Quantum switching at a mean-field instability of a Bose-Einstein condensate in an optical lattice

V. S. Shchesnovich and V. V. Konotop

1 Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André, SP, 09210-170 Brazil,
2 Centro de Física Teórica e Computacional, Universidade de Lisboa,
Complexo Interdisciplinar, Avenida Professor Gama Pinto 2,
Lisboa 1649-003, Portugal; Departamento de Física, Faculdade de Ciências,
Universidade de Lisboa, Campo Grande, Ed. C8, Piso 6, Lisboa 1749-016, Portugal

It is shown that bifurcations of the mean-field dynamics of a Bose-Einstein condensate can be related with the quantum phase transitions of the original many-body system. As an example we explore the intra-band tunneling in the two-dimensional optical lattice. Such a system allows for easy control by the lattice depth as well as for macroscopic visualization of the phase transition. The system manifests switching between two selftrapping states or from a selftrapping state to a superposition of the macroscopically populated selftrapping states with the step-like variation of the control parameter about the bifurcation point. We have also observed the magnification of the microscopic difference between the even and odd number of atoms to a macroscopically distinguishable dynamics of the system.

PACS numbers: 03.75.Lm; 03.75.Nt

Introduction.- Since the very beginning of the quantum mechanics its relation to the classical dynamics constitutes one of the central questions of the theory. Dependence of the energy levels distribution on the type of dynamics of the corresponding classical system, in general, and the quantum system response to variation of the bifurcation parameters controlling the qualitative changes of the classical behavior are among the major issues. One of the main tools in studies of the quantum-classical correspondence is the WKB approximation, where, loosely speaking, the Planck constant $\hbar$ is regarded as a small parameter.

On the other hand, for a $N$-boson system the limit $N \to \infty$ at a constant density, leading to the mean-field approximation, can also be understood as a semiclassical limit. This latter approach has received a great deal of attention during the last decade, due its high relevance to the theory of Bose-Einstein condensates (BECs), many properties of whose dynamics are remarkably well described within the framework of the mean-field models. More recently, it was shown that the mean-field description of a few-mode $N$-boson system can be recast in a form similar to the WKB approximation for a discrete Schrödinger equation, emergent for the coefficients of the wavefunction expansion in the associated Fock space, where $1/N$ plays the role similar to that of the Planck constant in the conventional WKB approximation.

The mean-field equations of a system of interacting bosons are nonlinear, hence, they naturally manifest many common features of the nonlinear dynamics, including bifurcations of the stationary solutions caused by variation of the system parameters. One of the well studied examples is a boson-Josephson junction, which can show either equally populated (symmetric) or strongly asymmetric states, characterized by population of only one of the sites (the well known phenomenon of selftrapping). Now, exploring parallels between the semiclassical approach and the mean-field approximation one can pose the natural question: what changes occur in a many-body system when a control parameter crosses an instability (e.g. bifurcation) point of the limiting mean-field system?

In the present Letter we give a partial answer showing that one of the possible scenarios is the quantum phase transition of the second type, associated with the switching of the wave-function in the Fock space between the “coherent” and “Bogoliubov” states possessing distinct features. Considering a flexible (time-dependent) control parameter, we have also found a strong sensitivity of the system to the parity of the total number of atoms $N$, showing parity-dependent structure of the energy levels and the macroscopically different dynamics for different parity of $N$. Observation of the discussed phenomena is feasible in the experimental setting available nowadays.

Quantum and mean-field models.- We consider the nonlinearity-induced intra-band tunneling of BEC between the two high-symmetry $X$-points of a two-dimensional square optical lattice (OL). The process is described by the two mode boson Hamiltonian (see for the details)

$$\hat{H} = \frac{1}{2N^2} \left\{ n_1^2 + n_2^2 + \Lambda \left[ 4n_1n_2 + (b_1^\dagger b_2)^2 + (b_2^\dagger b_1)^2 \right] \right\},$$

(1)

where $b_j$ and $b_j^\dagger$ are the annihilation and creation operators of the two $X$-states, $\Lambda (0 \leq \Lambda \leq 1)$ is the lattice parameter easily controllable by variation of the lattice depth (or period). The Schrödinger equation for the BEC in a state $|\Psi\rangle$ reads $i\hbar \partial_t |\Psi\rangle = \hat{H} |\Psi\rangle$, where $\hbar = 2/N$ and $\tau = (2g\rho/\hbar)t$, with $g = 4\pi\hbar^2a_s/m$. 

and the atomic density $\rho$. The link with the semiclassical limit is evident for the Hamiltonian in the form (1): the Schrödinger equation written in the Fock basis, $|k, N - k\rangle = \frac{b_k^\dagger b_{N-k}^\dagger}{\sqrt{k!(N-k)!}} |0\rangle$, depends only on the relative populations $k/N$ and $(N-k)/N$, while $h$ serves as an effective “Planck constant”.

Hamiltonian (1) represents a nonlinear version of the well-known boson-Josephson model (see, e.g. [9, 11]), where unlike in the previously studied models the states are coupled by the exchange of pairs of atoms. This is a fairly common situation for systems with four-wave-mixing, provided by the two-body interactions involving four bosons. The exchange of the bosons by pairs results in the coupling of the states with the same parity of the population and is reflected in the double degeneracy of all $(N + 1)/2$ energy levels for odd $N$, due to the symmetry relation $\langle 2k, N - 2k | \Psi_1 \rangle = \langle N - 2k, 2k | \Psi_2 \rangle$. For even $N$ the energy levels show quasi degeneracy (see below).

The mean-field limit of the system (1) can be formally obtained by replacing the boson operators $b_j$ in (1) by the c-numbers $b_1 \rightarrow \sqrt{N}e^{i\phi}/4$ and $b_2 \rightarrow \sqrt{N}(1 - x)e^{-i\phi}/4$, what gives the classical Hamiltonian [6]

$$\mathcal{H} = x(1 - x)[2\Lambda - 1 + \Lambda \cos \phi] + \frac{1}{2} \mathcal{H}_0$$

where $x = \langle a_1^\dagger a_1 \rangle/N$ is the population density and $\phi = \arg \langle b_1^\dagger b_2^\dagger b_2 b_1 \rangle$ is the relative phase. $\mathcal{H}$ possesses two stationary points describing equally populated $X$-states: the classical energy maximum $P_1 = (x = 1/2, \phi = 0)$ and minimum $P_2 = (x = 1/2, \phi = \pi)$. $P_1$ is dynamically stable in the domain $\Lambda > \Lambda_c = \frac{1}{4}$. For $\Lambda < \Lambda_c$ it looses its stability, and another set of stationary points $x = 1$ ($S_1$) and $x = 0$ ($S_2$) appears, which is a fairly general situation in nonlinear boson models. The appearing solutions describe the symmetry breaking leading to selftrapping.

Energy levels near the critical point.- To describe the spectrum of the Hamiltonian (1) in the vicinity of the critical value $\Lambda_c$ we rewrite $\mathcal{H}$ in terms of the operators $a_{1,2} = (b_1 \mp ib_2)/\sqrt{2}$

$$\mathcal{H} = \mathcal{H}_0 + \left(1 - \frac{\Lambda}{\Lambda_c}\right)\mathcal{V} + \mathcal{E}(\Lambda), \quad \mathcal{E}(\Lambda) = \frac{\Lambda + 1}{4} + \frac{\Lambda}{2N} \quad (3)$$

where $\mathcal{H}_0 = \Lambda k^2 a_1^\dagger a_1^\dagger a_2 a_2$ and $\mathcal{V} = \frac{1}{4N} \left(a_1^\dagger a_2 a_2 + a_2^\dagger a_1 a_1\right)^2$.

At the critical point the energy spectrum is determined by $\mathcal{H}_0$: $E_m = \frac{\Lambda}{N^2} m(N - m) + \mathcal{E}(\Lambda_c)$, where $m$ is the occupation number corresponding to the operator $a_1^\dagger a_1$. The spectrum of $\mathcal{H}_0$ is doubly degenerate (except for the top level for even $N$) due to the symmetry $m \rightarrow N - m$.

The ground state energy is $E_{\min}(\Lambda_c) = E_0 = E_N$, while the top energy level has $m = N/2$ for even $N$ and $m = (N \pm 1)/2$ for odd $N$. Restricting ourselves to even numbers of bosons we get $E_{\max}(\Lambda_c) = \frac{\Lambda}{2N}$.

Now consider small deviations of $\Lambda$ from the bifurcation point $\Lambda_c$. To this end, for a fixed $N$, one can use the basis consisting of the degenerate eigenstates of $\mathcal{H}_0$: $|E_m, j\rangle = (a_1^\dagger)^m(a_3^\dagger)^{N-m}\sqrt{m!(N-m)!}|0\rangle$, $j = 1, 2, m = 0, ..., \frac{N}{2}$.

The conditions for $\mathcal{V}$ to be treated as a perturbation depend on $m$ as is seen from the diagonal matrix elements:

$$\langle E_m, j | \mathcal{V} | E_m, j \rangle = \frac{1}{4N} + \frac{m}{2N} \left(1 - \frac{m}{N}\right). \quad (4)$$

At the lower levels ($m \ll N/2$) the energy gaps between the degenerate subspaces and the perturbation both scale as $\Delta E \sim N^{-1}$, hence the condition of applicability is $|\Lambda - \Lambda_c| \ll 1$ and the lower energy subspaces acquire simple shifts. At the upper energy levels ($m \sim N/2$) the above energy gaps behave as $\Delta E \sim N^{-2}$. Since $\langle \mathcal{V} \rangle \sim 1$ in this case, the perturbation theory is applicable only in an interval of $\Lambda$ on the order of $N^{-2}$. There is a dramatic transition in the energy levels, e.g. Fig. 1(b) shows the exchange of the double degeneracy of the top levels for even $N$ in this $N^{-2}$-small interval of $\Lambda$. By considering the phase of

$$\langle E_m, j | (b_2^\dagger b_1^\dagger)^2 | E_m, j \rangle = -\frac{N^2}{4} + \frac{N}{4} + \frac{3}{2} m(N - m), \quad (5)$$

it is easy to verify that the upper and lower eigenstates correspond, respectively, to the mean-field stationary points $P_1$ ($\phi = 0$) and $P_2$ ($\phi = \pi$).

FIG. 1: (a) The energy levels of $\mathcal{H}$ for $N = 200$ and (b) a detailed picture in the vicinity of $\Lambda_c$. The classical energy lines of the mean-field fixed points $P_1$ and $S_2$ are visibly formed. The top energy levels for sufficiently large $|\Lambda - \Lambda_c|$ are quasi-degenerate with the inter-level distances indistinguishable on the scale of the figure (see the discussion in the text below).

Spectrum in the limit $N \rightarrow \infty$. Coherent states and selftrapping states. - For $\Lambda_c^+ - \Lambda_c^- \gg N^{-2}$ the quantum states corresponding to $P_1$ can be obtained by quantizing the local classical Hamiltonian (2), i.e. by expanding it with respect to $x - 1/2$ and $\phi$ and setting $\phi = -ih\frac{\Lambda}{2N}$ (see also Ref. [12]; on this way one looses the term of order
The “wave function” $\psi(x) = \sqrt{N}C_k = \sqrt{N}\langle k, N-k|\psi \rangle$ satisfies

$$\left[ \frac{\hbar^2}{8} \frac{\partial^2}{\partial x^2} + (3\Lambda - 1) \left( \frac{1}{4} - \left( x - \frac{1}{2} \right)^2 \right) \right] \psi = E \psi. \quad (6)$$

Eq. (6) is the negative mass quantum oscillator problem with the frequency $\omega^2 = 8 \left( 3 - \frac{1}{x} \right)$. The respective descending energy levels read $E^{\text{(top)}}_n = E_{\text{max}} + \frac{1}{2} \left( \Lambda - 1 \right) - \frac{\hbar \omega}{2} \left( n + \frac{1}{2} \right)$. The eigenfunctions are localized in the Fock space, e.g. the $n = 0$ eigenfunction is $\psi_0(x) = C \exp \left[ -\frac{\hbar \omega}{2x} \left( x - \frac{1}{2} \right)^2 \right]$. In the original discrete variable $x = k/N$, there are even and odd eigenstates $C_{2k}$ and $C_{2k-1}$ related by the approximate symmetry $C_n \approx C_{n+1}$, hence the energy levels are quasi doubly degenerate [c.f. Fig. 1(b)].

The local approximation becomes invalid as $\Lambda^{-1} - \Lambda^{-1} \sim N^{-2}$ (the wave-function delocalizes). The other set of the stationary points, $S_{1,2}$, becomes stable for $\Lambda < \Lambda_c$ in the mean-field limit. In this case, however, the phase $\phi$ is undefined. Let us first consider the full quantum case, for example, the limit $\langle n_1 \rangle \ll N$ (i.e. the point $S_2$). The resulting reduced Hamiltonian can be either easily derived in the Fock basis or obtained by formally setting $b_2 = N$ and retaining the lowest-order terms in $b_1$ and $b_1^\dagger$.

$$\hat{H} \approx \hat{H}_{S_2} = \frac{1}{2} + \frac{2(\Lambda - 1)}{N} b_1^\dagger b_1 + \frac{\Lambda}{2N} (b_1^2 + b_1^2). \quad (7)$$

Hamiltonian (7) can be diagonalized by the Bogoliubov transformation $c = \cosh(\theta) b_1 - \sinh(\theta) b_1^\dagger$, where $\theta = \theta(\Lambda) > 0$ is determined from $\tanh(2\theta) = \Lambda/(1 - 2\Lambda)$. We get

$$\begin{equation}
\hat{H}_{S_2} = -\frac{\Lambda}{N \sinh(2\theta)} c^\dagger c + \frac{\Lambda \tanh \theta}{2N} + 1/2. \quad (8)
\end{equation}$$

Thus $c^\dagger c$ gives the number of negative-energy quasiparticles over the Bogoliubov (squeezed) vacuum solving $c|\text{vac} \rangle = 0$. In the atom-number basis $|\text{vac} \rangle$ is a superposition of the Fock states with $C^{\text{(vac)}}_{2k} = \tanh(k\theta)\sqrt{(2k)!/(2^kk!)} C_0$ and $C^{\text{(vac)}}_{2k-1} = 0$, ($C_0$ is a normalization constant).

The validity condition of the approximation (7), given by $\langle \hat{n} \rangle, \Delta n \ll N$, can be rewritten in the form $\tanh^{-2}(2\theta) \gg 1 + N^{-2}$, what is the same as $\Lambda^{-1} - \Lambda^{-1} \gg N^{-2}$. In this case, the eigenstates of (7) are well-localized in the atom-number Fock space, i.e. the coefficients $C_{2k}$ decay fast enough. The condition for this excludes the same small interval as in the perturbation theory, hence the transition between the coherent states and the selftrapping (Bogoliubov) states occurs on the interval of $\Lambda$ of order of $N^{-2}$. The convergence of the eigenstates of $\hat{H}_{S_2}$ to that of the full Hamiltonian (11) turns out to be remarkably fast as it is shown in Fig. 2(a). In Fig. 2(b) the dramatic deformation of the top energy eigenstate of $\hat{H}$ (corresponding to the $S_2$-$P_1$ transition) about the critical $\Lambda_c$ is shown. Finally, we note that for even $N$ the quasi double degeneracy of the energy levels for $\Lambda^{-1} - \Lambda^{-1} \gg N^{-2}$ (c.f. Fig. 1(b)) is due to the exchange symmetry between $S_1$ and $S_2$ resulting in equal energy levels of the Hamiltonians $\hat{H}_{S_1}$ and $\hat{H}_{S_2}$.

In the mean-field description of the stationary point $S_2$ the associated Hamiltonian is defined by replacing the boson operators in Eq. (7) by the c-numbers $b_1 = \sqrt{N}\alpha$ and $b_2 = \sqrt{N}\beta$. Using $|\alpha|^2 + |\beta|^2 = 1$ and fixing the irrelevant common phase by setting $\beta$ real we get the dynamical variables $\alpha$ and $\alpha^*$ and the classical Hamiltonian in the form $H_{S_2} = \frac{1}{2} + \frac{2}{2N} (1 + |\alpha|^2)(2(2\Lambda - 1)|\alpha|^2 + \Lambda|\alpha|^2 + (\alpha^*)^2)$, from which the stability of the point $S_2$ ($\alpha = 0$) for $\Lambda < \Lambda_c$ follows.

Thus, the passage through the bifurcation point $\Lambda_c$ of the mean-field model, corresponds to the phase transition in the quantum many-body system on an interval of the control parameter scaling as $N^{-2}$ and reflected in the deformation of the spectrum and dramatic change of the system wave-function in the Fock space. The described change of the system is related to the change of the symmetry of the atomic distribution, and thus it is the second order phase transition.

In our case this scenario corresponds to loss of stability of the selftrapping solutions $S_1$ and $S_2$ and appearance of the stable stationary point $P_1$. In the quantum description this happens by a set of avoided crossings of the top energy levels (and splitting of the quasi-degenerate energy levels for even $N$) as the parameter $\Lambda$ sweeps the small interval on the order of $N^{-2}$ about the critical value $\Lambda_c$ (see Fig. 11). For lower energy levels the avoided crossings appear along the two straight lines approximating the classical energies of the two involved stationary points: $H(P_1) = \frac{1}{2} + \frac{(3\Lambda - 1)}{4}$ (for $\Lambda < \Lambda_c$) and $E_{\text{max}} = \frac{1}{2}$ ($\Lambda > \Lambda_c$), see Fig. 11.
Dynamics of the phase transition.- Let us see how the quantum phase transition shows up in the system dynamics when \( \Lambda \) is time-dependent. The selftrapping states \( S_1 \) and \( S_2 \), eigenstates of the Hamiltonian (1), correspond to occupation of just one of the \( X \)-points. Such an initial condition can be experimentally created by switching on a moving lattice with \( \Lambda < \Lambda_c \) (see e.g. [3]). As the lattice parameter \( \Lambda(\tau) \) passes the critical value from below, the selftrapping states are replaced by the coherent states with comparable average occupations of the two \( X \)-points.

A more intriguing dynamics is observed when \( \Lambda(\tau) \) is a smooth step-like function between \( \Lambda_1 \) and \( \Lambda_2 \) such that \( \Lambda_1 < \Lambda_c < \Lambda_2 \). In this case, the system dynamics and the emerging states dramatically depend also on parity of the number of atoms. For fixed \( \Lambda_1, \Lambda_2 \) the system behavior crucially depends on the time that \( \Lambda(\tau) \) spends above \( \Lambda_c \). More specifically, one can identify two distinct scenarios, which can be described as a switching dynamics between the selftrapping states at the two \( X \)-points, Fig. 3(a),(b) or dynamic creation of the superposition of macroscopically distinct states, well approximated by

\[
\sum_{k,N} (C_k|k,N-k\rangle + C_{N-k}|N-k,k\rangle)
\]

with a small \( k_m/N \), Fig. 3(c),(d) (where \( k_m/N \approx 0.2 \)). In the case of macroscopic superposition the dynamics shows anomalous dependence on parity of \( N \), i.e. showing the same behavior for large \( N \) of the same parity but macroscopically distinct behavior for \( N \) and \( N+1 \), Fig. 3(c).

Note that the mean-field dynamics is close to the quantum one in the switching case, Fig. 3(a), while it is dramatically different in the superposition case, Fig. 3(c).

To estimate the physical time scale, \( t \equiv t_{ph}\tau = \frac{md^2\tau}{8\pi\hbar a_sN_{pc}} \), we assume that a condensate of \(^{87}\text{Rb} \) atoms is loaded in a square lattice with the mean density of \( N_{pc} = 20 \) atoms per cite. If the lattice constant \( d = 2 \mu m \) and the oscillator length of the tight transverse trap (to assure the two-dimensional approximation) \( \ell_t = 0.1 \mu m \), then \( t_{ph} \sim 0.2 \) ms and the time necessary for the creation of the macroscopic superposition of Fig. 3(c),(d) is about 20 ms.

Conclusion.- We have shown that behind the mean-field instability in the intra-band tunneling of BEC in an optical lattice is a quantum phase transition between macroscopically distinct states, giving a macroscopic magnification of the microscopic quantum features of the system. A spectacular demonstration of this is the dynamic formation of the superposition of macroscopically distinct states, which, besides being responsible for the difference between the mean-field and quantum dynamics (see also recent Ref. [13]), shows also an anomalous dependence on parity of BEC atoms reflecting distinct energy level structure for even and odd number of atoms.

The work of VSS was supported by the FAPESP of Brazil.

![FIG. 3: (Color online) The average population densities \( \langle n_1 \rangle/N \), (a) and (c), and the atom-number probabilities \( C_k^2 \), (b) and (d), for \( \Lambda(\tau) = \Lambda_1 + (\Lambda_2 - \Lambda_1) \left[ \tanh (\tau - \tau_1) - \tanh (\tau - \tau_2) \right] / 2 \). The corresponding classical dynamics is shown by the dash-dot lines in (a) and (c). Here \( \Lambda_1 = 0.25 < \Lambda_c \), \( \Lambda_2 = 0.5 > \Lambda_c \), \( \tau_1 = 50 \) and \( \tau_2 = 85 \) (a) with \( N = 500 \) and 501 (indistinguishable), while in (c) \( \tau_2 = 135 \) with \( N = 500 \) and 400 (the upper solid and dashed lines) and \( N = 501 \) and 401 (the lower lines). The initial state is \( |\text{vac}\rangle \) of \( H_{S_1} \), but using \( |N,0\rangle \) gives a similar picture.](image-url)