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Mean field loops versus quantum anti-crossing nets in trapped Bose-Einstein condensates

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Abstract. We study a Bose-Einstein condensate trapped in an asymmetric double well potential. Solutions of the time-independent Gross-Pitaevskii equation reveal intrinsic loops in the energy (or chemical potential) level behavior when the shape of the potential is varied. We investigate the corresponding behavior of the quantum (many-body) energy levels. Applying the two-mode approximation to the bosonic field operators, we show that the quantum energy levels create an anti-crossing net inside the region bounded by the loop of the mean field solution.

PACS. 03.75.Fi Phase coherent atomic ensembles; quantum condensation phenomena – 05.30.Jp Boson systems – 32.80.Pj Optical cooling of atoms; trapping

Experimental realizations of a Bose-Einstein condensate (BEC) in cooled and trapped atomic gases [1] are triggering many efforts to explore new quantum phenomena on a macroscopic level. The weak interaction between the condensate atoms allows for a precise tailoring that is not feasible experimentally with other superfluid systems such as the ^{4}He-II. In particular, interference phenomena have been investigated in the case of a condensate trapped in both double [2] and multiple [3] wells potentials, and the possibility of tunneling has resulted in an oscillatory (Josephson) atomic flow across adjacent traps [4]. A theoretical description of the process carried out within the mean field (Gross-Pitaevskii equation (GPE) [5]) approximation predicts a rich dynamical phase diagram [6]. Quantum corrections show that the mean field description remains valid for a very long but finite period of time up to the moment when the system is able to detect tiny differences in energy between the multi-particle levels [7–9].

The excitation of solitons and vortices in a condensate by an adiabatic deformation of the trapping potential has been recently investigated in [10,11]. However, we have found that some levels of the time-independent GPE reveal loop-like structures when varying a parameter of the potential [11]. Solutions of GPE which correspond to eigenvalues on those loops are typical of nonlinear equations and do not have a linear ($g_0 = 0$ in (4)) single particle counterpart. This class of GPE solutions has been investigated in [12] for a symmetric double well potential. The loop-like behavior in the solution of the GPE has been also observed for Bloch bands spectrum in reference [13]. There, the appearance of the loops results in the breakdown of the Bloch oscillations due to non-zero adiabatic tunneling into the upper band.

One may wonder about the quantum (multi-particle) equivalent of such loops. In this case, indeed, no loops are expected because the many-body Hamiltonian is a Hermitian operator. It has been proved in [14] that the ground state and the associated energy of GPE for repulsive atom-atom interactions (positive scattering length a_s) are asymptotically exact when the number of particles $N \to \infty$ while Na_s is kept constant. To the best of our knowledge there is no similar theorem concerning the negative a_s case and the excited eigenstates of the GPE. Therefore, it is important to understand how those mean-field loops are approached by the eigenenergies of the quantum Hamiltonian which, we remark, cannot form any loop.

The aim of the present paper is to investigate quantum multiparticle energy levels of an asymmetric double well potential in the regime where the GPE reveals loop-like structures. The structures can be observed even for a very weak interaction between particles, so we use a two-mode approximation (TMA) [6–9] in the quantum calculations. The results so obtained are compared with the GPE predictions, calculated both in the TMA and with a numerical integration in a 1D geometry.

We consider a condensate trapped in a harmonic cigar-like potential with an additional Gaussian perturbation. Freezing the transversal degrees of freedom tightly confining the condensate in the same direction, the potential

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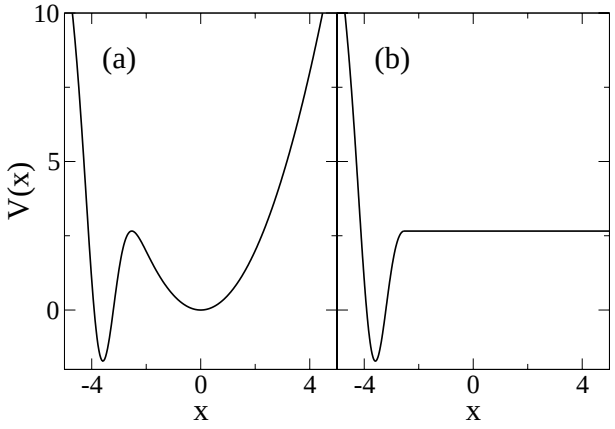

Fig. 1. (a) Plot of the potential (1) for $U_0 = 6.4$, $\sigma = 0.5$ and $x_0 = -3.7$. (b) Single well potential obtained by taking the left part of the potential plotted in panel (a) up to the point corresponding to the top of the barrier and in the remaining space the potential is kept constant. The lowest eigenstate of such a single well potential constitutes the mode $u_1(x)$. In an analogous way the mode $u_2(x)$ of the right potential well is defined.

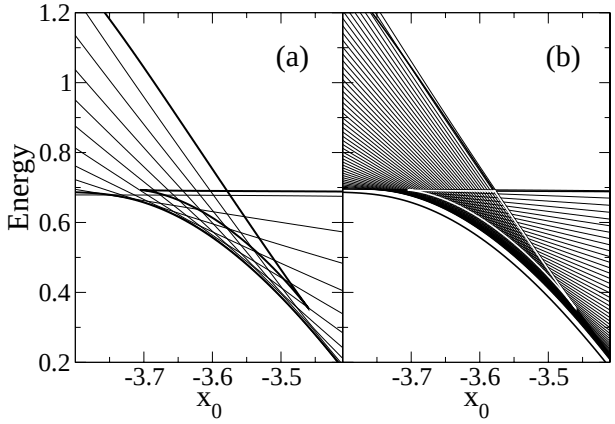

Fig. 2. Energy levels of a condensate per particle as a function of x_0, for $Ng_0 = 1$. The other potential parameters are: $U_0 = 6.4$ and $\sigma = 0.5$. Thick lines, in both panels, correspond to the solutions of the GPE (4), *i.e.* $E/N = \mu - (Ng_0/2)\int |\varphi(x)|^4 \mathrm{d}x$, while lines are the results of the quantum two-mode approximation (3) for number of particles $N = 10$ (a) and $N = 50$ (b).

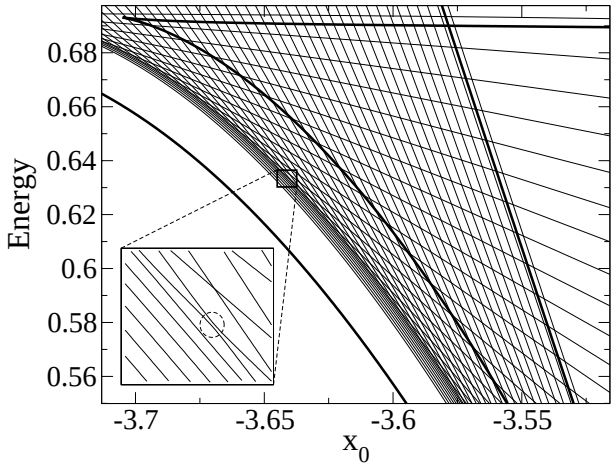

Fig. 3. Magnified anti-crossings structure of Figure 2b. Anti-crossings are so tiny that they become visible in the insert (in the circle).

(in units of a harmonic oscillator corresponding to the longitudinal direction) reads

$$V(x) = \frac{x^2}{2} + U_0 \arctan(x_0) \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right). \quad (1)$$

Within a certain window of parameters, the potential (1) has a double well shape [10,11]. The many-body Hamiltonian governing the full N-particle problem [15] is,

$$\hat{H} = \int \mathrm{d}x \left[\hat{\psi}^\dagger H_0 \hat{\psi} + \frac{g_0}{2}\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}\hat{\psi}\right], \quad (2)$$

where $H_0 = -(\mathrm{d}^2/\mathrm{d}x^2)/2 + V(x)$. $\hat{H}$ can be approximated expanding the field operators in terms of the local modes, $\hat{\psi} \approx u_1(x)\hat{c}_1 + u_2(x)\hat{c}_2$. $u_j(x)$ are localized solutions of the Schrödinger equation solved for each well of the potential separately (see below). This, provided that $\int u_1^*(x)u_2(x)\mathrm{d}x \approx 0$, yields

$$\hat{H} \approx E_1\hat{c}_1^\dagger\hat{c}_1 + E_2\hat{c}_2^\dagger\hat{c}_2 + \frac{\Omega}{2}(\hat{c}_2^\dagger\hat{c}_1 + \hat{c}_1^\dagger\hat{c}_2) + \frac{g_0}{2V_1}(\hat{c}_1^\dagger)^2(\hat{c}_1)^2 + \frac{g_0}{2V_2}(\hat{c}_2^\dagger)^2(\hat{c}_2)^2, \quad (3)$$

where $E_j = \int u_j^*(x)H_0u_j(x)\mathrm{d}x$, $\Omega = 2\int u_1^*(x)H_0u_2(x)\mathrm{d}x$ and the effective mode volume of each well $V_j^{-1} = \int |u_j(x)|^4\mathrm{d}x$.

The Bose operators $\hat{c}_j$, that annihilate a particle at the respective well of the potential, obey the usual commutation relation $[\hat{c}_j, \hat{c}_k^\dagger] = \delta_{jk}$. To define the modes $u_j(x)$, we have separated each well from the potential (1) as shown in Figure 1 [17]. Given the modes one can immediately calculate the parameters of the Hamiltonian (3).

The solutions of the time-independent GPE,

$$H_0\varphi(x) + Ng_0|\varphi(x)|^2\varphi(x) = \mu\varphi(x), \quad (4)$$

where $|\varphi(x)|^2$ is normalized to unity and N denotes the number of particles in a BEC, give the chemical potential levels μ of the condensate [5]. For a very small nonlinearity parameter, Ng_0, changing the parameter of the potential x_0 (for $U_0 = 6.4$ and $\sigma = 0.5$), a narrow avoided crossing between the ground and first excited levels occurs around $x_0 = -3.6$ [10]. However, when Ng_0 increases the usual avoided crossing turns into a more complicated structure where the excited level reveals a loop-like character, see Figure 2. To compare this single-particle description of the system with the quantum multi-particle picture we have diagonalized the Hamiltonian (3) for $N = 10$ and $N = 50$ adjusting g_0 so that $Ng_0 = 1$ in both cases. Figure 3 shows that quantum energy levels undergo a net of anti-crossings and the GPE solutions provide an envelope of this anti-crossings structure. The lowest quantum energy level corresponds to the ground state of the BEC while the highest one corresponds to all particles occupying the

Rapid Note

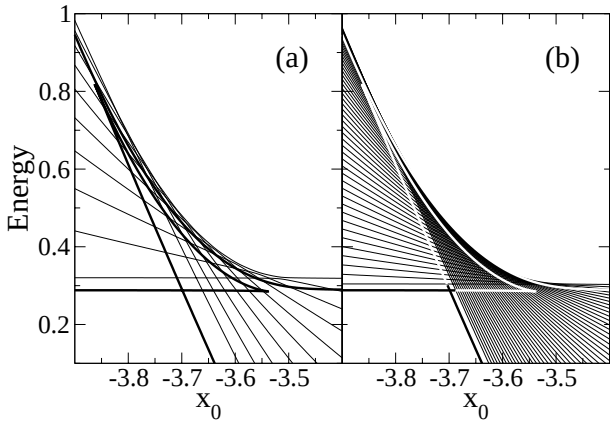

Fig. 4. The same as in Figure 2 but for $Ng_0 = -1$.

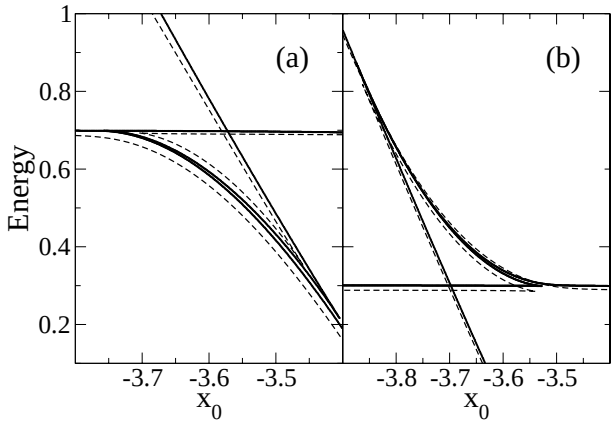

Fig. 5. Comparison of the two-mode approximation applied to the GPE (solid lines) with the solutions of the full GPE (dashed lines). Panel (a) corresponds to $Ng_0 = 1$, panel (b) to $Ng_0 = -1$.

upper level of the trap. Both states can be calculated by solving the GPE equation. However, in the middle of the figure not only the lowest and highest energy states can be represented by a mean field wavefunction which corresponds to all atoms in the same one-particle state. Indeed, the existence of the loop indicates that there are two more of such states.

As expected, also in the attractive case we observe a loop-like structure (see Fig. 4) which, however, is on the ground state energy level. In the two-mode approximation, the conditions for the formation of loops can be easily calculated analytically (see below).

Switching to the quantum two-mode approximation we found that the energy levels reveal (similarly as for the repulsive interaction) an anti-crossing structure located within the loop of the mean field results (Fig. 4).

Let us now carry out the two-mode approximation also in the mean field description. Replacing the ansatz wavefunction $\varphi(x) = (c_1 u_1(x) + c_2 u_2(x))/\sqrt{N}$ in (4) we get a pair of coupled equations,

$$\begin{cases} c_1 E_1 + c_2 \Omega/2 + |c_1|^2 c_1 g_0/V_1 = c_1 \mu \\ c_2 E_2 + c_1 \Omega/2 + |c_2|^2 c_2 g_0/V_2 = c_2 \mu \end{cases}, \tag{5}$$

which (with the additional constraint $|c_1|^2 + |c_2|^2 = N$) allow us to calculate the coefficients c_j and the chemical potential. In the range of the parameter x_0 where there is no loop of the GPE, we get only two solutions of (5), while in the inner region there are four of them forming a loop. In Figure 5 we compare the classical two-mode approximation with the results of the GPE both for repulsive and attractive interaction between particles. The results of the classical two-mode approximation are in a good agreement with the full GPE solutions and, therefore, we expect that the quantum two-mode will also be a good approximation of the full quantum multi-particle problem. We note that the expression for the energy of the N-particle condensate in the classical two-mode approximation,

$$H = E_1|c_1|^2 + E_2|c_2|^2 + \frac{\Omega}{2}(c_1 c_2^* + c_1^* c_2) + \frac{g_0}{2V_1}|c_1|^4 + \frac{g_0}{2V_2}|c_2|^4, \tag{6}$$

is of the same form as the corresponding quantum Hamiltonian (3), but with c_j being c-numbers.

By increasing the number of atoms in the BEC keeping Ng_0 fixed, the values of the extremal quantum energy levels reproduce the classical two-mode approximation results more and more accurately.

In [10] we have suggested that starting with a condensate in the ground state of a harmonic trap and sweeping the trap with a laser beam (which actually leads to the potential (1) where x_0 changes from some negative value to zero) can be used to excite a BEC solitary wave by means of a diabatic passage through an avoided crossing. In the mean field description, the presence of a loop does not break the process because the ground state wavefunction on one side of such a strange avoided crossing structure (*i.e.* a loop) is basically the same as the wavefunction of the first excited state on the other side so the diabatic scenario applies [11]. Switching to the quantum description we see that one avoided crossing of GPE levels, which has to be passed by each one of the N particles, is just replaced by many smaller ones in the multi-particle level structure. We expect that when the laser beam is swept with appropriate velocity it will transfer the atoms from the ground energy level on the left hand side of Figure 2 (or Fig. 4) to the highest energy levels on the right hand side of Figure 2 (or Fig. 4). To test such a hypothesis we have carried out quantum time dependent calculations within the TMA starting with the system in a ground state of the pure harmonic trap [18]. In Figure 6 we show the results of a laser sweep, *i.e.* a change of x_0 from -5 to 0 according to $x_0(t) = -5 + 0.05t$. In the case of the noninteracting particle system ($g_0 = 0$), if the excitation probability of a particle from the ground state to the first excited state in the single particle description is less than 1 (although close to unity), the corresponding multiparticle picture reveals population of a bunch of the eigenstates as shown in Figure 6a [10]. Switching on the interaction the effect of the laser sweep is unchanged — similarly as in the noninteracting particle case the highest energy eigenstates of

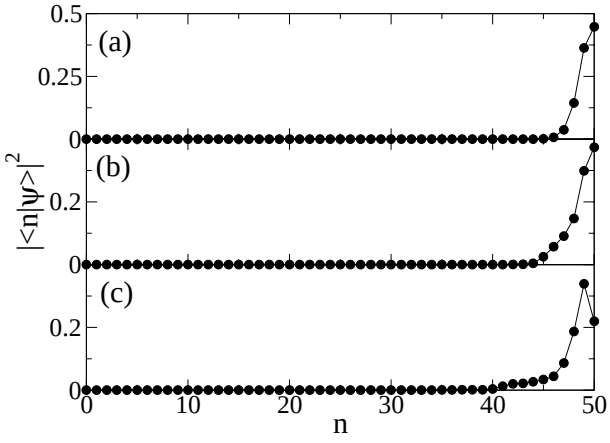

Fig. 6. Overlaps $|\langle n|\psi\rangle|^2$ of the wavefunction on the energy eigenstates of the $N = 50$ particle system in the harmonic trap at the end of the laser sweep. Starting with the ground state of the harmonic trap, *i.e.* $|\psi(0)\rangle = |n = 0\rangle$, we change the potential (1) according to $x_0(t) = x_0(0) + 0.05t$ with $x_0(0) = -5$. At the end of the sweep the highest energy eigenstates become populated — panel (a) corresponds to the noninteracting particle case (*i.e.* $g_0 = 0$), panel (b) to $g_0N = 1$ and (c) to $g_0N = -1$.

the system become populated, see Figures 6b and 6c. Of course, this is a simplified picture in the two-mode approximation that is valid only for a weak interaction between atoms. For stronger interactions further investigations are necessary.

In reference [13] a loop-like behavior was observed in solutions of the GPE for a BEC in a periodic lattice, implying breakdown of Bloch oscillations and adiabatic tunneling into the upper band. The approximation method performed here can be easily applied in that case. This allows one to identify which multi-particle eigenstates are populated in the tunneling process.

To summarize, we have considered the behavior of the energy levels of an asymmetric double well potential when the shape of the potential is changed. Using the two-mode approximation in the quantum multi-particle Hamiltonian we have found that the energy levels undergo a net of avoided crossings. Solutions of the Gross-Pitaevskii equation reveal a loop structure which provides an envelope to the quantum avoided-crossings net. We finally note that since the two-mode approximation, applied to the mean field description, is in a very good agreement with the full numerical solution of the Gross-Pitaevskii equation, the quantum two-mode approximation can also be considered a good approximation of the full quantum multi-particle problem at least in the regime of weak interaction between atoms studied here.

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15. In the harmonic oscillator units, $g_0 = g/(\hbar\omega_{||}a_{||})$ where the coefficient $g = 4\pi\hbar^2 a_s/(m\pi a_\perp^2)$ is renormalized by the transverse condensate length $a_\perp$ in reducing the dimensionality of the problem from 3D to 1D [16]
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17. The modes may be defined in many ways, *e.g.* as states of potentials obtained by expanding equation (1) around a center of each well up to the second order (which, however, is a poor approximation for the Gaussian-like well which we deal with in our problem) or as symmetric and antisymmetric eigenstates combinations. Such states can be calculated as solutions of the Gross-Pitaevskii equation (providing, in general, a more accurate two-mode approximation [6]). In the present paper, however, the localized wave-functions have been calculated by neglecting the (in our case very small) non-linearity
18. In the time dependent calculations we have defined modes as the two lowest eigenstates of the potential (1). It allows us to describe the system not only when the potential (1) reveals double well structure but in the full range of the potential parameter x_0