Quantum Fluctuation Driven First-order Phase Transitions in Optical Lattices

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We study quantum fluctuation driven first-order phase transitions of a two-species bosonic system in a three-dimensional optical lattice. Using effective potential method we find that the superfluid-Mott insulator phase transition of one type of bosons can be changed from second-order to first-order by the quantum fluctuations of the other type of bosons. The study of the scaling behaviors near the quantum critical point shows that the first-order phase transition has a different universality from the second-order one. We also discuss the observation of this exotic phenomenon in the realistic cold-atom experiments.

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Introduction.—Near quantum critical points (QCPs) the quantum fluctuations play an important role and control various intriguing properties of the physics. Of particular interest is the effect of quantum fluctuation driven first-order phase transitions. The QCPs may become unstable in the appearance of competing orders. The nature of the phase transition can be changed from second to first-order by the quantum fluctuations. This phenomenon was first discussed by S. Coleman and E. Weinberg \cite{1}. They investigated a theory of a massless charged meson coupled to the electrodynamic field using effective potential method. Starting from a model without symmetry breaking at tree level they found that the one-loop effective potential indicated that a new energy minimum was developed away from the origin. Independently, Halperin, Lubensky, and Ma \cite{2} discovered the same phenomenon in the Ginzburg-Landau theory of superconductor to normal metal transition and showed that the fluctuations of the electromagnetic field induce a first-order transition. Recently, there have appeared more examples of the nature of the quantum phase transition is predicted to become discontinuous as the QCP is approached \cite{3,4}. For instance, the quantum fluctuations may give rise to a first-order phase transition in a heavy-fermion metal near the metallic antiferromagnetic QCP \cite{4}.

The flexible control of cold atoms and the lattice potential provide exquisite tools to study quantum phase transitions and quantum criticality. One celebrated example is the paradigmatic superfluid to Mott insulator transition in an optical lattice \cite{10,12}, which confirmed the predictions of the Bose-Hubbard model \cite{13,14}. Multi-component bosonic systems have also been studied both experimentally \cite{15,18} and theoretically \cite{19,26}. With multi-species, the zero-temperature diagrams of quantum phases are much richer than the simple duplication of the single species. Recently, the researches of quantum criticality in cold-atom systems have attracted a great deal of interest. Several schemes were proposed to determine the critical properties by extracting the universal scaling functions from the atomic density profiles \cite{27,29}. The experimental observations of quantum critical behavior of ultracold atoms have also been reported \cite{30,31}. As a clean and highly controllable system, cold atoms can be a good play ground to study various quantum critical behaviors.

In this letter we investigate the quantum fluctuation driven first-order phase transitions of a two-species boson system in a three dimensional optical lattice. The effective potential method \cite{1} developed in quantum field theory is implemented to calculate the quantum corrections to the classical action up to one-loop level. We find that with the quantum fluctuation taken into account a first-order phase transition is encountered as one approaches to the QCP. To our knowledge, this phenomenon and universality have not be sufficiently explored in condensed matter physics. We study the scaling behaviors near the first-order phase transition and give a feasible proposal to observe this phenomenon in cold-atom systems.

Two-species Bose-Hubbard model and the Coleman-Weinberg effective potential.— To describe Bose-Bose mixtures loaded into optical lattices, we consider the following two-species Bose-Hubbard Hamiltonian,

\[ H = - \sum_{\alpha, <ij>} t_{\alpha} (\hat{b}_{\alpha i}^{\dagger} \hat{b}_{\alpha j} + \hat{b}_{\alpha j}^{\dagger} \hat{b}_{\alpha i}) - \sum_{\alpha,i} \mu_{\alpha} \hat{n}_{\alpha i} + \sum_{\alpha,i} U_{\alpha} \hat{n}_{\alpha i} (\hat{n}_{\alpha i} - 1) + U_{AB} \sum_{i=1}^{N} \hat{n}_{1i} \hat{n}_{2i}. \] (1)

Here \( b_{\alpha i}^{\dagger} \) creates a boson of sort \( \alpha = A, B \) at site \( i \). The first term in the Hamiltonian represents the hopping of bosons of types \( A \) and \( B \) between the nearest-neighbor pairs of sites \( <ij> \) with hopping amplitudes \( t_{A} \) and \( t_{B} \). \( \hat{n}_{\alpha i} \equiv b_{\alpha i}^{\dagger} b_{\alpha i} \) is the number operator of the \( \alpha \) type boson at the site \( i \). We have two chemical potential \( \mu_{A} \) and \( \mu_{B} \) to fix the total number of type \( A \) and \( B \) bosons. \( U_{\alpha} \) and \( U_{AB} \) denote the intra- and inter-species on-site interaction strengths.
The mean-field analysis shows that the system has three different phases [21]: (I) both species A and B stay in the superfluid phases; (II) one species is in the superfluid phase and the other one is in the Mott insulator phase; and (III) both species are in the Mott insulator phases. Two examples of the phase diagrams are shown in Fig. 1. To study the quantum fluctuation effects in the vicinity of QCPs we may take the limit of vanishing lattice constant and finally write down a continuum quantum field theory to describe the phase transitions. This can be done by following a standard procedure [32]: (I) writing the partition function in the coherent state path integral representation; (II) decoupling the hoping terms by introducing two auxiliary fields \( \phi_1 \) and \( \phi_2 \) through the Hubbard-Stratonovich transformation; and (III) integrating out the fields \( b_{Ai} \), \( b_{Ai}^\dagger \), \( b_{Bi} \) and \( b_{Bi}^\dagger \). Then the action can be written as

\[
S = \int d^{3}x \left\{ u_1 \phi_1^2 \partial_x \phi_1 + v_1 \partial_x \phi_1^2 + w_1 |\nabla \phi_1|^2 + u_2 \phi_2^2 \partial_x \phi_2 + v_2 \partial_x \phi_2^2 + w_2 |\nabla \phi_2|^2 + r_1 |\phi_1|^2 + r_2 |\phi_2|^2 + g_1 |\phi_1|^4 + g_2 |\phi_2|^4 + g_3 |\phi_1|^2 |\phi_2|^2 \right\}. \tag{2}
\]

The average of the two Hubbard-Stratonovich field \( \phi_1 \) and \( \phi_2 \) are proportional to \( (b_{Ai}(x,r)) \) and \( (b_{Bi}(x,r)) \). Hence, they can be taken as the superfluid order parameters. All the coefficients in Eq. (2) can be expressed in terms of the hopping amplitudes, the chemical potentials, and the on-site interaction strengths. For instance, \( r_1 = \frac{1}{\mu_A - U_A n_{A0}^\dagger n_{B0} + U_A n_{A0} n_{B0}} \) and \( r_2 = \frac{n_{B0}^\dagger}{\mu_A + U_A (n_{A0}^\dagger - 1) + U_A n_{A0} n_{B0}} \).

The equation \( r_1 = 0 \) and \( r_2 = 0 \) generate the mean-field phase boundaries in Fig. 1. Furthermore, the two-species Bose-Hubbard model obeys a \( U(1) \times U(1) \) gauge symmetry, which implies that the model is invariant under the transformation \( b_{\alpha}(\tau) \rightarrow b_{\alpha}(\tau)e^{i\theta_{\alpha}(\tau)} \), \( \phi_{\alpha}(\tau) \rightarrow \phi_{\alpha}(\tau)e^{i\theta_{\alpha}(\tau)} \) and \( \mu_a \rightarrow \mu_a + i\partial_\tau \theta(\tau) \), where \( \alpha = A, B \). This gauge invariance helps to fix the coefficients of the first-order time derivatives \( u_1 \) and \( u_2 \) as \( u_1 = -\frac{1}{t_1} \frac{\partial \mu_A}{\partial t_1} \) and \( u_2 = -\frac{1}{t_2} \frac{\partial \mu_B}{\partial t_2} \) on the mean-field phase boundaries [32]. Hence, at the tips of the insulating lobes coefficients \( u_1 \) and \( u_2 \) vanish. The action of Eq. (2) is deduced to a relativistic theory.

For simplicity we consider the QCPs at the tips of the insulating lobes, where \( r_1 = r_2 = 0 \). The classical potential of this theory is posed right on the edge of the symmetry breaking. We wonder whether the quantum fluctuations will break the symmetry or not. To answer this question we implement the effective potential method [1] to calculate the quantum corrections to the action of Eq. (2). The notion of the effective potential has been found to be very useful in connection with theories exhibiting spontaneously broken symmetry. It allows one to calculate quantum corrections to the classical picture of spontaneous symmetry breaking. Following the general method proposed by Coleman and Weinberg [1] the effective potential of our action up to one-loop level can be calculated as

\[
V_{\text{eff}} = \frac{g_1}{2} |\phi_1|^2 + \frac{g_2}{2} |\phi_2|^2 + g_3 |\phi_1|^2 |\phi_2|^2 + \frac{1}{64\pi^2} \left\{ m_1^2 m_2^2 + m_1^2 m_4^2 + m_2^2 m_4^2 \ln m_2^4 + m_4^4 \ln m_2^2 \right\} + B_1 |\phi_1|^2 + B_2 |\phi_2|^2 + C_1 |\phi_1|^2 + C_2 |\phi_2|^2 + C_3 |\phi_1|^2 |\phi_2|^2 \tag{3}
\]

where \( m_1^2 = \frac{g_1}{2} |\phi_1|^2 + \frac{g_2}{2} |\phi_2|^2 \), \( m_2^2 = |g_2| |\phi_2|^2 + |g_3| |\phi_1|^2 \) and \( m_4^2 = \frac{1}{2} \left( |g_1| + g_2 \right) |\phi_1|^2 + \left( |g_2| + g_3 \right) |\phi_2|^2 \geq \sqrt{|(3g_1 - g_2)| |\phi_1|^2 - (3g_2 - g_3)| |\phi_2|^2 + 16g_5^2 |\phi_1|^2 |\phi_2|^2} \). The terms with coefficients \( B_1 \), \( B_2 \), \( C_1 \) and \( C_3 \) are the renormalization counterterms. They can be fixed by imposing the renormalization conditions \( \frac{\partial V_{\text{eff}}}{\partial \phi_1^2} |_{\phi_1=0,\phi_2=0} = 0 \), \( \frac{\partial V_{\text{eff}}}{\partial \phi_2^2} |_{\phi_1=0,\phi_2=0} = 0 \), \( V_{\text{eff}}(\phi_1 = M, |\phi_2| = 0) = \frac{g_1}{2} M^2 \), \( V_{\text{eff}}(\phi_1 = 0, |\phi_2| = M) = \frac{g_2}{2} M^2 \), \( V_{\text{eff}}(\phi_1 = M, |\phi_2| = M) = \left( \frac{g_1}{2} + \frac{g_2}{2} + g_3 \right) M^4 \), where \( M \) is the renormalization parameter and can be chosen arbitrarily.

The minima of the effective potential actually give the true vacuum states with the quantum fluctuation corrections. Compared with the classical potential where the vacuum is right at the origin, the one-loop effective potential in Eq. (3) exhibits new vacua away from the origin. Hence, the quantum fluctuations indeed induce the breaking of the \( U(1) \times U(1) \) symmetry. This can be shown in the three-dimensional and contour plots of the effective potential in Fig. 2. Without loss of generality we already simplified the effective potential by fixing the complex fields to their real directions so that the effective potential can be easily visualized in Fig. 2. That is, we take \( \phi_1 \rightarrow \phi_{1R} \) and \( \phi_2 \rightarrow \phi_{2R} \), \( \phi_{1R} \) and \( \phi_{2R} \) are real fields. In graph (a) and (b) of Fig. 2 we set the interac-
tion couplings $g_1 = g_2$. For this specific case the vacua are degenerate. New vacua appear in both $\phi_1 \phi_0 = 0$ and $\phi_2 \phi_0 = 0$ direction. The system can break down to any of the vacua. In graph (c) and (d) of Fig. 2 the coupling $g_2$ is stronger than $g_1$. The vacua appear only in $\phi_1 \phi_0 = 0$ direction. Hence, the $U(1) \times U(1)$ symmetry is spontaneously broken to $U(1)$ symmetry by the quantum fluctuations. At the new vacuum the field $\phi_2$ stays in the insulator phase and field $\phi_1$ is in the superfluid phase.

Detailed calculations show that this spontaneous symmetry breaking of $\phi_1$ is actually induced by the quantum fluctuations from the interactions between $\phi_1$ and $\phi_2$. In order to see this we take the direction of $\phi_2 \phi_0 = 0$ in the effective potential to explore the vacuum. Along this direction the effective potential can be reduced to

$$V_{\text{eff}} = g_1/2 (\phi_1^2)^2 + \frac{1}{64\pi^2} g_2^2 (\phi_1^2)^2 \left[ \ln \frac{(\phi_1^2)}{M^2} - 3 \right].$$

The effective potential of Eq. 4 includes a term of $\ln \frac{(\phi_1^2)}{M^2}$. The logarithm of a small number is negative. That is, the one-loop corrections can turn the minimum at the origin into a maximum and cause a new minimum to appear away from the origin. Now the new energy minimum is at $|\phi_1|^2 = \rho^2$, where $\rho^2 \equiv M^2 \exp[3 - \frac{64\pi^2 g_2^2}{2 g_1^2}]$. The new vacuum is illustrated in Fig. 3. As $g_3$ gets stronger the vacuum becomes deeper.

The excitation spectrum around the new vacuum can be calculated by expanding the effective action around the new vacuum of $|\phi_1|^2 = \rho^2$, $|\phi_2|^2 = 0$. Let us write $\phi_1 \rightarrow \rho + \delta \phi_1$, $\phi_2 \rightarrow \delta \phi_2$. Up to the quadratic order of the fields $\delta \phi_1$ and $\delta \phi_2$ a straightforward computation yields $S = \int d^d x \left[ \sqrt{g} \left( \frac{1}{2} (\partial_\mu \delta \phi_1)^2 + (\partial_\mu \delta \phi_2)^2 + (\mathbf{\nabla} \delta \phi_2)^2 - \frac{\delta \phi_2^2}{64 \pi^2 \rho^4} + \frac{3 g_2^2}{64 \pi^2 \rho^2} (\delta \phi_1^2 + \delta \phi_1^2 + 2 \delta \phi_1 \delta \phi_2) + g_3 \delta \phi_1 \delta \phi_2 \right) \right]$. The diagonalization of the mass term of field $\delta \phi_1$ generates two mass eigenvalues $m_1^2 = \frac{3 g_2^2}{32 \pi^2 \rho^2}$ or 0. The massless excitation is the Goldstone mode, which indicates the break down of $U(1)$ symmetry of field $\phi_1$. The field $\delta \phi_2$ has two modes with the same mass $m_2^2 = g_3 \rho^2$.

Nature of the phase transition—We investigate the effective potential with non-zero parameter $r_1$ and $r_2$. For large enough $r_1$ and $r_2$ the vacuum of the effective potential is at the origin. Now we vary the coefficient $r_1$ to study how the vacuum changes. Along the direction of $\phi_2 \phi_0 = 0$ the effective potential is obtained as $V_{\text{eff}} = r_1 |\phi_1|^2 + g_2 (|\phi_1|^2)^4 + \frac{r_2 + g_3 (|\phi_1|^2)^2}{32 \pi^2} \ln(r_2 + g_3 (|\phi_1|^2)^2) - \frac{r_2^2 \ln(r_2 + g_3 (|\phi_1|^2)^2)^2}{32 \pi^2}$. For simplicity we choose $M^2 = (\phi_1^2)^2$, where $(\phi_1^2)$ is the vacuum expectation value of the field $\phi_1$. Using the condition of $\frac{\partial V_{\text{eff}}}{\partial \phi_1} |_{\phi_1 = 0} = 0$ the effective potential can be simplified as

$$V_{\text{eff}} = r_1 (r_1 + r_2) + \frac{(r_2 + g_3 (|\phi_1|^2)^2)^2}{32 \pi^2} \ln(r_2 + g_3 (|\phi_1|^2)^2) - \frac{(r_1 + r_2 + g_3 (|\phi_1|^2)^2)^2}{32 \pi^2} \ln(r_2 + g_3 (|\phi_1|^2)^2) - \frac{(r_2 + g_3 (|\phi_1|^2)^2)^2}{16 \pi^2 (\phi_1^2)^2} \ln(r_2 + g_3 (|\phi_1|^2)^2) - \frac{g_3}{32 \pi^2} (r_2 + g_3 (|\phi_1|^2)^2).$$

As we lower the parameter $r_1$ the vacuum of above effective potential jumps from the origin to a new vacuum at $\phi_1 \phi_0 = (\phi_1^2)$ and $\phi_2 \phi_0 = 0$, where type B bosons stay in the insulator phase and the type A bosons become superfluid. This phase transition occurs at a finite value of $r_1$. The changing of the vacuum is shown in graph (a) of Fig. 4. As $r_1$ approaches to the critical value $r_{1c}$ there is a first-order phase transition, where critical value of $r_1$ is

$$r_{1c} = \frac{1}{16 \pi^2 (\phi_1^2)} \left[ r_2^2 \ln r_2 + \frac{g_3}{32 \pi^2} (r_2 + g_3 (|\phi_1|^2)^2) - \frac{r_2}{16 \pi^2 (\phi_1^2)^2} (r_2 + g_3 (|\phi_1|^2)^2)^2 \ln(r_2 + g_3 (|\phi_1|^2)^2).$$
In graph (b) of Fig. 4 we show the dependence of \( T_{\text{ara}} \) frequencies. With high temperature approximation of the effective potential by sums over the Matsubara first order. \( r_{1c} \) of the first-order phase transition of type A bosons as a function of coefficient \( r_2 \).

In graph (b) of Fig. 4 we show the dependence of \( r_{1c} \) on the parameter \( r_2 \). As \( r_2 \) gets larger the critical value \( r_{1c} \) becomes smaller and even goes to zero, where the second-order phase transition will take place. That is, if the field \( \phi_2 \) is deeply in the insulator phase the first-order phase transition of \( \phi_1 \) can not be induced. This quantum fluctuation driven first-order phase transition can only happen near the QCP with the appearance of competing orders.

At a first-order phase transition certain physical quantities, such as the order parameter and the energy density, have a discontinuous behavior and the correlation lengths remain generally finite. Hence, there is no true critical behavior. However, it turns out to be useful to develop a scaling approach for these transitions \([33,34]\) with scaling exponents such as \( \beta = 0, \alpha = \gamma = 1, \nu = 1/(d + z) \) and \( \delta = \infty \). In our case the effective potential at the metastable minimum \( \phi_1^2(\phi_1) = (\phi_1^2)^2 \) can be written as \( V_{\text{eff}}((\phi_1)) = 1/2(r_1 - r_{1c})^2(\phi_1)^2 \). Introducing a parameter \( \delta = r_1 - r_{1c} \), which measures the distance to the critical value \( r_{1c} \), we have \( V_{\text{eff}} \propto |\delta|^{2-\alpha} \). We can identify that \( \alpha = 1 \), which reflects the nature of the phase transition is first order.

The finite temperature case can be studied through replacing the frequency integrations in the calculation of the effective potential by sums over the Matsubara frequencies. With high temperature approximation \( T \gg r_{1c} \) the effective potential is written as \( V_{\text{eff}} = V_{\text{eff}}(T = 0) - 2^{\frac{d-2}{2}} \frac{T^4}{(T + T_0)^4} + (r_1 - r_{1c})^2(\phi_1^2)^2 + (2g_1 + g_3)\phi_1^2\phi_0^2 \frac{g_3}{g_1} T^2 \), where \( V_{\text{eff}}(T = 0) \) is the effective potential in Eq. (5) and we take \( k_B = 1 \). The first-order phase transition at finite temperature occurs at \( r_1 - r_{1c} = r_{1c} \), where \( r_{1c} \) is the critical value in Eq. (4). Then the critical temperature of the first-order phase transition is \( T_c = \sqrt{\frac{12(r_{1c} - r_1)}{2g_1 + g_3}} \). Furthermore, at high temperature the effective potential can be cast in a scaling form \( V_{\text{eff}} = \frac{1}{2}|\delta|^{2-\alpha}(\phi_1^2)^2(1 - \frac{4\pi T^2}{4g_1^2(\phi_1^2)^2}) = |\delta|^{2-\alpha}F[\frac{T}{T_X}] \), where the crossover line is \( T_X = |\delta|^\nu = |\delta|^{\frac{\nu}{\nu}} \). We can identify that \( \nu = 1/4 \) with \( z = 1 \) in our case. This satisfies the hyperscaling relation \( 2 - \alpha = \nu(d + z) \) and the universality of first-order phase transition, where \( \nu = \frac{1}{2} \) \([34]\). Finite temperature phase diagram is shown in Fig. 5.

**Experimental proposals.**—The study of quantum criticality in cold-atom systems is based on in situ density measurements \([27,24,31]\). General arguments show that the observables obey universal scaling relations near the QCPs. The density can be cast as \( n(\mu, T) - n_c(\mu, T) = T^{\frac{g}{2} - 1} G(\frac{\mu - \mu_c}{T^{\frac{g}{2} - 1}}) \), where \( \mu_c \) is the critical value of the chemical potential, \( n_c \) is the regular part of the density and \( G(x) \) is a universal function describing the singular part of the density. Following the scheme developed by Q. Zhou and T.-L. Ho \([27]\) we can plot the “scaled density” \( A(\mu, T) = T^{\frac{g}{2} - 1} G(\frac{\mu - \mu_c}{T^{\frac{g}{2} - 1}}) \) versus \( (\mu - \mu_c)/T^{1/2} \). The scaled density curves for all temperatures will collapse into a single curve. Here it’s important to notice that our calculation of \( \nu = \frac{1}{4} \) with respect to the argument \( \delta = r_1 - r_{1c} \). However, in the realistic cold-atom experiments we use \( \mu_c - \mu_c \) to measure the distance to the QCP. Hence, a critical exponent \( \tilde{\nu} \) with respect to the argument \( \mu_c - \mu_c \) should be obtained. As we approach the tip of the insulator lob by varying the chemical potential we have \( \delta = r_1 - r_{1c} \sim (\mu_c - \mu_c)^{\frac{1}{2}} \) \([13]\). A straightforward calculation yields \( \tilde{\nu} = 2 \nu = \frac{1}{2} \). Then the scaled density will be in form of \( A(\mu, T) = T^{-2}(n(\mu, T) - n_c) \) near the first-order QCP, where we have \( z = 1, d = 3 \) and \( \tilde{\nu} = \frac{1}{4} \). In order to distinguish this case with the second-order phase transition we also calculate the scaled density near the second-order QCP, which belongs to the three-dimensional XY universality class, where \( z = 1 \) and \( \tilde{\nu} = 1 \) \([13]\). Then the scaled density is \( A(\mu, T) = T^{-2}(n(\mu, T) - n_c) \). By testing which form the measured scaled density obeys we can determine whether the phase transition is first or second order.

**Conclusions**—In summary, we have investigated the quantum fluctuation effects in two-species bosons in a three-dimensional optical lattice. We find that nature of the superfluid-Mott insulator phase transition of one type of bosons can be changed from second-order to first-order
by the quantum fluctuations of the other type of bosons. This novel phenomenon occurs near the QCP with the appearance of competing orders. The scaling behavior of this first-order phase transition was studied and the critical exponents were calculated. Finally, we discussed the observation of this phenomenon in a realistic cold-atom experiment.

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