Quantum Switching at a Mean-Field Instability of a Bose-Einstein Condensate in an Optical Lattice

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It is shown that bifurcation of the mean-field dynamics of a Bose-Einstein condensate can be related to the quantum phase transition of the original many-body system. As an example we explore the intraband 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 self-trapping states or from a self-trapping state to a superposition of the macroscopically populated self-trapping states with a steplike 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.

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Introduction.—Since the very beginning of quantum mechanics its relation to classical dynamics constitutes one of the central questions of the theory. The dependence of the energy levels distribution on the type of dynamics of the corresponding classical system [1], in general, and the quantum system response to variation of the bifurcation parameters controlling the qualitative changes of the classical behavior [2] are among the major issues [3]. 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 [4], 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 [5]. More recently, it was shown [6,7] 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 [8], emergent for the coefficients of the wave-function 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 [9], 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 self-trapping [10]). 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 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 number of BEC 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 intraband tunneling of BEC between two high-symmetry X points of the same band of a square optical lattice (OL). The process is described by the two-mode boson Hamiltonian (see [6] for the details)

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

where b_j and $b_j^\dagger$ are the annihilation and creation operators of the two X states, Λ ($0 \le \Lambda \le 1$) is the lattice parameter, easily controllable by variation of the lattice depth (or period). The Schrödinger equation for BEC in a state $|\Psi\rangle$ reads $ih\partial_\tau|\Psi\rangle = \hat{H}|\Psi\rangle$, where $h = 2/N$ and $\tau = (2g\rho/\hbar)t$, with $g = 4\pi\hbar^2 a_s/m$ and the atomic density ρ. The link with the semiclassical limit is evident for the

Hamiltonian in the form (1): the Schrödinger equation written in the Fock basis, $|k, N-k\rangle = \frac{(b_1^\dagger)^k (b_2^\dagger)^{N-k}}{\sqrt{k!(N-k)!}}|0\rangle$, 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 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 $2k \to N-2k$ (relating different sets of values for odd N). For even N the energy levels show quasidegeneracy (see below).

The mean-field limit of Hamiltonian (1) can be formally obtained by replacing the boson operators b_j in (1) by the c numbers $b_1 \to \sqrt{Nx}e^{i\phi/4}$ and $b_2 \to \sqrt{N(1-x)}e^{-i\phi/4}$. We get [6]

$$\mathcal{H} = x(1-x)[2\Lambda - 1 + \Lambda\cos\phi] + \tfrac{1}{2}, \qquad (2)$$

where $x = \langle n_1\rangle/N$ is the population density and $\phi = \arg\langle (b_2^\dagger)^2 b_1^2\rangle$ is the relative phase. $\mathcal{H}$ possesses two stationary points corresponding to equally populated X states: the classical energy maximum $P_1 = (x=\frac{1}{2}, \phi = 0)$ and minimum $P_2 = (x = \frac{1}{2}, \phi = \pi)$. P_1 is dynamically stable in the domain $\Lambda > \Lambda_c = \frac{1}{3}$. 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 self-trapping.

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

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

where $\hat{H}_0 = \frac{2\Lambda}{N^2} a_1^\dagger a_1 a_2^\dagger a_2$ and $\hat{V} = \frac{1}{4N^2}(a_1^\dagger a_2 + a_2^\dagger a_1)^2$. At the critical point the energy spectrum is determined by $\hat{H}_0$: $E_m = \frac{2\Lambda_c}{N^2} m(N-m) + \mathcal{E}(\Lambda_c)$, where m is the occupation number corresponding to the operator $a_1^\dagger a_1$. The spectrum of $\hat{H}_0$ is doubly degenerate (except for the top level for even N) due to the symmetry $m \to N-m$. The ground state energy is $\mathcal{E}_{\min}(\Lambda_c) = E_0 = E_N$, 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 number of bosons we get $\mathcal{E}_{\max}(\Lambda_c) = \frac{1}{2} + \frac{\Lambda_c}{2N}$.

Now consider small deviations of Λ from the bifurcation point Λ_c. To this end, for a fixed N, one can use the basis consisting of the degenerate eigenstates of $\hat{H}_0$: $|E_m, j\rangle = \frac{(a_j^\dagger)^m (a_{3-j}^\dagger)^{N-m}}{\sqrt{m!(N-m)!}}|0\rangle$, $j = 1, 2$, $m = 0, \ldots, \frac{N}{2}$. The conditions for $\hat{V}$ to be treated as a perturbation depend on m as is seen from the diagonal matrix elements:

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

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 of the perturbation theory 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 $\langle \hat{V}\rangle \sim 1$ in this case, the perturbation theory is applicable only in a very small interval of Λ 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 Λ. By considering the phase of

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

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 ($\phi = \pi$).

Spectrum in the limit $N \to \infty$. Coherent states and self-trapping states.—For $\Lambda_c^{-1} - \Lambda^{-1} \gg N^{-2}$ 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 ϕ and setting $\phi = -ih\frac{\partial}{\partial x}$ (see also Ref. [12]; in this way one loses the term of order $1/N$

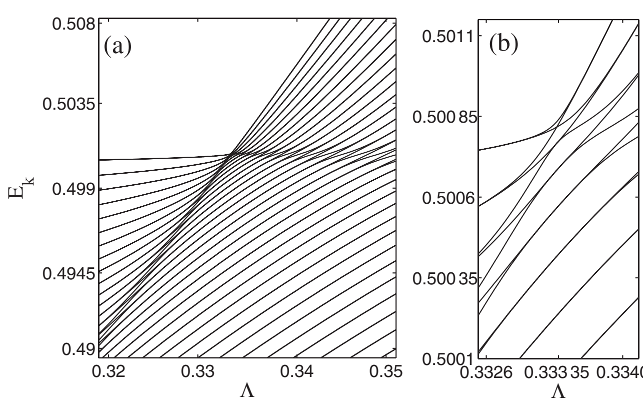

FIG. 1. (a) The energy levels of $\hat{H}$ for $N = 200$ and (b) a detailed picture in the vicinity of Λ_c. The classical energy lines of the mean-field fixed points P_1 and S_2 are visibly formed. The top energy levels for sufficiently large $|\Lambda - \Lambda_c|$ are quasidegenerate with the interlevel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

in $\mathcal{E}_{\max}$). The "wave function" $\psi(x) = \sqrt{N} C_k \equiv \sqrt{N}\langle k, N-k|\psi\rangle$ satisfies

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

Equation (6) is the negative mass quantum oscillator problem with the frequency $\omega^2 = 8(3 - \frac{1}{\Lambda})$. Hence, the descending energy levels read $E_{(N/2)-n} = \mathcal{E}_{\max} + \frac{1}{4}(\frac{\Lambda}{\Lambda_c} - 1) - \frac{h\Lambda\omega}{4}(n + \frac{1}{2})$. The eigenfunctions are localized in the Fock space, e.g., the $n = 0$ eigenfunction is $\psi_0(x) = C\exp[-\frac{\omega}{2h}(x - \frac{1}{2})^2]$. In the original discrete variable $k = Nx$, there are even and odd eigenstates C_{2k} and C_{2k-1} related by the approximate symmetry $C_l \approx C_{l+1}$; hence, the energy levels are quasi doubly degenerate [cf. Fig. 1(b)].

The local approximation becomes invalid as $\Lambda_c^{-1} - \Lambda^{-1} \sim N^{-2}$ (the wave function delocalizes). Two other stationary points ($S_{1,2}$) corresponding to $x = 1$ and $x = 0$ become stable for $\Lambda < \Lambda_c$ in the mean-field limit. In this case, however, the phase ϕ is undefined. Let us first consider the full quantum case, for example, when $\langle n_1\rangle \ll N$ (point S_2). The resulting reduced Hamiltonian can be either derived in the Fock basis or obtained by formally setting $b_2 = N$ and retaining the lowest-order terms in b_1 and $b_1^\dagger$:

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

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

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

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 $C_{2k}^{(\text{vac})} = \tanh^k(\theta) \times \sqrt{(2k)!}/(2^k k!) C_0$ and $C_{2k-1}^{(\text{vac})} = 0$ (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 $\Lambda^{-1} - \Lambda_c^{-1} \gg N^{-2}$. 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 self-trapping (Bogoliubov) states occurs on the interval of Λ of order of N^{-2}. The convergence of the eigenstates of $\hat{H}_{S_2}$ to that of the full Hamiltonian (1) 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 Λ_c is shown. Finally, we note that for even N the quasi double degeneracy of the energy levels for $\Lambda^{-1} - \Lambda_c^{-1} \gg N^{-2}$ [cf. Fig. 1(b)] is due to equal energy levels of the Hamiltonians $\hat{H}_{S_2}$ and $\hat{H}_{S_1}$ and the sharp localization of their eigenstates at the points $k = 0$ and $k = N$.

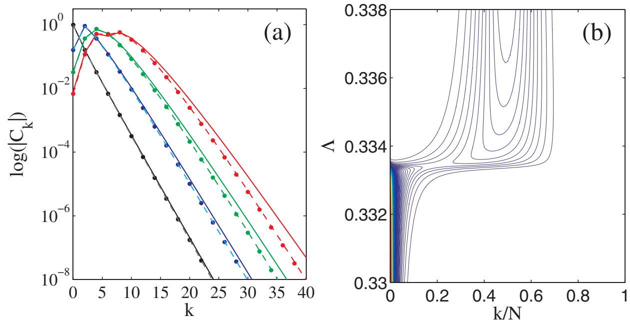

FIG. 2 (color online). (a) Convergence of the four upper eigenstates of the Hamiltonian (1) to the eigenstates of $\hat{H}_{S_2}$ (shown by dots) for $N = 100$ (solid lines) and $N = 1000$ (dashed lines), for $\Lambda = \Lambda_c - 0.1$. (b) The contour plot of the state corresponding to the top energy level in the vicinity of Λ_c for $N = 200$.

The associated mean-field Hamiltonian for description of the stationary points $S_{1,2}$ is defined by replacing the boson operators in Eq. (1) by c numbers $b_1 = \sqrt{N}\alpha$ and $b_2 = \sqrt{N}\beta$. For S_2, using $|\alpha|^2 + |\beta|^2 = 1$ and fixing the irrelevant common phase by setting β real we get the dynamical variables α and α^* and the classical Hamiltonian in the form $\mathcal{H} = \frac{1}{2} + \frac{1}{2}(1 - |\alpha|^2) \times \{2(2\Lambda - 1)|\alpha|^2 + \Lambda[\alpha^2 + (\alpha^*)^2]\}$, from which the dynamic stability for $\Lambda < \Lambda_c$ of the point S_2 ($\alpha = 0$) follows.

Thus, the passage through the bifurcation point Λ_c of the two-mode mean-field model, corresponds to the phase transition in the quantum N-boson 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 self-trapping 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 quasidegenerate energy levels for even N) as the parameter Λ sweeps the small interval on the order of N^{-2} about the critical value Λ_c (see Fig. 1). For lower energy levels the avoided crossings appear along the two straight lines approximating the classical energies of the two involved stationary points: $\mathcal{H}(P_1) = \frac{1}{2} + \frac{(3\Lambda - 1)}{4}$ (for $\Lambda < \Lambda_c$) and $\mathcal{H}(S_{1,2}) = \frac{1}{2}$ ($\Lambda > \Lambda_c$), see Fig. 1.

Dynamics of the phase transition.—Let us see how the quantum phase transition shows up in the system dynamics when Λ is time dependent. The self-trapping states at $S_{1,2}$ are eigenstates of Hamiltonian (1) correspond to occupa-

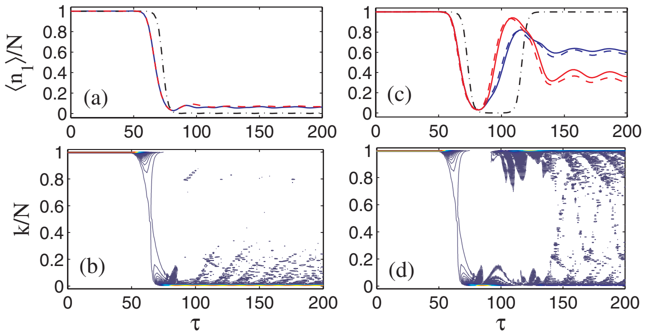

FIG. 3 (color online). The average population densities $\langle n_1 \rangle / N$, (a) and (c), and the atom-number probabilities $|C_k|^2$, (b) and (d), for $\Lambda(\tau) = \Lambda_1 + (\Lambda_2 - \Lambda_1)[\tanh(\tau - \tau_1) - \tanh(\tau - \tau_2)]/2$. The corresponding classical dynamics is shown by the dash-dot lines in (a) and (c). Here $\Lambda_1 = 0.25 < \Lambda_{\rm cr}$, $\Lambda_2 = 0.5 > \Lambda_{\rm cr}$, $\tau_1 = 50$ 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 $|{\rm vac}\rangle$ of H_{S_1}, but using $|N, 0\rangle$ gives a similar picture.

tion 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., [7]). As the lattice parameter $\Lambda(\tau)$ passes the critical value from below, the self-trapping states are replaced by the coherent states with comparable average occupations of the two X points.

A more rich dynamics is observed when $\Lambda(\tau)$ is a smooth steplike function between Λ_1 and Λ_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 $\Lambda_{1,2}$ the system behavior crucially depends on the time that $\Lambda(\tau)$ spends above Λ_c. More specifically, one can identify two distinct scenarios, which can be described as a switching dynamics between the self-trapping states at the two X points, Figs. 3(a) and 3(b) or a dynamic creation of the superposition of macroscopically distinct states, well approximated by the expression $\sum_{k<k_m}(C_k|k, N-k\rangle + C_{N-k}|N-k, k\rangle)$ with a small k_m/N, Figs. 3(c) and 3(d) (where $k_m/N \approx 0.2$). In the macroscopic superposition case 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, $t \equiv t_{\rm ph}\tau = \frac{md^2\ell_\perp}{8\pi\hbar a_s \mathcal{N}_{\rm pc}}\tau$, we assume that a condensate of ^{87}Rb atoms is loaded in a square lattice with the mean density of $\mathcal{N}_{\rm pc} = 20$ 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) is $\ell_\perp = 0.1\ \mu$m, then $t_{\rm ph} \sim 0.2$ ms and the time necessary for the creation of the macroscopic superposition of Figs. 3(c) and 3(d) is about 20 ms.

Conclusion.—We have shown that behind the mean-field instability in the intraband tunneling of BEC in a square 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 self-trapping 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.

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