Scaling of the density profiles of cold atoms near the quantum critical point in two- and three-dimensional optical lattices

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We study the critical behavior near the quantum critical point of strongly interacting bosons placed in an optical lattice. Using the combined Bogoliubov method and the quantum rotor approach, we map the Hamiltonian of strongly interacting bosons onto $U(1)$ phase action in order to calculate analytically the density profiles as a function of hopping and reduced chemical potential. Our approach allows us to explicitly compute the scaling form of the density n_s for systems confined in two-dimensional square and three-dimensional cubic lattices. We find a good convergence of n_s with the universal scaling function in a wide temperature range that is accessible in the current experiments on the density profiles in cold bosonic systems.

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I. INTRODUCTION

During recent years enormous progress was made in the experimental study of cold atoms in optical lattices [1]. The great advantage of optical lattices as analog simulators of strongly correlated Hamiltonians lies in the ability of optical lattices to accurately implement lattice models without impurities or defects. Furthermore, ultracold atoms confined in optical lattice structure provide a very clean experimental realization of a strongly correlated many-body problem [2]. Strong correlation effects, which imply enhanced quantum fluctuations, are playing an increasingly important role in recent experiments on dilute quantum gases [3].

The concept of a critical transition between different phases of matter at temperature $T = 0$ is central to many complex phenomena in strongly correlated systems [4]. Quantum critical points (QCPs) give rise to unusual features through a range of temperatures, and may be responsible for heavy fermion [5], non-Fermi-liquid properties [6], as well as the anomalous normal state of cuprate superconductors [7,8]. In the context of bosons in optical lattices the nonthermal tuning parameters offer a convenient organizing principle to facilitate the theoretical analysis, but systematic experimental access to quantum criticality in these systems turns out to be difficult. The problem lies in the setup where phase transitions can be traversed through nonthermal perturbations in the low-temperature limit. In experiment, one can measure the density profiles of bosons trapped in optical lattice, which is given by a single-particle Green's function integrated over momenta [9,10]. Quite recently, a numerical evaluation of the density profiles in a scaling form has been performed using large-scale quantum Monte Carlo simulations for strongly interacting bosons in a two-dimensional optical lattice [11].

It is our goal in the present paper to calculate analytically the density profiles in the quantum critical region for the system of bosons in two- and three-dimensional optical lattices. We use a theory that goes beyond the simple Bogoliubov approximation that has been recently developed and incorporates the phase degrees of freedom via the quantum rotor approach to describe regimes beyond the very weakly interacting one [12]. This scenario provided a picture of quasiparticles and energy excitations in the strong interaction limit, where the transition between the superfluid and the Mott state is driven by phase fluctuations. Taking advantage of the macroscopically populated condensate state, we have separated the problem into the amplitude of the Bose field and the fluctuating phase that was absent in the original Bogoliubov problem [13]. We further quantitatively demonstrate the universal scaling properties near the superfluid–Mott-insulator quantum phase transition point through the finite temperature density profile in a trapped system. The plan of the paper is as follows: in Sec. II, we introduce the microscopic Bose-Hubbard model relevant for the description of strongly interacting bosons in an optical lattice. In the following section, we briefly present our approach and calculate density profiles of bosons in optical lattice. In Sec. IV, results of our calculations are plotted in a scaling form of normalized density profiles. Finally, we conclude in Sec. V.

II. MODEL HAMILTONIAN

From a theoretical point of view, a description of the bosons in optical lattice can be achieved through the definition of a microscopic Hamiltonian that can capture the main physics of these systems: the Bose-Hubbard Hamiltonian. Within this model, the bosons move on a lattice within a tight-binding scheme and correlation is introduced through an on-site repulsive term, since in real Bose gases the interaction between atoms cannot be neglected in the physical description of the gas. We consider a second quantized, bosonic Hubbard Hamiltonian in the form [14,15]

$$\mathcal{H} = -t \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} [a^\dagger(\mathbf{r})a(\mathbf{r}') + a^\dagger(\mathbf{r}')a(\mathbf{r})] + \frac{U}{2} \sum_{\mathbf{r}} n^2(\mathbf{r}) - \overline{\mu} \sum_{\mathbf{r}} n(\mathbf{r}). \quad (1)$$

The constant t represents the nearest-neighbors tunneling matrix element and is responsible for the dynamical hopping of bosons from one optical lattice site to another. During a jump between two neighboring sites a boson gains energy t. The constant U is the strength of the on-site repulsive interaction of bosons. Adding a boson to an already occupied

site costs energy U. Furthermore, $\overline{\mu} = \mu + \frac{U}{2}$, where μ is a chemical potential controlling the average number of bosons. The operators $a^\dagger(\mathbf{r})$ and $a(\mathbf{r}')$ create and annihilate bosons on sites $\mathbf{r}$ and $\mathbf{r}'$ of a regular two-dimensional (2D) lattice with the nearest-neighbors hopping denoted by summation over $\langle \mathbf{r},\mathbf{r}' \rangle$. A total number of sites is equal to N and the boson number operator $n(\mathbf{r}) = a^\dagger(\mathbf{r})a(\mathbf{r})$. We use the Hamiltonian in Eq. (1) to describe a homogeneous (translationally invariant) system, omitting the effect of the external magnetic potential that is usually superimposed on top of the optical lattice potential in order to additionally trap the atoms. The external potential can be included in the Hamiltonian as $\sum_{\mathbf{r}} \epsilon(\mathbf{r})n(\mathbf{r})$ and would couple to the chemical potential term. The realization of the Bose-Hubbard Hamiltonian using optical lattices has the advantage that the interaction matrix element U and the tunneling matrix element t can be controlled by adjusting the intensity of the laser beams. The Hamiltonian and its descendants have been widely studied within the last years. The phase diagram and ground-state properties include the mean-field ansatz [16], strong coupling expansions [17–19], the quantum rotor approach [20], methods using the density matrix renormalization group (DMRG) [21–24], and quantum Monte Carlo (QMC) simulations [25–28].

III. CRITICAL SCALING OF PARTICLE DENSITY PROFILES

We start with the singular part of the free energy, which near the critical transition line becomes divergent. General arguments show that when the dimensionality d is below the upper critical dimension d_c, the singular part of the particle density $n_s = n - n_r = \partial f_s/\partial\mu$ can be expressed near the transition line in the scaling form as follows [29,30]:

$$n(\mu,T) - n_r(\mu,T) = T^{\frac{d}{z}+1-\frac{1}{\nu z}}\mathcal{G}\left(\frac{\mu-\mu_c}{T^{1/\nu z}}\right), \tag{2}$$

where z is the dynamical exponent, ν is the correlation length exponent, n_r is the regular part of the density, and $\mathcal{G}(x)$ is a universal function describing the singular part of the density near criticality. Besides, μ_c denotes the chemical potential at $T = 0$ where the phase transition takes place. For a boson Mott insulator, n_r is an integer and in the first Mott lobe $n_r = 1$ (see Ref. [31]).

The statistical sum of the system defined by Eq. (1) can be written in a path integral form with use of complex fields $a(\mathbf{r}\tau)$ depending on the imaginary time $0 \leqslant \tau \leqslant \beta \equiv 1/k_B T$ (with T being the temperature) that satisfy the periodic condition $a(\mathbf{r}\tau) = a(\mathbf{r}t + \beta)$:

$$Z = \int [\mathcal{D}\overline{a}\mathcal{D}a] e^{-\mathcal{S}[\overline{a},a]}, \tag{3}$$

where the action $\mathcal{S}$ is equal to

$$\mathcal{S}[\overline{a},a] = \int_0^\beta d\tau \left[\mathcal{H}(\tau) + \sum_{\mathbf{r}} \overline{a}(\mathbf{r}\tau)\frac{\partial}{\partial\tau}a(\mathbf{r}\tau)\right]. \tag{4}$$

Referring to the microscopic Hamiltonian, the number of particles is given by

$$n = \frac{1}{\beta N}\sum_{\mathbf{k}\ell} G(\mathbf{k}\omega_\ell), \tag{5}$$

where the Green's function is given by

$$G(\mathbf{r}\tau;\mathbf{r}'\tau') = \langle a(\mathbf{r}\tau)\overline{a}(\mathbf{r}'\tau')\rangle, \tag{6}$$

with averaging performed with respect to action in Eq. (4). In order to proceed, we perform a local gauge $U(1)$ transformation to new bosonic variables,

$$a(\mathbf{r}\tau) = b(\mathbf{r}\tau)\zeta(\mathbf{r}\tau), \tag{7}$$

where

$$\zeta(\mathbf{r}\tau) = e^{i\phi(\mathbf{r}\tau)} \tag{8}$$

with $\phi(\mathbf{r}\tau)$ being the $U(1)$ phase variable [12]. The superfluid order parameter is defined by

$$\Psi_B = \langle a(\mathbf{r}\tau)\rangle = \langle b(\mathbf{r}\tau)\rangle\psi_B. \tag{9}$$

However, a nonzero value of the amplitude $\langle b(\mathbf{r}\tau)\rangle$ is not sufficient for superfluidity. Also, the $U(1)$ phase variables must become coherent, which leads to the phase order parameter

$$\psi_B = \langle e^{i\phi(\mathbf{r}\tau)}\rangle_\phi. \tag{10}$$

In order to calculate the Green's function in Eq. (5), we proceed according to the procedure described in Ref. [12]. According to Eq. (7), the Green's function in Eq. (6) splits into the product of Green's functions of $U(1)$ phase field ζ and bosonic b sectors,

$$G(\mathbf{r}\tau;\mathbf{r}'\tau') = G_\zeta(\mathbf{r}\tau;\mathbf{r}'\tau')G_b(\mathbf{r}\tau;\mathbf{r}'\tau'), \tag{11}$$

where

$$\begin{aligned} G_\zeta(\mathbf{r}\tau;\mathbf{r}'\tau') &= \langle\zeta(\mathbf{r}\tau)\overline{\zeta}(\mathbf{r}'\tau')\rangle_\zeta \\ G_b(\mathbf{r}\tau;\mathbf{r}'\tau') &= \langle b(\mathbf{r}\tau)\overline{b}(\mathbf{r}'\tau')\rangle_b. \end{aligned} \tag{12}$$

The averagings appearing over ζ and b in Eq. (12) refer to averaging with respect to actions dependent of the pertinent fields. Proceeding along these lines we obtain

$$\begin{aligned} n = \frac{\overline{\mu}}{U} &- (1-2\psi_B^2)v\left(\frac{\overline{\mu}}{U}\right) \\ &- \frac{1}{N}\sum_{\mathbf{k}}\coth\left\{\frac{\beta U}{2}\left[\Xi_{\delta\lambda}(\mathbf{k}) + v\left(\frac{\overline{\mu}}{U}\right)\right]\right\} \\ &+ \frac{1}{N}\sum_{\mathbf{k}}\coth\left\{\frac{\beta U}{2}\left[\Xi_{\delta\lambda}(\mathbf{k}) - v\left(\frac{\overline{\mu}}{U}\right)\right]\right\}, \end{aligned} \tag{13}$$

where:

$$\Xi_{\delta\lambda}(\mathbf{k}) = \sqrt{\frac{\delta\lambda}{U} + \frac{2t}{U}b_0^2(\varepsilon_{\mathbf{0}} - \varepsilon_{\mathbf{k}}) + v^2\left(\frac{\overline{\mu}}{U}\right)}, \tag{14}$$

$\varepsilon_{\mathbf{k}}$ is the dispersion of the square two-dimensional ($\gamma = 0$) or cubic three-dimensional ($\gamma = 1$) lattice

$$\varepsilon_{\mathbf{k}} = \cos(ak_x) + \cos(ak_y) + \gamma\cos(ak_z), \tag{15}$$

b_0 is the bosonic amplitude

$$b_0^2 = 2d\frac{t}{U} + \frac{\overline{\mu}}{U}, \tag{16}$$

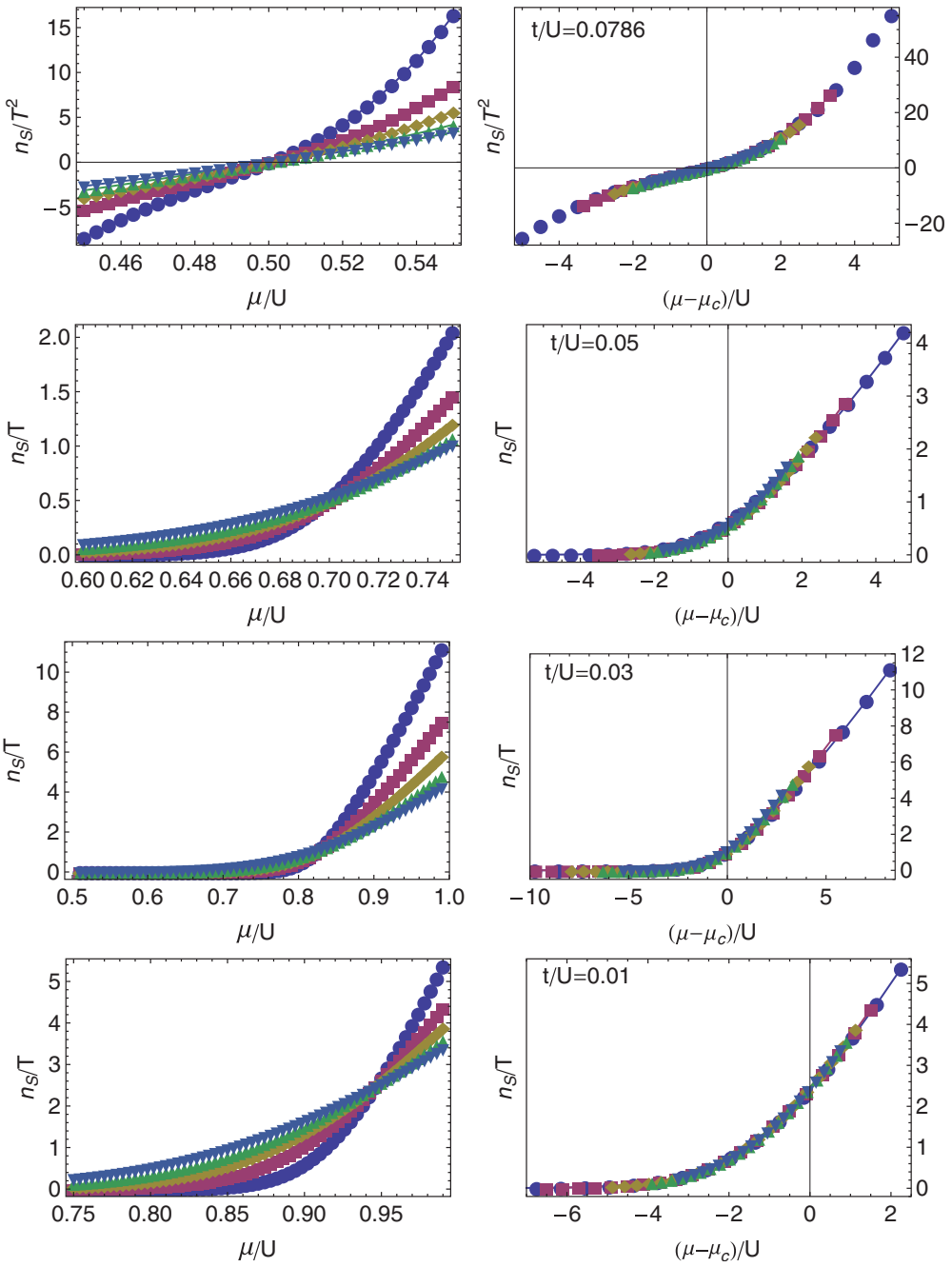

FIG. 1. (Color online) Dependence of the density $n_s/T^{\frac{d}{z}+1-\frac{1}{\nu z}}$ as a function of chemical potential μ/U (left side) and scaling of density profiles $n_s/T^{\frac{d}{z}+1-\frac{1}{\nu z}}$ vs reduced chemical potential $(\mu-\mu_c)/T$ (right side) for bosons in a square lattice for various temperatures. The plots are paired for selected values of interaction t/U. The value 0.0786 denotes the tip of the lobe, which results in the critical exponent $z=1$, different than for the other values of t/U ($z=2$). Symbols denote temperatures (k_BT/U) from the range of 0.02 to 0.06 (0.02: circles, 0.03: squares, 0.04: diamonds, 0.05: up-pointing triangles, 0.06: down-pointing triangles).

and, finally, $v(x)=x-[x]-1/2$, with $[x]$ being the floor function, which gives the greatest integer less than or equal to x. Here, $\delta\lambda=\lambda-\lambda_0$, where λ is the Lagrange multiplier that enforces (on average) the unimodular constraint on the $\zeta(\mathbf{r}\tau)$ variables in Eq. (8). In the whole low-temperature ordered phase (superfluid) the Lagrange multiplier λ is constant and equal to the saddle-point value λ_0

$$\lambda_0-2tb_0^2\varepsilon_{\mathbf{0}}+K^{-1}(\omega_{\ell=0})=0, \tag{17}$$

with $K^{-1}(\tau-\tau')$ being the inverse of the phase-phase correlator (see Ref. [12]), whose Fourier transform reads

$$K^{-1}(\omega_\ell)=\frac{U}{4}-U\left[v\left(\frac{\overline{\mu}}{U}\right)+\frac{i\omega_\ell}{U}\right]^2. \tag{18}$$

This leads to $\delta\lambda=0$ in the superfluid region. Outside the ordered region, $\delta\lambda$ is positive and has to be determined

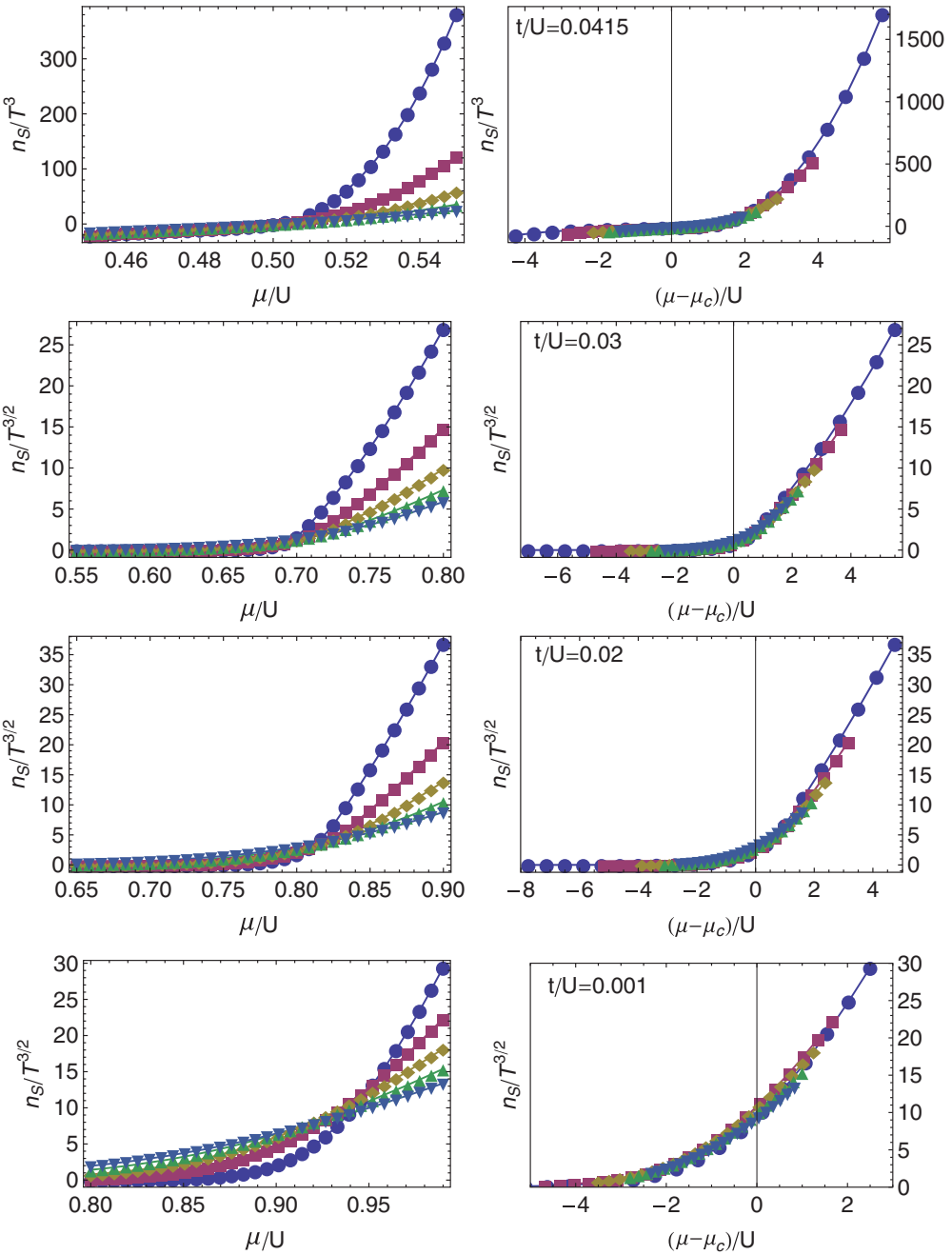

FIG. 2. (Color online) Dependence of the density $n_s/T^{\frac{d}{z}+1-\frac{1}{\nu z}}$ as a function of chemical potential μ/U (left side) and scaling of density profiles $n_s/T^{\frac{d}{z}+1-\frac{1}{\nu z}}$ vs reduced chemical potential $(\mu-\mu_c)/T$ (right side) for bosons in cubic lattice for various temperatures. The plots are paired for selected values of interaction t/U. The value 0.0415 denotes the tip of the lobe, which results in the critical exponent $z=1$, different than for the other values of t/U ($z=2$). Symbols denote temperatures (k_BT/U) from the range of 0.02 to 0.06 (0.02: circles, 0.03: squares, 0.04: diamonds, 0.05: up-pointing triangles, 0.06: down-pointing triangles).

numerically from the equation,

$$1=\Omega(\delta\lambda), \tag{19}$$

where

$$\Omega(\delta\lambda)=\frac{1}{4N}\sum_{\mathbf{k}}\frac{\coth\left\{\frac{\beta U}{2}\left[\Xi_{\delta\lambda}(\mathbf{k})-v\left(\frac{\mu}{U}\right)\right]\right\}}{\Xi_{\delta\lambda}(\mathbf{k})} + \frac{1}{4N}\sum_{\mathbf{k}}\frac{\coth\left\{\frac{\beta U}{2}\left[\Xi_{\delta\lambda}(\mathbf{k})+v\left(\frac{\mu}{U}\right)\right]\right\}}{\Xi_{\delta\lambda}(\mathbf{k})}. \tag{20}$$

On the other hand, the phase order parameter ψ_B is equal to zero in the disordered phase (in particular, the Mott insulator for $T=0$), while in the superfluid region is determined from

$$1-\psi_B^2=\Omega(\delta\lambda=0), \tag{21}$$

which for $\psi_B=0$ becomes the equation for the critical line.

IV. RESULTS

Now, we turn to the analysis of the critical properties of a Bose system in optical lattice in two and three dimensions. Using the relation in Eq. (13), we have calculated normalized density profiles. It is well known that the critical exponents in Eq. (2) read $z = 2$ and $\nu = 1/2$ at the tip of the lobe and $z = 1$, $\nu = 1$, elsewhere in the t/U vs μ/U zero-temperature phase diagram [29]. As a result, the value of the exponent $\frac{d}{z} + 1 - \frac{1}{\nu z}$ for a two-dimensional system is equal to 2 at the tip of the lobe and 1 elsewhere, while for a three-dimensional system it reads 3 at the tip of the lobe, and 3/2 in the remaining parts of the phase diagram. Furthermore, for every chosen ratio of t/U, we have plotted curves of $n_s/T^{\frac{d}{z}+1-\frac{1}{\nu z}}$ as a function of μ/U at different temperatures. Their intersection sets the value of the critical chemical potential μ_c (as a result, μ_c is not temperature dependent). After determination of μ_c, we have plotted the density of bosons $n_s/T^{\frac{d}{z}+1-\frac{1}{\nu z}}$ as a function of the rescaled chemical potential $(\mu - \mu_c)/T$. We find a good convergence for the universal scaling function [see Eq. (2)] in a wide temperature range $0.02U$–$0.06U$ (see Fig. 1 for square and Fig. 2 for cubic system, respectively).

V. CONCLUSION

The possibility of exploring novel quantum phases of matter using ultracold atoms trapped in optical lattices has raised the interest of many researchers. In the present paper, we have shown that important features of interacting bosons in an optical lattice occur close to the quantum critical point. In particular, we show the rescaled singular density $(n_s/T^{\frac{d}{z}+1-\frac{1}{\nu z}})$ as a function of rescaled chemical potential, $(\mu - \mu_c)/T$, in the quantum rotor model and find a very nice convergence for the universal scaling function $\mathcal{G}$ [see Eq. (2)] in a wide temperature range. We can compare part of our results that pertain to the two-dimensional lattice with the outcome of quantum Monte Carlo calculations (see Ref. [11]). For example, plots for $t/U = 0.3$ in Fig. 1 correspond to Figs. (3a) and (3b) in Ref. [11], where the agreement between rescaled densities is quite good. This is clear evidence of the scaling theory near the critical point of the superfluid–Mott-insulator transition. From the experimental point of view, however, it is somehow more important to know the characteristic temperature, T^*, below which the universal scaling behavior is observable. Recent experiments have reported temperatures on the order of $k_B T/t \approx 0.9$. At such temperatures, the effects of excited states become important, motivating investigations into the finite temperature phase diagram, quantum versus thermal transitions, and the location of the phase boundary. Accurate thermometry is of the essence in the observation of universal scaling behavior. Our theoretical model can provide the information that within this range of temperature the universal scaling of the model under study should be visible. We hope that our results can be directly applied to the current experiment on quantum gases in optical lattices and will stimulate future investigations in this area.

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