Reentrant Phenomenon in Quantum Phase Diagram of Optical Boson Lattice

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We calculate the location of the quantum phase transitions of a gas of bosons trapped in an optical lattice as a function of effective scattering length $a_{\rm eff}$ 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* $a_{\rm eff}$.

1) Optical lattices offer the possibility to investigate the properties of Bose-Einstein condensates (BECs) at varying interaction strengths [1, 2]. 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, up to a trivial additive constant,

$$\epsilon(\mathbf{k}) = 2J \sum_{i=1}^{3} [1 - \cos(k_i \delta)] \,. \tag{1}$$

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 [3]

$$J = \frac{4}{\sqrt{\pi}}\, E_r \left(\frac{V_0}{E_r}\right)^{3/4} \exp\left[-2\left(\frac{V_0}{E_r}\right)^{1/2}\right] . \tag{2}$$

Due to the low-density of the system, a repulsive potential $V(\mathbf{x}) = g\delta^{(3)}(\mathbf{x})$ with the coupling constant $g = 4\pi^2\hbar^2 a/M$ 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 δ-function interaction with strength [2, 3] $g_{\rm eff}/\delta^D = U \equiv g \int d^D x\, w^4(\mathbf{x}) = (a/a_0) 2\hbar\omega_0/\sqrt{2\pi} = (2\pi a/\lambda)\sqrt{8/\pi} E_r (V_0/E_r)^{3/4}$. The importance of the interactions between the particles in the periodic traps is measured by the ratio $\gamma \equiv U/J$ between interaction energy $U = g_{\rm eff} n$ with $g_{\rm eff} = 4\pi^2\hbar^2 a_{\rm eff}/M_{\rm eff}$ and kinetic energy $J = \hbar^2 n^{2/3}/2M_{\rm eff}$, where n is the particle density ($= f/\delta^3$ for filling factor f). This leads to $\gamma = 8\pi a_{\rm eff}\, n^{1/3}$.

The experimental optical lattice of Ref. [4] is made of laser beams with wavelength $\lambda = 2\delta$=852 nm and contains about 2×10^5 atoms ^{87}Rb with $a \approx 4.76$ nm [5]. Its energy scale is $E_r \approx \hbar \times 20\,\text{kHz} \approx k_B \times 150\,\text{nK}$ 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, $\hbar\omega_0/E_r$ increases from 0.36 to 0.57. Expanding the small-$\mathbf{k}$ behavior of the band energy (1) as $\hbar^2\mathbf{k}^2/2M_{\rm eff} + \dots$, the band width $4J$ 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 $n^{-1/3}$ of a few thousand Å, their 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 [4] for temperatures near zero we have $\gamma = 0.0248 \exp(2\sqrt{V_0/E_r})$, 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.

Above the quantum phase transition, 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].

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 $T_c^{(0)} = 2\pi\hbar^2/M_{\rm eff} k_B [\zeta(3/2)/n]^{2/3}$ 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 nK to 1.93 nK, implying that $T_c^{(0)}/E_r$ drops from 0.094 to 0.013. Hence J and $k_B T$ (k_B = Boltzmann constant, T = temperature) are much smaller than $\hbar\omega_0$, so that we can ignore all higher bands.

The purpose of this note is to derive the full temperature dependence of this transition, thereby predicting a surprising reentrant phenomenon [7].

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

$$\mathcal{A}[\psi^*, \psi] = \int_0^{\hbar\beta} d\tau \int d^D x \Big\{ \psi^*(\mathbf{x},\tau)[\hbar\partial_\tau + \epsilon(-i\hbar\boldsymbol{\nabla}) - \mu] \times \psi(\mathbf{x},\tau) + \frac{g_{\rm eff}}{2}\, \psi(\mathbf{x},\tau)^2 \psi^*(\mathbf{x},\tau)^2 \Big\} , \tag{3}$$

where μ is the chemical potential, and $\beta \equiv 1/k_B T$. To describe the phase transition in this gas we calculate its effective energy. We expand the Bose fields $\psi(\mathbf{x},\tau)$ around a constant background Ψ, i.e. $\psi(\mathbf{x},\tau) = \Psi + \delta\psi(\mathbf{x},\tau)$, and perform the functional integral for the partition func-

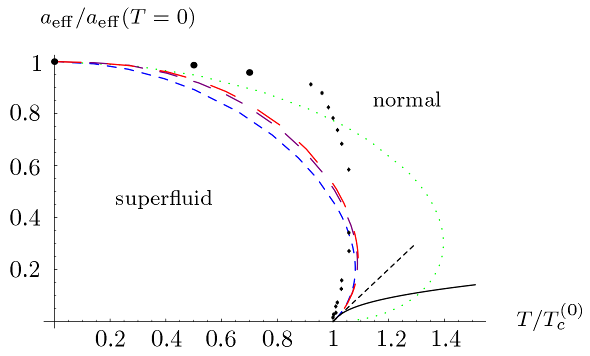

FIG. 1: Phase diagram of Bose-Einstein condensation in variationally improved one-loop approximation without (dotted) and with properly imposed higher-loop slope properties at $T_c^{(0)}$ (dashed length increasing with order of variational perturbation theory). Short solid curve starting at $T_c^{(0)}$ is due to Arnold et al. [22]. Dashed straight line indicates the slope of our curve extracted either from Monte-Carlo data [18, 19] or recent analytic results [20, 21]. Diamonds correspond to the Monte-Carlo data of Ref. [17] and dots stem from Ref. [23], both scaled to their critical value $a_{\rm eff}(T=0)\approx 0.63$.

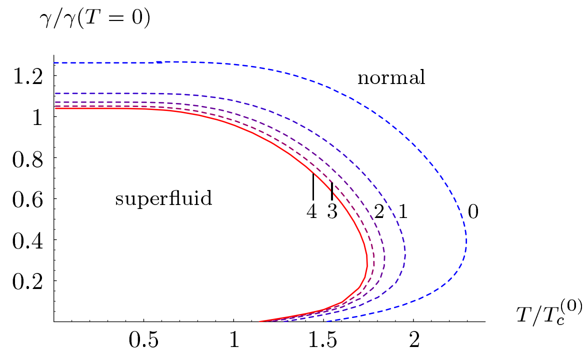

FIG. 2: Phase diagram of the superfluid-Mott insulator transition for increasing hopping order (right to left). The quantity γ is the ratio U/J.

tion including only the harmonic fluctuations in $\delta\psi(\mathbf{x},\tau)$. This yields the one-loop approximation to the effective potential

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

with quasiparticle energies

$$E(\mathbf{k})=\sqrt{\{\epsilon(\mathbf{k})-\mu+2g_{\rm eff}|\Psi|^2\}^2-g_{\rm eff}^2|\Psi|^4}\,. \tag{5}$$

An expansion parameter $\eta=1$ has been introduced whose power serves to count the loop order. The extremum of the effective potential (4) with respect to the condensate density $n_0=\Psi^*\Psi$ yields the grand-canonical potential $\Omega(\mu,T)$. The chemical potential μ is fixed by the total particle density $n(\mu,T)=-V^{-1}\partial\Omega(\mu,T)/\partial\mu$. Eliminating μ in favor of the condensate density n_0 via $n_0=|\Psi|^2=\mu/g_{\rm eff}+\mathcal{O}(\eta)$, and keeping only terms of order $\mathcal{O}(\eta)$ on the right-hand side of Eq. (4), the so-called Popov approximation [8], we find for the particle density

$$n-n_0 = \frac{\eta}{V}\sum_{\mathbf{k}}\frac{\epsilon(\mathbf{k})+g_{\rm eff}n_0}{\sqrt{\epsilon(\mathbf{k})^2+2g_{\rm eff}n_0\epsilon(\mathbf{k})}} \times\left(\frac{1}{2}+\frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2+2g_{\rm eff}n_0\epsilon(\mathbf{k})}}-1}\right). \tag{6}$$

This result 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 on the right-hand side. Thus we obtain for the physical value $\eta=1$

$$n-n_0 = \frac{1}{V}\sum_{\mathbf{k}}\frac{\epsilon(\mathbf{k})+g_{\rm eff}n}{\sqrt{\epsilon(\mathbf{k})^2+2g_{\rm eff}n\epsilon(\mathbf{k})}} \times\left(\frac{1}{2}+\frac{1}{e^{\beta\sqrt{\epsilon(\mathbf{k})^2+2g_{\rm eff}n\epsilon(\mathbf{k})}}-1}\right). \tag{7}$$

The location of the quantum phase transition for all T is obtained by solving this equation for $n_0=0$ [13, 14]. The evaluation will be discussed in in the next two paragraphs for different one-particle spectra $\epsilon(\mathbf{k})$.

Note that a more satisfactory approach to derive the self-consistent Eq. (7) from (6) proceeds by applying variational perturbation theory to according to the rules developed in [9, 10], and applied successfully to critical phenomena in [11] as well as many other strong-coupling problems [11, 12]. In $\mathcal{V}(\Psi,\Psi^*)$ one introduces a dummy variational parameter $\tilde\mu$ by replacing $\mu\to\tilde\mu+\eta r$ with $r\equiv(\mu-\tilde\mu)/\eta$, and re-expand $\mathcal{V}$ consistently at fixed r up to the first power in η. After this one re-inserts $r\equiv(\mu-\tilde\mu)/\eta$ and extremizes the resulting expression with respect to $\tilde\mu$ and $\Psi\Psi^*$. The result turns out to be precisely Eq. (7).

3) 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 the sum in (7) reduces 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 we obtain in $D=3$ dimensions the following equation for the transition curve in the $T-a_{\rm eff}$ plane [7]:

$$a_{\rm eff}\,n^{1/3}\left[1+\frac{3\alpha}{16}I(\alpha)\right]^{2/3}=\left(\frac{9\pi}{64}\right)^{1/3}. \tag{8}$$

Here $I(\alpha)$ abbreviates the integral

$$I(\alpha)=\int_0^\infty dx\,\frac{x\alpha+8}{2\sqrt{x\alpha+16}\,(e^{\sqrt{x^2\alpha/16+x}}-1)}\,, \tag{9}$$

and α is the dimensionless parameter

$$\alpha \equiv \left(\frac{t}{a_{\rm eff}\, n^{1/3}\zeta(3/2)^{2/3}}\right)^2 , \qquad (10)$$

with $t \equiv T/T_c^{(0)}$ being the reduced temperature. The result is shown in Fig. 1. For small temperatures, the transition curve behaves like

$$a_{\rm eff} n^{1/3} = a_0 + a_1\alpha + a_2\alpha^2 + \mathcal{O}\left(\alpha^3\right) , \qquad (11)$$

with the dimensionless expansion coefficients $a_0 = (9\pi/64)^{1/3} \approx 0.762$, $a_1 \approx -0.3132$, and $a_2 \approx 0.1996$. The interaction causes an upward shift of the critical temperature from $t_c^{(0)} = 1$ to

$$t_c = 1 + \frac{4\sqrt{2\pi}}{3\zeta(3/2)^{2/3}}\sqrt{a_{\rm eff} n^{1/3}} + \mathcal{O}\left(a_{\rm eff} n^{1/3}\right) . \qquad (12)$$

This has the square-root behavior found before in Ref. [15, 16], with the positive sign agreeing with Ref. [16].

As announced in the abstract, the phase diagram in Fig. 1 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, 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 [17] as shown in Fig. 1.

Recent Monte-Carlo simulations [18, 19] and precise high-temperature calculations [20, 21] indicate, however, that the approximation (12) is unreliable near $T_c^{(0)}$, the leading critical temperature shift being linear in the scattering length $a_{\rm eff}$:

$$t_c = 1 + c_1 a_{\rm eff} n^{1/3} + \mathcal{O}\left(a_{\rm eff}^2 n^{2/3}\right), \qquad (13)$$

with a coefficient $c_1 \approx 1.3$.

It is possible to improve our self-consistent approximation (8) to accommodate the high-loop result (13). This can be done with the help of variational perturbation theory [9, 11, 12, 24]. For this we use the expansion (11) with a few exact coefficients and add two more trial coefficients to enforce the behavior (13). This produces a sequence of improved transition curves shown in Fig. 1 as dashed curves [7].

4) We now consider the true band spectrum (1) where the wave vectors $\mathbf{k}$ are restricted to the Brillouin zone $k_i \in (-\pi/\delta, \pi/\delta)$, and the sum in (7) reduces to the integral $\sum_{\mathbf{k}} \to V\prod_{i=1}^{D}\int_{-\pi/\delta}^{\pi/\delta} dk_i/2\pi$. The integral is evaluated using the *hopping expansion* [25], in which one expands the integrand in powers of the cosines in (1). 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

$$F_D\left(\frac{k_B T_c}{J}, \frac{U}{J}\right) = 0 , \qquad (14)$$

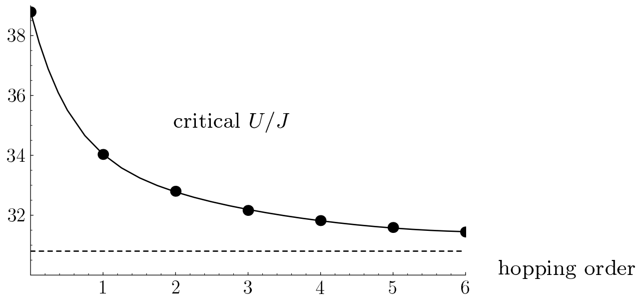

FIG. 3: Convergence of hopping expansion for the critical value of U/J at the zero-temperature quantum phase transition. The limiting value is $(U/J)_c^{T=0} \approx 30.8$.

where in zeroth hopping order

$$F_D^{(0)}(x,y) = x - \frac{2\sqrt{D^2+Dy}}{\ln\dfrac{4\sqrt{D^2+Dy}+y+2D}{4\sqrt{D^2+Dy}-y-2D}} . \qquad (15)$$

The resulting transition curve for $D = 3$ and the next three approximations coming from successive hopping orders are shown in Fig. 2. A fast convergence is observed, with the approximation sequence of transition 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. 3.

Thus our value is smaller than the mean-field result $(U/J)_c^{T=0} \approx 34.8$ derived from Bose-Hubbard model [1, 26–28] and the experimental number $(U/J)_c^{T=0} \approx 36$ [4]. The associated hopping sequence of transition temperatures at $U = 0$ converges to $T_c^{(0)} \approx 3.6\, J/k_B$.

The higher-loop slope for the lattice spectrum of $\epsilon(\mathbf{k})$ is unknown, so that 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.

For the experimentalist it is important to know whether this phenomenon persists if the optical lattice is stabilized by an overall weak magnetic trap of a typical frequency $\omega_{\rm trap} \approx 2\pi \times 24$ Hz which is necessary to prevent the particles from escaping the optical lattice. According to the result of Ref. [29], the nose in the transition curve could disappear since for the free-particle spectrum an external trap causes a reversal of the slope of the transition curve at $T_c^{(0)}$ [30, 31], the shift (13) becoming

$$t_c \approx 1 - 3.427\sqrt{r_1}\times r_2 \times a_{\rm eff} n^{1/3} = 1 - 0.136\sqrt{r_1}\times r_2 \times U/J, \qquad (16)$$

where $r_1 \equiv k_B T_c^{(0)}/2\pi\hbar\omega_{\rm trap}$ and $r_2 \equiv 1/\lambda_{\omega_{\rm trap}} n^{1/3}$ is the ratio between the length scale $\delta/f^{1/3}$ and the width of the trap $\lambda_{\omega_{\rm trap}} \equiv \sqrt{\hbar/M_{\rm eff}\omega_{\rm trap}}$. These numbers have the ranges $r_1 \in (0.27, 2.0)$ and $r_2 \in (0.52, 1.4)$ so that $0.136 \times \sqrt{r_1} \times r_2$ lies between 0.037 and 0.27, experimentally.

Note added in proof: After this paper appeared on the Los Alamos server, P.J.H. Denteneer drew our attention to a preprint of his written with D.B.M. Dickerscheid, D. van Oosten, and H.T.C. Stoof (eprint: `cond-mat/0306573`) in which they also found a nose in the phase diagram (see their Figure 6). According to his private communication they did not, however, interpret their nose as a signal for a reentrant transition but considered it as an artefact of their slave boson approach.

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