# Reentrant Phenomenon in the Quantum Phase Transitions of a Gas of Bosons Trapped in an Optical Lattice

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We calculate the location of the quantum phase transitions of a Bose gas trapped in an optical lattice as a function of effective scattering length $a_{\text{eff}}$ and temperature $T$. Knowledge of recent high-loop results on the shift of the critical temperature at weak couplings is used to locate a *nose* in the phase diagram above the free Bose-Einstein critical temperature $T_c^{(0)}$, thus predicting the existence of a reentrant transition *above* $T_c^{(0)}$, where a condensate should form when *increasing* $a_{\text{eff}}$. At zero temperature, the transition to the normal phase produces the experimentally observed Mott insulator.

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Optical lattices offer the intriguing possibility of investigating properties of Bose-Einstein condensates (BECs) at varying effective interaction strengths [1,2]. Because of Bloch's theorem, particles loaded into such lattices behave in some ways like particles in an ordinary continuous space. Thus they may form a BEC condensate in the zero-momentum state in the same way as in the continuum.

Because of the lattice structure, the bosons in an optical lattice exhibit another phase transition which does not exist in the continuum [3]. It produces a state in which the atoms are frozen to their individual optical potential wells on the lattice and require an activation energy to be moved. This state is referred to as a *Mott insulator* due to its analogy to a state described long ago by Mott for fermionic systems [4]. For bosons on a lattice, a Mott insulator is generally expected to exist for integer filling factors at all temperatures if the repulsion between the atoms is larger than $k_BT$ so that the atoms have no place to escape from their optical potential wells.

At very low temperature, the existence of this state has recently been demonstrated by determining the critical effective scattering length [5]. It is generally expected that at zero temperature the Mott transition should coincide with the superfluid-normal transition. At the critical point, the excitation energies of the bosons acquire a gap which pins the atoms to their potential wells. Expressed differently, the Goldstone modes of translations have become massive and the associated phase fluctuations decoherent, in accordance with the criterion found in Ref. [6].

Standard treatments of this situation proceed by analytic or numeric studies of the Bose-Hubbard model [1,2,7,8]. The purpose of this Letter is to simplify the model by focusing the attention upon systems with low density where physics takes place in the lowest energy band. There simple field-theoretic techniques can be applied to calculate the whole quantum phase diagram for the superfluid-normal transition. Our main point will be to include recent high-loop results near $T_c$ of the weakly coupled system to predict an interesting characteristic reentrant transition. In addition we observe that our calculated superfluid-normal transition point at zero temperature agrees with the experimentally observed Mott transition point.

(i) If bosons of mass $M$ are trapped in a three-dimensional cubic periodic potential $V(\mathbf{x})$ of lattice vectors $\boldsymbol{\delta}$, i.e., $V(\mathbf{x}) = V_0 \sum_{i=1}^{3} \sin^2(q_i x_i)$ with $q_i = \pi/\delta$, the wave vector $\mathbf{q}$ defines an energy scale $E_r = \hbar^2\mathbf{q}^2/2M$. If the individual potential wells are deep, i.e., $V_0 \gg E_r$, the single particle Wannier functions $w(\mathbf{x})$ in the nearly harmonic wells are given by oscillator ground-state wave functions at the lattice sites $\boldsymbol{\delta}$ with size $A_0 = \sqrt{\hbar/M\omega_0}$ and energy $\hbar\omega_0 \approx 2E_r(V_0/E_r)^{1/2}$. The lowest energy band arising due to Bloch's theorem reads $\epsilon_B(\mathbf{k}) = 2J\sum_{i=1}^{3}[1-\cos(k_i\delta)]$ up to a trivial additive constant. Here $J$ follows from the tight-binding approximation as $J = \int d^3x w(\mathbf{x})[-\hbar^2\boldsymbol{\nabla}^2/2M + V(\mathbf{x})]w(\mathbf{x}+\boldsymbol{\delta})$ and is equal to $J = 4E_r(V_0/E_r)^{3/4}e^{-2(V_0/E_r)^{1/2}}/\sqrt{\pi}$ [9]. Because of the low density of the system, a repulsive potential $V(\mathbf{x}) = g\delta^{(3)}(\mathbf{x})$ with the coupling constant $g = 4\pi\hbar^2 a/M$ approximates well all relevant spherically symmetric short-range two-particle interactions, where $a$ is the $s$-wave scattering length. In an optical lattice, this gives rise to an effective repulsive $\delta$-function interaction with strength $U \equiv g\int d^3x w^4(\mathbf{x}) = (a/A_0)2\hbar\omega_0/\sqrt{2\pi} = (2\pi a/\lambda) \times \sqrt{8/\pi}E_r(V_0/E_r)^{3/4}$ [2,9]. The importance of the interactions between the particles in the periodic traps is measured by the ratio $\gamma \equiv U/J$ between interaction energy $U = g_{\text{eff}}n$ with $g_{\text{eff}} = 4\pi\hbar^2 a_{\text{eff}}/M_{\text{eff}}$ and kinetic energy $J = \hbar^2 n^{2/3}/2M_{\text{eff}}$, where $n$ is the particle density ($=f/\delta^3$ with filling factor $f$). This leads to $\gamma = 8\pi a_{\text{eff}} n^{1/3}$.

The experimental optical lattice of Ref. [5] is made of laser beams with wavelength $\lambda = 2\delta = 852$ nm and con-

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tains about $2 \times 10^5$ atoms $^{87}$Rb with $a \approx 4.76$ nm [10]. Its energy scale is $E_r \approx \hbar \times 20$ kHz $\approx k_B \times 150$ nK and $V_0/E_r$ is raised from 12 to 22. In this range, $J/E_r$ drops from 0.014 to 0.002, $U/E_r$ increases from 0.36 to 0.57, and $\hbar\omega_0/E_r$ increases from 0.36 to 0.57. Expanding the small-$\mathbf{k}$ behavior of the band energy $\epsilon_B(\mathbf{k})$ as $\hbar^2\mathbf{k}^2/2M_{\rm eff} + \ldots$, the bandwidth $4J$ defines an effective mass $M_{\rm eff}$ of the particles $M_{\rm eff} = \hbar^2/2J\delta^2$. In a typical BEC with $a_{\rm eff}$ of the order of Å and particle distances of a few thousands Å, this ratio is extremely small. For the particles tightly bound in an optical lattice, however, $a_{\rm eff}n^{1/3}$ can be made quite large. In the experiment of Ref. [5], for temperatures near zero we have $\gamma \approx 0.0248 \times \exp(2\sqrt{V_0/E_r})$, so that the increase of the potential depth $V_0/E_r$ from 12 to 22 raises $a_{\rm eff}n^{1/3}$ from 1 to 11.7.

For increasing temperatures, we expect the critical $a_{\rm eff}n^{1/3}$ to decrease until it hits zero as $T$ reaches roughly the free BEC critical temperature $T_c^{(0)} = 2\pi\hbar^2[n/\zeta(3/2)]^{2/3}/M_{\rm eff}k_B$ with $\zeta(3/2) \approx 2.6124$. In the above experiment where $V_0/E_r$ is raised from 12 to 22, the temperature $T_c^{(0)}$ drops from 14.2 to 1.93 nK, implying that $T_c^{(0)}/E_r$ drops from 0.094 to 0.013. Hence $J$ and $k_BT$ are much smaller than $\hbar\omega_0$, so that we can ignore all higher bands.

The purpose of this Letter is to derive the full temperature dependence of this transition, thereby predicting a surprising reentrant phenomenon.

(ii) We begin by considering a $D$-dimensional Bose gas in the dilute limit where the two-particle $\delta$-function interaction is dominant. In the grand-canonical ensemble it is described by the Euclidean action

$$\mathcal{A}[\psi^*, \psi] = \int_0^{\hbar\beta} d\tau \int d^D x \Big\{ \psi^*(\mathbf{x},\tau)[\hbar\partial_\tau + \epsilon(-i\hbar\nabla) - \mu]\psi(\mathbf{x},\tau) + \frac{g_{\rm eff}}{2}\psi(\mathbf{x},\tau)^2\psi^*(\mathbf{x},\tau)^2 \Big\}, \qquad (1)$$

where $\mu$ is the chemical potential, and $\beta \equiv 1/k_BT$. To describe the phase transitions in this gas we calculate its effective energy. We expand the Bose field $\psi(\mathbf{x},\tau)$ around a constant background $\Psi$, i.e., $\psi(\mathbf{x},\tau) = \Psi + \delta\psi(\mathbf{x},\tau)$, and perform the functional integration for the grand-canonical partition function including only the harmonic fluctuations in $\delta\psi(\mathbf{x},\tau)$. This yields the one-loop approximation to the effective potential

$$\mathcal{V}(\Psi, \Psi^*) = V\Big(-\mu|\Psi|^2 + \frac{g_{\rm eff}}{2}|\Psi|^4\Big) + \frac{\eta}{2}\sum_{\mathbf{k}} E(\mathbf{k}) + \frac{\eta}{\beta}\sum_{\mathbf{k}} \ln[1 - e^{-\beta E(\mathbf{k})}], \qquad (2)$$

with $E(\mathbf{k}) = \sqrt{\{\epsilon(\mathbf{k}) - \mu + 2g_{\rm eff}|\Psi|^2\}^2 - g_{\rm eff}^2|\Psi|^4}$ denoting the quasiparticle energies. An expansion parameter $\eta = 1$ has been introduced whose power serves to count the loop order. The effective potential (2) is extremized with respect to the background field $\Psi$, yielding the condensate density

$$n_0 = \Psi^*\Psi = \frac{\mu}{g_{\rm eff}} - \frac{\eta}{V}\sum_{\mathbf{k}} \frac{2\epsilon(\mathbf{k}) + \mu}{\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}} \times \Big(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}} - 1}\Big) + \mathcal{O}(\eta^2) \qquad (3)$$

and the grand-canonical potential

$$\frac{\Omega(\mu, T)}{V} = -\frac{\mu^2}{2g} + \frac{\eta}{2V}\sum_{\mathbf{k}}\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})} + \frac{\eta}{\beta V}\sum_{\mathbf{k}} \ln(1 - e^{-\beta\sqrt{\epsilon(\mathbf{k})^2 + 2\mu\epsilon(\mathbf{k})}}) + \mathcal{O}(\eta^2). \qquad (4)$$

The chemical potential $\mu$ is fixed by the total particle density $n(\mu, T) = -V^{-1}\partial\Omega(\mu, T)/\partial\mu$. Eliminating $\mu$ in favor of the condensate density $n_0$ via (3), we find for the particle density

$$n - n_0 = \frac{\eta}{V}\sum_{\mathbf{k}} \frac{\epsilon(\mathbf{k}) + g_{\rm eff}n_0}{\sqrt{\epsilon(\mathbf{k})^2 + 2g_{\rm eff}n_0\epsilon(\mathbf{k})}} \times \Big(\frac{1}{2} + \frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2 + 2g_{\rm eff}n_0\epsilon(\mathbf{k})}} - 1}\Big) + \mathcal{O}(\eta^2). \qquad (5)$$

This result is the so-called Popov approximation [11,12]. It is derived only for a small right-hand side where $n \approx n_0$. A standard way to extend such a relation to $n \gg n_0$ is by making the equation self-consistent, replacing $n_0$ by $n$ (and $\eta$ by 1) on the right-hand side. The location of the quantum phase transition for all $T$ is obtained by solving this equation for $n_0 = 0$ [13,14]. The evaluation is discussed in the next two paragraphs.

Note that a more systematic approach to derive the self-consistent Popov approximation (5) proceeds by applying variational perturbation theory to (3) and (4) according to the rules developed in [15,16] and applied successfully to critical phenomena in [17] as well as many other strong-coupling problems [18]. There one introduces a dummy variational parameter $\tilde{\mu}$ by replacing $\mu \to \tilde{\mu} + \eta r$ with $r \equiv (\mu - \tilde{\mu})/\eta$ and reexpands consistently at fixed $r$ up to the first power in $\eta$. After this one reinserts $r \equiv (\mu - \tilde{\mu})/\eta$ and extremizes the resulting expression with respect to $\tilde{\mu}$. The result turns out to be precisely the self-consistent version of the Popov approximation (5) (see also the related discussion of the self-consistent Hartree-Fock-Bogoliubov-Popov approximation in one-dimensional optical lattices [7,8]).

(iii) We first discuss the formation of a condensate for the free-particle spectrum $\epsilon(\mathbf{k}) = \hbar^2\mathbf{k}^2/2M_{\rm eff}$, where momentum sums reduce to $\sum_{\mathbf{k}} \to V\int d^Dk/(2\pi)^D$. The integral of the zero-temperature contribution can now be evaluated analytically, and in $D = 3$ dimensions for the transition curve in the $T - a_{\rm eff}$ plane we obtain

$$a_{\rm eff} n^{1/3}\left[1 + \frac{3\alpha}{16} I(\alpha)\right]^{2/3} = \left(\frac{9\pi}{64}\right)^{1/3}. \qquad (6)$$

Here $I(\alpha)$ abbreviates the integral

$$I(\alpha) = \int_0^\infty dx \frac{x\alpha + 8}{2\sqrt{x\alpha + 16}(e^{\sqrt{x^2\alpha/16 + x}} - 1)}, \qquad (7)$$

and $\alpha \equiv t^2/a_{\rm eff}^2 n^{2/3}\zeta(3/2)^{4/3}$ is a dimensionless parameter, with $t \equiv T/T_c^{(0)}$ being the reduced temperature. The result is shown in Fig. 1(a). For small temperatures, the transition curve behaves like

$$a_{\rm eff} n^{1/3} = a_0 + a_1\alpha + a_2\alpha^2 + \mathcal{O}(\alpha^3), \qquad (8)$$

with the dimensionless expansion coefficients $a_0 = (9\pi/64)^{1/3} \approx 0.762$, $a_1 = -\pi^2 a_0/24 \approx -0.3132$, $a_2 \approx 0.1996$, and $a_3 \approx -0.207$. The interaction causes an upward shift of the critical temperature from $t_c^{(0)} = 1$ to $t_c = 1 + 4\sqrt{2\pi}\sqrt{a_{\rm eff} n^{1/3}}/3\zeta(3/2)^{2/3} + \mathcal{O}(a_{\rm eff} n^{1/3})$. This has the square-root behavior found before in Refs. [26,27].

As announced in the abstract, the phase diagram has the interesting property that there exists a *reentrant transition* above the critical temperature $T_c^{(0)}$ of the free system, which shows up as a *nose* in the transition curve,

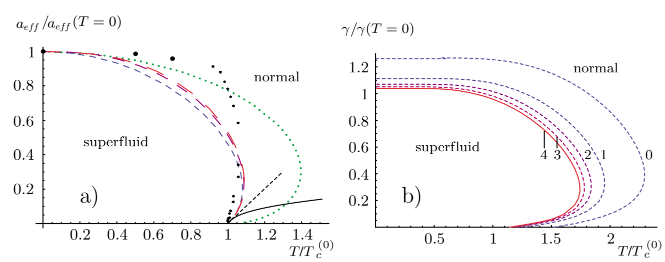


FIG. 1 (color online). (a) Quantum phase diagram of a homogeneous dilute Bose gas in variationally improved one-loop approximation without (dotted line) and with properly imposed higher-loop slope properties at $T_c^{(0)}$ [dashed length increasing with variational perturbation theory order from 1 to 3]. The short solid curve starting at $T = T_c^{(0)}$ is due to a second-order finite-temperature calculation of Arnold *et al.* [19]. The dashed straight line indicates the slope of our curve extracted either from Monte Carlo data [20,21] or precise high-temperature calculations [22,23]. The diamonds correspond to the Monte Carlo data of Ref. [24] and the dots stem from Ref. [25], both scaled to their respective values $a_{\rm eff}(T = 0)$. (b) Quantum phase diagram of optical boson lattice calculated for increasing hopping order (right to left). The quantity $\gamma = U/J$ is proportional to the effective scattering length $a_{\rm eff}$. At zero temperature, the transition takes the superfluid into a Mott insulator. Near $T_c$, higher corrections are needed due to infrared singularities. Since these are the same as in the continuum model, the correct curve should start out with a similar slope as in (a).

where a condensate can be produced by *increasing* $a_{\rm eff}$, which disappears upon a further increase of $a_{\rm eff}$. Our curves agree qualitatively with early Monte Carlo simulations [24] as shown in Fig. 1(a).

Recent Monte Carlo simulations [20,21] and precise high-temperature calculations [22,23] indicate, however, that the square-root approximation is unreliable near $T_c^{(0)}$, the leading critical temperature shift being linear in the scattering length $a_{\rm eff}$ with a coefficient $c_1 \approx 1.3$:

$$t_c = 1 + c_1 a_{\rm eff} n^{1/3} + \mathcal{O}(a_{\rm eff}^2 n^{2/3}). \qquad (9)$$

It is possible to improve our self-consistent approximation (6) to accommodate the high-loop result (9). This can be done with the help of variational perturbation theory [15,17,18,28]. For this we use the expansion (8) with a few exact coefficients and add two more trial coefficients to enforce the behavior (9). This produces a sequence of improved transition curves shown in Fig. 1(a) as dashed curves.

(iv) We now consider an optical lattice where the wave vectors $\mathbf{k}$ of the band spectrum $\epsilon_B(\mathbf{k})$ are restricted to the Brillouin zone $k_i \in (-\pi/\delta, \pi/\delta)$, and momentum sums become $V\prod_{i=1}^D \int_{-\pi/\delta}^{\pi/\delta} dk_i/2\pi$. The integral is evaluated using the *hopping expansion* [29], in which one expands the integrand in powers of the cosines in $\epsilon_B(\mathbf{k})$. By doing so, we express the result in terms of the lattice interaction $U = g_{\rm eff} n$. The transition curve is now determined by the implicit equation $F_D(k_B T/J, U/J) = 0$, where in zeroth hopping order $F_D^{(0)}(x, y) = x - 2\sqrt{D^2 + Dy}/\ln[4\sqrt{D^2 + Dy} + y + 2D]/[4\sqrt{D^2 + Dy} - y - 2D]$. The resulting transition curve for $D = 3$ and the next four approximations coming from successive hopping orders are shown in Fig. 1(b). A fast convergence is observed, with the approximation sequence of transition points at $T = 0$ corresponding to $(U/J)_c^{T=0} = 6(3 + 2\sqrt{3}) \approx 38.8, 34.1, 32.2, 31.8, 31.6\ldots$ which converge to roughly 30.8, as shown in Fig. 2. Thus our value is slightly smaller than the mean-field result $(U/J)_c^{T=0} \approx 34.8$ derived from the Bose-Hubbard model [1,30–32] and the experimental number $(U/J)_c^{T=0} \approx 36$ [5]. The associated

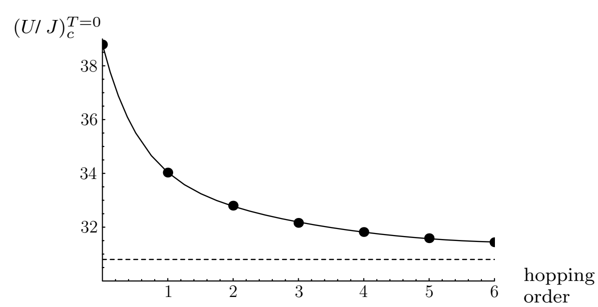


FIG. 2. Convergence of hopping expansion for the critical value of $U/J$ at the zero-temperature quantum phase transition. The limiting value for $(U/J)_c^{T=0}$ is 30.8.

hopping sequence of transition temperatures at $U = 0$ converges to $T_c^{(0)} \approx 3.6J/k_B$.

For the lattice spectrum (1) we cannot improve the result near $T_c^{(0)}$ in the same way as for the free-particle spectrum. By analogy, we may, however, assume that the characteristic reentrant transition will also here survive higher-loop corrections.

An important question is whether the nose survives the experimental setup of an optical lattice where the particles require an extra weak overall magnetic trap to keep them together. Indeed, if the magnetic trap is harmonic as in all present experiments with typical frequency $\omega_{\rm trap} \approx 2\pi \times 24$ Hz, the nose is expected to disappear since by analogy with a continuum calculation, the external trap reverses the slope of the transition curve at $T_c^{(0)}$ [33,34] (see also Chap. 7 of [15]). However, a nose will definitely be seen if the experiment is performed with a magnetic trap which has an approximate boxlike magnetic shape. This can be experimentally realized by using optical dipolar traps and lasers with square profiles. It will be interesting to study experimentally the dependence of the slope of the transition line on the shape of the magnetic trap potential as it is distorted from harmonic to a boxlike shape. For a powerlike shape of the trap [35] there should be a critical power where the nose appears [36].

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