming from the mean field approach. Properties of the Gross-Pitaevskii equation provide that if the value of the function $\Phi_0(x)$ is zero for some x it will stay zero there during the whole evolution. It is not true for the one-particle density predicted by an exact solution.

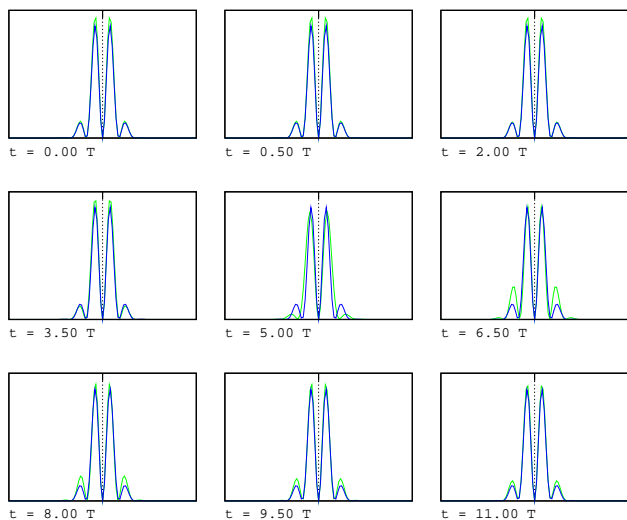


FIG. 9: This figure is counterpart of the Fig. 8 and presents a one-particle momentum distribution predicted by Gross-Pitaevskii solution (blue line) and an exact solution for the 1st orbital (green line). It shows once more that Gross-Pitaevskii equation describes properly the dynamics of the first orbital only.

lattices when two atoms occupy each site. We show one-particle momenta distributions for different initial states and compare them to those obtained from the mean-field dynamics. The differences between the two signify the two atom entanglement. The momentum distribution is directly measured by exposure of the system to a resonant light after ballistic expansion and therefore creation of entanglement in the two particle system can be easily traced in time and compared to exact solutions.

Acknowledgments

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