Finite-size scaling for quantum criticality above the upper critical dimension: Superfluid–Mott-insulator transition in three dimensions

Yasuyuki Kato* and Naoki Kawashima

Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa, Chiba 277-8581, Japan

(Received 30 September 2009; published 19 January 2010)

The validity of modified finite-size scaling above the upper critical dimension is demonstrated for the quantum phase transition whose dynamical critical exponent is $z=2$. We consider the N-component Bose-Hubbard model, which is exactly solvable and exhibits mean-field type critical phenomena in the large-N limit. The modified finite-size scaling holds exactly in that limit. However, the usual procedure, taking the large system-size limit with fixed temperature, does not lead to the expected (and correct) mean-field critical behavior because of the limited range of applicability of the finite-size scaling form. By quantum Monte Carlo simulation, it is shown that the modified finite-size scaling holds in the case of $N=1$.

DOI: 10.1103/PhysRevE.81.011123 PACS number(s): 64.60.an, 67.25.dj, 64.70.Tg, 37.10.Jk

I. INTRODUCTION

Since the quantum phase transition to the Mott insulator from a superfluid was observed in the optical lattice system [1], this quantum critical phenomenon has been a hot topic [2]. This system is effectively described by the Bose-Hubbard (BH) Hamiltonian [3]. The zero-temperature phase diagram of the BH model has been well investigated [4–6]. There are phase transition points called multicritical points with the dynamical critical exponent of $z=1$ and a line of the other type of phase transition called generic transition, the dynamical critical exponent of which is $z=2$ on the zero-temperature phase diagram. In this paper, we consider the generic transition (i.e., $z=2$) in three-dimensional systems. Three dimensions ($d=3$) are above the upper critical dimension $d_u=2$. Therefore, this phase transition is exactly classified and its critical exponents should be identical to those of the mean-field theory. To estimate the locations of critical points quantitatively, we frequently apply finite-size scaling to the data of finite-size systems calculated by the quantum Monte Carlo (QMC) method.

Above the upper critical dimension, a finite-size scaling (FSS) should be modified because of a dangerous irrelevant variable [7]. In contrast to the conventional FSS below d_u, the modified finite-size scaling (MFSS) [8] is not justified by renormalization group or scaling theories. However, its validity has been demonstrated for the five-dimensional Ising model [7,9,10], the $O(n)$ model [11], and the ϕ^4 model in a large-N limit [9,12]. For the quantum phase transition with $z=1$, below the upper critical dimension, a simple application of the FSS is trivially possible by identifying the inverse temperature β as merely an additional dimension. Actually, to estimate the multicritical point quantitatively, Šmakov and Sørensen [13] applied the FSS with the additional argument β/L to the multicritical point in the $d=2$ case where the system is below the upper critical dimension because $d+z<4$. For the quantum phase transition with $z\neq 1$, below the upper critical dimension, the application of FSS is also possible with the additional argument β/L^z instead of β/L on the ground where the ratio between the correlation time ξ_τ and the correlation length ξ to the zth power is $\xi_\tau/\xi^z=O(1)$ [4]. Zhao *et al.* applied the FSS to the case of $z=2$ and $d=2$, which is just the upper critical dimension, and succeeded in estimating the phase boundary on the zero-temperature phase diagram of their model [14]. The purpose of the present paper is to demonstrate the validity of the MFSS in the case where $d>d_u$ and $z\neq 1$, both by Monte Carlo simulation and by exact solutions. We consider the case of $z=2$ and $d=3$, i.e., above the upper critical dimension. It seems a natural extension to add the argument β/L^2 to the scaling function of MFSS [15]. Namely, we assume that the singular part of the free energy F_s has the scaling form

$$F_s(r,\eta,\beta,L) \sim \tilde{Y}_F(\delta L^{(d+2)/2}, \eta L^{3(d+2)/4}, \beta/L^2) \qquad (1)$$

with a universal scaling function $\tilde{Y}_F$, where the definition of the free energy is $F\equiv -\ln \Xi$ with the partition function Ξ, r indicates the coefficient of the term including the square of the order parameter in the Hamiltonian [e.g., the chemical potential μ or the hopping amplitude t in model (2) described below], δ indicates the difference from the quantum critical point (e.g., $\delta=r-r_c$), and η is the field inducing the order parameter.

The critical exponents for the finite-temperature behavior at the quantum critical point should be identical to those of the mean-field theory, e.g., $\chi\sim T^{-3/2}$ where χ is susceptibility. However, as shown in Sec. III, the exponents derived by the limit $L\to\infty$ of the scaling form (e.g., $\chi\sim T^{-5/4}$) are different from those of the mean-field theory. The reason for this apparent contradiction is that scaling form (1) is valid only when $\beta/L^2=O(1)$. That is, we cannot infinitize L in Eq. (1) while keeping β finite. In this paper, we show that the application of MFSS to the $z=2$ quantum critical point is reliable if the condition of validity is satisfied, just as the conventional FSS is below the upper critical dimension.

In Sec. II, we define the N-component BH model. In Sec. III, we focus on the $N=1$ case and show the application of the MFSS to the numerical result of the QMC simulation. In Sec. IV, we focus on the $N=\infty$ case, which is exactly solvable even for finite systems, to show that the susceptibility

*katoyasu@issp.u-tokyo.ac.jp

 ©2010 The American Physical Society

obeys the MFSS form. In Sec. V, we give a discussion and summary of this paper.

II. *N*-COMPONENT BOSE-HUBBARD MODEL

We consider the N-component BH model on the hypercubic lattice with a Hamiltonian is described as

$$\mathcal{H}_N = -\frac{t}{Z}\sum_{\alpha=1}^{N}\sum_{\langle i,j\rangle}(b_{\alpha i}^{\dagger}b_{\alpha j} + b_{\alpha i}b_{\alpha j}^{\dagger}) - \mu\sum_{\alpha=1}^{N}\sum_{i} b_{\alpha i}^{\dagger}b_{\alpha i} + \frac{U}{2N}\sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}\sum_{i} b_{\alpha i}^{\dagger}b_{\beta i}^{\dagger}b_{\beta i}b_{\alpha i}, \tag{2}$$

where $b_{\alpha i}^{\dagger}(b_{\alpha i})$ creates (annihilates) an α-type boson at site i, and $\langle i,j\rangle$ runs over all pairs of nearest-neighbor sites. The symbols t, U, and μ denote the hopping amplitude, the on-site interaction between bosons, and the chemical potential, respectively. The coordination number in the hypercubic lattice is $Z=2d$. We take the lattice spacing as our unit of distance. For concreteness, we consider only the three-dimensional case in this paper (i.e., $Z=6$). The generalization to arbitrary dimensions should be straightforward.

Here, we define the free energy F_η as

$$F_\eta \equiv -\frac{1}{N}\ln \mathrm{Tr}[e^{-\beta(\mathcal{H}_N-\eta\mathcal{Q})}], \tag{3}$$

$$\mathcal{Q} \equiv \sum_{\alpha=1}^{N}\sum_{i}(b_{\alpha i}^{\dagger} + b_{\alpha i}), \tag{4}$$

with the field η inducing the order parameter.

The N-component BH model (2) is solvable in the large-N limit. In Sec. IV, we demonstrate that MFSS (1) exactly describes the asymptotic behavior of model (2) in the large-N limit. We note here that an exactly solvable model similar to the present one was investigated in the 1980s [16,17]. The model was defined with Bose field operators in the continuous space. In those papers, the critical behavior in the thermodynamic limit near the quantum critical point was discussed. As a result, the mean-field-type criticality was confirmed above the upper critical dimension (e.g., $\chi\sim\delta^{-1}$).

III. NUMERICAL VERIFICATION OF MODIFIED FINITE-SIZE SCALING

In this section, we apply MFSS to the result of QMC simulation for the single-component BH model [18,19]. We focus on the superfluid to Mott-insulator transition. The zero-temperature phase diagram is shown in Fig. 2; it consists of Mott lobes and a superfluid region. The phase boundary was estimated using the Mott gap [6]. At the tip of the Mott lobe, which is a multicritical point, the dynamical critical exponent z is 1 because of the asymptotic particle-hole symmetry [4,13]. The rest of the critical lines correspond to the generic transition with the dynamical critical exponent $z=2$. In this section, we fix the chemical potential as $\mu/U=0.1$ and vary the hopping amplitude t/U. Namely, δ in the first argument of the scaling functions corresponds to $\delta=t/U-(t/U)_c$ in the present case.

We study compressibility κ and susceptibility χ. Their definitions are

$$\kappa \equiv \frac{1}{\rho^2}\frac{\partial\rho}{\partial\mu} \tag{5}$$

and

$$\chi \equiv -\frac{1}{2L^d\beta}\frac{\partial^2 F_\eta}{\partial\eta^2}\bigg|_{\eta=0}, \tag{6}$$

where

$$\rho \equiv -\frac{1}{L^d\beta}\frac{\partial F_0}{\partial\mu}. \tag{7}$$

The scaling forms of κ and χ are derived using the scaling form of the free energy (1) as

$$\kappa \sim \tilde{Y}_\kappa(x,y), \quad \chi \sim L^{5/2}\tilde{Y}_\chi(x,y), \tag{8}$$

where

$$x = \delta L^{5/2}, \quad y = \frac{\beta t}{L^2}. \tag{9}$$

We fix the second argument as $y=0.375$ and estimate the critical value of t/U as $(t/U)_c=0.088\,935(7)$ at $\mu/U=0.1$ by MFSS of κ and χ, as shown in Figs. 1(a) and 1(b). In these plots, we used the mean-field values for the exponents, leaving the critical value of t/U as the only fitting parameter.

It is also possible to estimate the positions of the quantum critical points using the Mott gap [5]. To compare the estimations using the Mott gap and MFSS, we estimate the Mott gap at $t/U=0.088\,935$ and $\mu/U=0.5$, and plot the corresponding points in the inset of Fig. 2. As we can see in the figure, the agreement is very good.

Here, a remark on the range of validity of the MFSS form is appropriate. We consider the finite-temperature behavior of χ at the quantum critical point $\delta=0$. If we neglect the applicability condition of the MFSS form and take the limit $L\to\infty$ while keeping βt finite, the finite-temperature dependence of χ is derived as

$$\chi \sim L^{5/2}\left(\frac{\beta t}{L^2}\right)^{5/4} \sim T^{-5/4}(\mathrm{error}) \tag{10}$$

from the scaling form (8). This exponent, $-5/4$, is different from that of mean-field theory, $-3/2$. As shown in Sec. IV, the reason for this error is that scaling form (8) or (1) is valid only under the condition of $\beta t/L^2=O(1)$. To confirm the mean-field exponent, we show the finite-temperature dependence of χ at the quantum critical point in Fig. 3.

The superfluid density ρ_S is one of the most important quantities characterizing superfluidity. However, it is not straightforward to derive the MFSS form of ρ_S because it is not directly obtained from the free energy by simple differentiation. The superfluid density ρ_S is proportional to the fluctuation of the winding number $\boldsymbol{W}=(W_x,W_y,W_z)$ and is defined as $\rho_S\equiv\langle \boldsymbol{W}^2\rangle/(\beta t L)$ within the framework of QMC simulation [20]. In Appendix B, we show that $\rho_S=\chi/(\beta L^d)$,

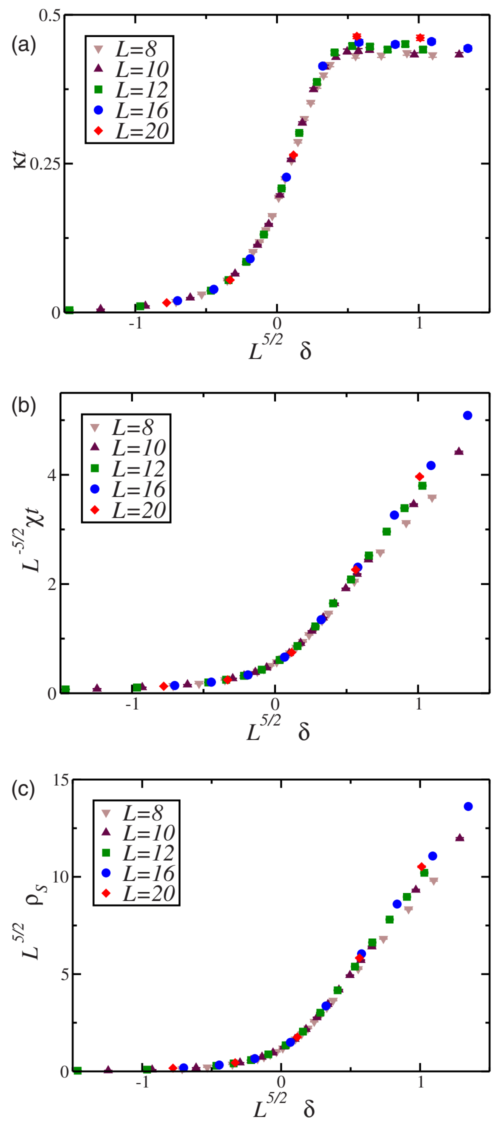

FIG. 1. (Color online) MFSS plots of single-component BH model where $\mu/U=0.1$ and $\beta t/L^2=0.375$. $\delta \equiv t/U-(t/U)_c$ with $(t/U)_c=0.088\,935$. (a) Compressibility, (b) susceptibility, and (c) superfluid density.

for model (2) in the large-N limit under the condition, $\beta t/L^2 \geq O(1)$, $d>2$, and $\beta t \gg 1$. By MFSS for χ, we obtain

$$\rho_S \sim L^{-5/2}\tilde{Y}_{\rho_S}(x,y). \tag{11}$$

Although this form is derived only for the exactly solvable model, we believe that it holds in general for the mean-field-type critical behavior. We apply this MFSS form to the result of ρ_S estimated by QMC simulations. As can be seen in Fig. 1(c), MFSS (11) describes the data well.

IV. LARGE-N LIMIT OF N-COMPONENT BOSE-HUBBARD MODEL

In this section, we consider model (2), which is known to exhibit a mean-field-type critical phenomenon, to see whether MFSS is applicable to such a model. We consider

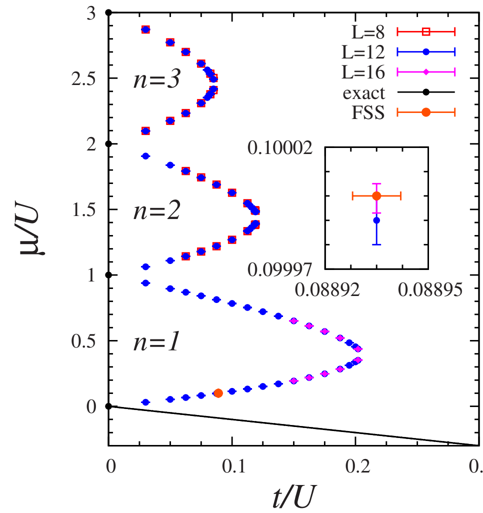

FIG. 2. (Color online) Zero-temperature phase diagram of single-component BH model in three dimensions. Almost all the quantum critical points ($L=8$,12, and 16), which is estimated using the Mott gap, is from our previous paper [6]. FSS indicates the result of MFSS. Inset is an enlarged view of the region near the critical point estimated by MFSS in Fig. 1.

the model on the d-dimensional hypercubic lattice in the large-N limit and show that the MFSS form Eq. (1) is exactly applicable to this case. To derive the self-consistent equation of χ in the large-N limit, we represent the partition function as a functional integral by making use of a coherent state basis at first. Then, we use the Stratonovitch-Hubbard transformation and the saddle-point method, which is also called the steepest descent method. Thus, the self-consistent equation of susceptibility χ in the large-N limit is derived exactly as

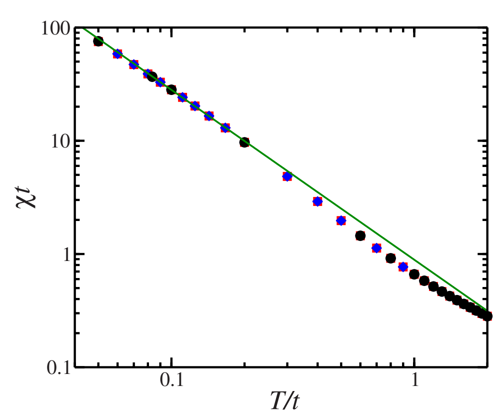

FIG. 3. (Color online) Temperature dependence of χ at the quantum critical point estimated by MFSS $[\mu/U=0.1,(t/U)_c=0.088\,935]$. The solid line is $A(T/t)^{-3/2}$, where $A=0.89$. The data points are obtained for $L=24$, 32, and 48. There is no visible size dependence on this scale. The statistical error is smaller than the size of symbols.

$$\chi^{-1} = -\mu - t + \frac{U}{L^d}\sum_{\mathbf{k}} \frac{1}{\exp\left[\beta\chi^{-1} + \frac{2\beta t}{Z}\sum_{\delta=1}^{d}(1-\cos k_\delta)\right] - 1}. \tag{12}$$

See Appendix A 1 for details of the derivation. By expanding the summand with respect to $\exp[-\{\beta\chi^{-1}+\frac{2\beta t}{Z}\Sigma_{\delta=1}^{d}(1-\cos k_\delta)\}]$, we obtain

$$\chi^{-1} = -\mu - t + \frac{U}{L^d}\sum_{\nu=1}^{\infty} e^{-\nu\beta\chi^{-1}} \times\left[\sum_{n=1}^{L}\exp\left\{-\frac{2\nu\beta t}{Z}\left[1-\cos\left(\frac{2\pi n}{L}\right)\right]\right\}\right]^d. \tag{13}$$

Below, we show that this equation has a solution such that $\chi \sim O((\beta t)^{(d+2)/4})$. Therefore, we assume $\chi \sim O((\beta t)^{(d+2)/4})$ for χ in the right-hand side (r.h.s.) of Eq. (13). Then, as shown in Appendix A 2, the approximation formula

$$\sum_{\nu=1}^{\infty} e^{-\nu\beta\chi^{-1}}\left[\sum_{n=1}^{L}\exp\left\{-\frac{2\nu\beta t}{Z}\left[1-\cos\left(\frac{2\pi n}{L}\right)\right]\right\}\right]^d \simeq \beta^{-1}\chi \tag{14}$$

becomes exact in the limit $\beta t\to\infty$ under the condition that $d>2$, $\beta t/L^2 \geq O(1)$. Using the self-consistent Eq. (13) and approximation (14), we arrive at a simple equation, $\chi^{-1} = -\mu - t + U\chi\beta^{-1}L^{-d}$. Its solution can be cast into the form

$$\frac{\chi t}{Z} \simeq \left(\frac{\beta t}{Z}\right)^{(d+2/4)} P_\chi^{UZ/t}\left[\left(\frac{\beta t}{Z}\right)^{(d+2/4)} Z\left(-\frac{\mu}{t}-1\right), \left(\frac{\beta t}{L^2 Z}\right)^{-(d/2)}\right]$$
$$\simeq L^{(d+2/2)} P_\chi^{UZ/t}\left[L^{(d+2/2)} Z\left(-\frac{\mu}{t}-1\right), \frac{\beta t}{L^2 Z}\right], \tag{15}$$

with the scaling function

$$P_\chi^{u}(x,y) \equiv \frac{2}{x+\sqrt{x^2+4uy^{-1}}}. \tag{16}$$

At the critical point $(\mu=-t)$, we obtain $\chi t \sim (\beta t)^{(d+2)/4} \times (\beta t/L^2)^{-d/4}$. To make this consistent with $\chi = O((\beta t)^{(d+2)/4})$ assumed initially and the condition $\beta t/L^2 \geq O(1)$, we must set $\beta t/L^2 = O(1)$. Thus, we have proved that Eq. (13) has the solution $\chi = O((\beta t)^{(d+2)/4})$ that satisfies Eq. (15), and MFSS form (8) has been derived as a formula that is asymptotically exact under the conditions of $d>2$ and $\beta t/L^2 = O(1)$.

To verify the validity of the form of scaling function (16), we demonstrate the MFSS plot of susceptibility in $d=3$. We solve the self-consistent Eq. (13) without using Eq. (14) and plot the results in Figs. 4(a) and 4(b). As shown in Fig. 4(b), the MFSS form fits well in the region $\beta t/L^2 = O(1)$.

V. DISCUSSION AND SUMMARY

In Secs. III and IV, we demonstrated that MFSS (1) is efficient in locating quantum critical points with the dynamical critical exponent $z=2$. It has been shown that MFSS is valid only if the second argument of scaling function $\beta t/L^2$ is $O(1)$. In particular, it is not permitted to infinitize L in scaling forms (8) and (11) while β is constant. This explains the apparent contradiction between MFSS and the mean-field critical exponents. It should be noted here that similar situations appear in classical models. Suppose we attempt to apply MFSS to a finite-temperature phase transition of a classical system and infinitize the system size in some (not all) of the directions while keeping the size in other directions fixed [15,21]. Singh and Pathria [21] considered a system of size $L^{d-d'} \times L'^{d'}$, where d is larger than the upper critical dimension and d' is less than the lower critical dimension. They analyzed a spin model with $O(n)$ symmetry in the limit of $L'\to\infty$ [21]. Then they derived the scaling form of susceptibility χ_0 as

$$\chi_0 \sim L^{[2(d-d')/(4-d')]} Y_{\chi_0}^{d'}(\tilde{t}L^{[2(d-d')/(4-d')]}), \tag{17}$$

where $\tilde{t} \equiv (T-T_c)/T_c$. Then, $\chi_0 \sim L^{2(d-d')/(4-d')}$ at the critical point $\tilde{t}=0$. On the other hand, if we keep L/L' finite, the MFSS form is

$$\chi_0 \sim L^{d/2}\bar{Y}_{\chi_0}^{d'}(\tilde{t}L^{d/2}, L/L'), \tag{18}$$

with the additional argument L/L' [15]. If we ignore the validity condition of MFSS (18) and take the limit $L'\to\infty$, we reach an erroneous conclusion, that is, $\chi_0 \sim L^{d/2}$ at $\tilde{t}=0$.

In summary, MFSS is applied to the quantum critical phenomenon with the dynamical critical exponent $z=2$. Using

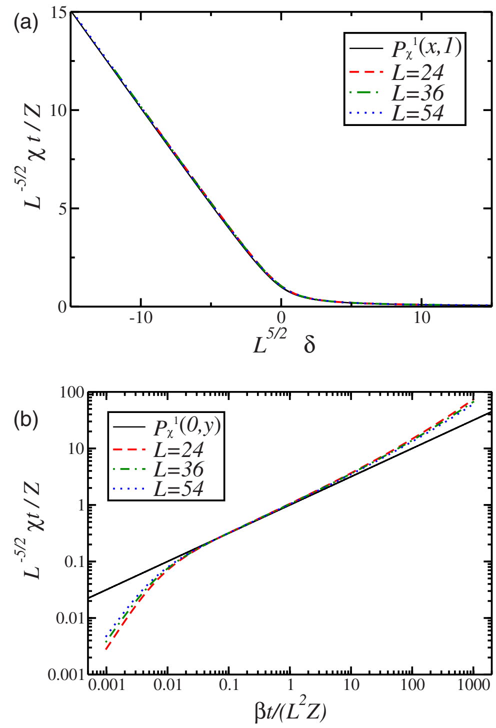

FIG. 4. (Color online) MFSS plots of susceptibility at $U/(t/Z) = 1$. (a) The x dependence of scaling function of susceptibility $P_\chi^{UZ/t}(x,y)$ and the solution of self-consistent Eq. (13) with $y \equiv \beta t/(ZL^2) = 1$, (b) y dependence of $P_\chi^{UZ/t}(x,y)$ and the solution of self-consistent Eq. (13) at quantum critical point $\delta=0$.

the N-component BH model, the MFSS form of the susceptibility Eq. (15) is exactly derived in the large-N limit with the applicability conditions $d>2$ and $\beta t/L^2=O(1)$. We also apply MFSS to the numerical results obtained by QMC simulation. As a result, we see that the position of the quantum critical point estimated by MFSS is identical to that estimated using the Mott gap within the statistical error. Finally, note that the scaling function derived in this paper, $P_\chi^u(x,y)$, is in complete agreement with the scaling function of the ϕ^4 model reported in Ref. [9]. While the scaling function is not justified by the renormalization group or scaling theories in contrast to the standard FSS below the upper critical dimension, the agreement strongly indicates that the mean-field scaling function above the upper critical dimension is universal.

ACKNOWLEDGMENTS

The present work was financially supported by a MEXT Grant-in-Aid for Scientific Research (B) (Grant No. 19340109), a MEXT Grant-in-Aid for Scientific Research on Priority Area “Novel States of Matter Induced by Frustration” (Grant No. 19052004), a Grant-in-Aid for JSPS Fellows, and by the Next Generation Supercomputing Project, Nanoscience Program, MEXT, Japan. The quantum Monte Carlo simulations were executed at the Supercomputer Center, Institute for Solid State Physics, University of Tokyo.

APPENDIX A: CALCULATION OF LARGE-N LIMIT

1. Self-consistent equation of χ

Here, we derive the self-consistent Eq. (13) of Hamiltonian (2). The partition function is expressed as

$$Z_N=\int \mathcal{D}\boldsymbol{\psi}_i(\tau)\mathcal{D}\boldsymbol{\psi}_i^*(\tau)e^{-(S_0+S_1)},$$

$$S_0=\int_0^\beta d\tau\Bigg[\sum_i\{\boldsymbol{\psi}_i^*(\tau)\cdot(\partial_\tau\boldsymbol{\psi}_i(\tau))-\mu\boldsymbol{\psi}_i^*(\tau)\cdot\boldsymbol{\psi}_i(\tau)\}-\frac{t}{Z}\sum_{\langle i,j\rangle}(\boldsymbol{\psi}_i^*(\tau)\cdot\boldsymbol{\psi}_j(\tau)+\boldsymbol{\psi}_j^*(\tau)\cdot\boldsymbol{\psi}_i(\tau))\Bigg],$$

$$S_1=\int_0^\beta d\tau\frac{U}{2N}\sum_i[\boldsymbol{\psi}_i^*(\tau)\cdot\boldsymbol{\psi}_i(\tau)]^2, \tag{A1}$$

by the path-integral representation with $\boldsymbol{\psi}_i(\tau)$ being an N-component complex field. Using the Stratonovitch-Hubbard transformation, the partition function is written as

$$Z_N=\int \mathcal{D}\boldsymbol{\psi}_i(\tau)\mathcal{D}\boldsymbol{\psi}_i^*(\tau)\mathcal{D}s_i(\tau)e^{-S_0}\times\exp\Bigg[-\int_0^\beta d\tau\Bigg\{\sum_i\Bigg\{\frac{N}{2}s_i^2(\tau)-i\sqrt{U}s_i(\tau)[\boldsymbol{\psi}_i^*(\tau)\cdot\boldsymbol{\psi}_i(\tau)]\Bigg\}\Bigg\}\Bigg],$$

$$Z_N=\int\mathcal{D}s_i(\tau)e^{-(N/2)\int_0^\beta d\tau\sum_i s_i^2(\tau)}[Z_1(\{s\})]^N, \tag{A2}$$

$$Z_1[(s)]\equiv\int\mathcal{D}\psi_i^\alpha(\tau)\mathcal{D}\psi_i^{\alpha*}(\tau)\exp\Bigg[-\int_0^\beta d\tau\Bigg[\sum_i\{\psi_i^{\alpha*}(\tau)\times[\partial_\tau\psi_i^\alpha(\tau)]-[\mu+i\sqrt{U}s_i(\tau)]\psi_i^{\alpha*}(\tau)\psi_i^\alpha(\tau)\}-\frac{t}{Z}\sum_{\langle i,j\rangle}[\psi_i^{\alpha*}(\tau)\psi_j^\alpha(\tau)+\psi_j^{\alpha*}(\tau)\psi_i^\alpha(\tau)]\Bigg]\Bigg], \tag{A3}$$

where $s_i(\tau)$ is an auxiliary field and the integral with respect to $s_i(\tau)$ is defined as

$$\int\mathcal{D}s_i(\tau)=\prod_{i,\tau}\sqrt{\frac{N}{2\pi}}\int_{-\infty}^{\infty}ds_i(\tau). \tag{A4}$$

In the large-N limit, by the saddle-point method, the auxiliary field $s_i(\tau)$ is replaced by $\bar{s}$ (see Ref. [12] and its references), which makes the exponents of the partition function maximum. Using Fourier transformation, we obtain

$$Z_N=Ae^{-(N\beta L^d/2)\bar{s}^2}[Z_1(\bar{s})]^N, \tag{A5}$$

$$Z_1(\bar{s})=\prod_{\boldsymbol{k}}(1-e^{-\beta\lambda_{\boldsymbol{k}}})^{-1}, \tag{A6}$$

$$\lambda_{\boldsymbol{k}}=-\mu-i\sqrt{U}\bar{s}-\frac{2t}{Z}\sum_{\delta=1}^{d}\cos k_\delta, \tag{A7}$$

where A is a real number originating from the fluctuation of $s_i(\tau)$ from $\bar{s}$, and does not contribute to the following discussion, and the product of $\boldsymbol{k}$ runs over the first Brillouin zone $\boldsymbol{k}=(2\pi/L)(m_1,\cdots,m_d)$, with $m_i=1,2,\cdots,L$. The stationary solution $\bar{s}$ must satisfy

$$\frac{\partial}{\partial\bar{s}}\Bigg[-\frac{N\beta L^d}{2}\bar{s}^2-\sum_{\boldsymbol{k}}\ln(1-e^{-\beta\lambda_{\boldsymbol{k}}})\Bigg]=0, \tag{A8}$$

which yields

$$\bar{s}=\frac{i\sqrt{U}}{L^d}\sum_{\boldsymbol{k}}[e^{\beta\lambda_{\boldsymbol{k}}}-1]^{-1}. \tag{A9}$$

The susceptibility χ is related to $\bar{s}$ by

$$\chi\equiv\frac{1}{N}\int_0^\beta d\tau\sum_i\langle\boldsymbol{\psi}_i^*(\tau)\cdot\boldsymbol{\psi}_0(0)\rangle=(-\mu-t-i\sqrt{U}\bar{s})^{-1}. \tag{A10}$$

Therefore, χ satisfies

$$\chi^{-1}=-\mu-t+\frac{U}{L^d}\sum_{\boldsymbol{k}}\frac{1}{\exp\Bigg[\frac{2\beta t}{Z}\sum_{\delta=1}^{d}(1-\cos k_\delta)+\beta\chi^{-1}\Bigg]-1}. \tag{A11}$$

2. Derivation of Eq. (14)

In Sec. IV, we derived $\chi=O((\beta t/Z)^{(2+d)/4})$ by self-consistent analysis. Namely, assuming the condition χ

$=O((\beta t/Z)^{(2+d)/4})$, we proved the resulting solution satisfies this condition. Here, assuming

$$(\beta t/Z)^{(2+d)/4}\chi^{-1}=O(1), \tag{A12}$$

we provide the approximation form

$$\sum_{\nu=1}^{\infty} e^{-\nu\beta\chi^{-1}}\left[\sum_{n=1}^{L}\exp\left\{-\frac{2\nu\beta t}{Z}\left[1-\cos\left(\frac{2\pi n}{L}\right)\right]\right\}\right]^{d}\simeq\beta^{-1}\chi, \tag{A13}$$

which becomes exact under the conditions that

$$d>2, \tag{A14}$$

$$\beta t/L^2\geq O(1), \tag{A15}$$

and

$$\beta t\gg 1. \tag{A16}$$

To begin with, we rewrite the left-hand side as

$$\begin{aligned}\sum_{\nu=1}^{\infty} e^{-\nu\beta\chi^{-1}}&\left[\sum_{n=1}^{L}\exp\left\{-\frac{2\nu\beta t}{Z}\left[1-\cos\left(\frac{2\pi n}{L}\right)\right]\right\}\right]^{d}\\ &=\sum_{\nu=1}^{\infty} e^{-\nu\beta\chi^{-1}}(1+A_\nu)^d,\\ &=\sum_{\nu=1}^{\infty} e^{-\nu\beta\chi^{-1}}+\sum_{\nu=1}^{\infty} e^{-\nu\beta\chi^{-1}}\left[\sum_{\alpha=1}^{d}\frac{d!}{\alpha\,!\,(d-\alpha)!}A_\nu^\alpha\right],\end{aligned} \tag{A17}$$

where

$$A_\nu\equiv e^{-4\nu\beta t/Z}+2\sum_{n=1}^{-1+L/2}\exp\left[-\frac{2\nu\beta t}{Z}\left\{1-\cos\left(\frac{2\pi n}{L}\right)\right\}\right]. \tag{A18}$$

Here, we note that $\beta\chi^{-1}\simeq 0$. [This is because $\beta\chi^{-1}=O((\beta t)^{-(d-2)/4})$ [because of condition (A12)], and because of condition (A14), it vanishes in the limit of Eq. (A16).] Since $\beta\chi^{-1}\simeq 0$, the first term of the r.h.s. of Eq. (A17) is approximated by

$$\sum_{\nu=1}^{\infty} e^{-\nu\beta\chi^{-1}}=\beta^{-1}\chi+O((\beta\chi^{-1})^0)=O((\beta t)^{(d-2)/4}). \tag{A19}$$

Below, we show that the second term of Eq. (A17) is a correction term that vanishes in the limit of $\beta t\to\infty$. At first, A_ν is bounded as

$$\begin{aligned}0<A_\nu&\leq 2\sum_{n=1}^{L/2}\exp\left[-\frac{2\nu\beta t}{Z}\left\{1-\cos\left(\frac{2\pi n}{L}\right)\right\}\right],\\ 0&\leq 2\int_0^{L/2}dp\,\exp\left[-\frac{2\nu\beta t}{Z}\left\{1-\cos\left(\frac{2\pi p}{L}\right)\right\}\right],\\ 0&\leq 2\int_0^{L/2}dp\,\exp\left[-\frac{2\nu\beta t}{Z}\left(\frac{8p^2}{L^2}\right)\right],\\ 0&\leq\sqrt{\frac{\pi L^2 Z}{16\nu\beta t}}.\end{aligned} \tag{A20}$$

Then, the second term of Eq. (A17) is evaluated as

$$\begin{aligned}0&<\sum_{\alpha=1}^{d}\frac{d!}{\alpha\,!\,(d-\alpha)!}\left[\sum_{\nu=1}^{\infty}e^{-\nu\beta\chi^{-1}}A_\nu^\alpha\right],\\ &\leq\sum_{\alpha=1}^{d}\frac{d!}{\alpha\,!\,(d-\alpha)!}\left[\sum_{\nu=1}^{\infty}e^{-\nu\beta\chi^{-1}}\left\{\frac{\pi L^2Z}{16\nu\beta t}\right\}^{\alpha/2}\right],\\ &\leq\sum_{\alpha=1}^{d}\frac{d!}{\alpha\,!\,(d-\alpha)!}\left\{\frac{\pi L^2 Z}{16\beta t}\right\}^{\alpha/2}\left[\int_0^\infty dp e^{-p\beta\chi^{-1}}p^{-\alpha/2}\right],\\ &=\sum_{\alpha=1}^{d}\frac{d!}{\alpha\,!\,(d-\alpha)!}\left\{\frac{\pi Z}{16(\beta t/L^2)}\right\}^{\alpha/2}\left[\int_0^\infty dq e^{-q}q^{-\alpha/2}\right]\\ &\quad\times(\beta\chi^{-1})^{(\alpha-2/2)}.\end{aligned} \tag{A21}$$

Since $\beta t/L^2\geq O(1)$ and $\beta\chi^{-1}\ll 1$, the $\alpha=1$ term is dominant. Therefore, the second term is of the same order as $(\beta t/L^2)^{-1/2}(\beta\chi^{-1})^{-1/2}$. Because of condition (A12), this is $O((\beta t/L^2)^{-1/2}\times(\beta t)^{(d-2)/8})$. Therefore, the ratio of the second to the first term of Eq. (A17) becomes less than $O((\beta t/L^2)^{-1/2}\times(\beta t)^{-(d-2)/8})$. This vanishes because of conditions (A14), (A15), and (A16). Thus Eq. (A13) is derived.

APPENDIX B: SCALING FUNCTION OF SUPERFLUID DENSITY IN LARGE-N LIMIT

In this section, we provide the MFSS form of superfluid density using the N-component BH model. The outline of this section is as follows. First, we obtain the explicit definition of superfluid density, which is estimated using the winding number in the QMC simulation, with an infinitesimal twist of the phase of the bosonic operator. Next, we calculate the superfluid density of the N-component BH model exactly. The result reveals that the superfluid density ρ_S is proportional to the susceptibility χ. Then, we derive the MFSS form of ρ_S as that of χ.

To start with, we derive an expression for the superfluid density ρ_S, introducing an infinitesimal twist of the phase of the bosonic operators. Namely, we modify Hamiltonian (2) by $b_{\alpha i}^\dagger\to b_{\alpha i}^\dagger e^{i\theta r_i^z}$, $b_{\alpha i}\to b_{\alpha i}e^{-i\theta r_i^z}$, where r_i^z is the z coordinate of site i. (Because of the periodic boundary condition, θ should be discrete. That is, $\theta=2\pi n/L$, where n is an integer. However, considering a sufficiently large system, we regard θ as a continuous real number.) Then, we define the twisted Hamiltonian $\mathcal{H}_{N\theta}$, the partition function $Z_{N\theta}$ and the free energy $F_{N\theta}$ as

$$\mathcal{H}_{N\theta} = -\frac{t}{Z}\sum_{\alpha=1}^{N}\sum_{\langle i,j\rangle}(b_{\alpha i}^{\dagger}b_{\alpha j}e^{i\theta(r_i^z-r_j^z)} + b_{\alpha i}b_{\alpha j}^{\dagger}e^{-i\theta(r_i^z-r_j^z)}) - \mu\sum_{\alpha=1}^{N}\sum_{i}b_{\alpha i}^{\dagger}b_{\alpha i} + \frac{U}{2N}\sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}\sum_{i}b_{\alpha i}^{\dagger}b_{\beta i}^{\dagger}b_{\beta i}b_{\alpha i}, \quad \text{(B1)}$$

$$Z_{N\theta} = \mathrm{Tr}[e^{-\beta\mathcal{H}_{N\theta}}], \quad \text{(B2)}$$

$$F_{N\theta} = -\frac{1}{N}\ln Z_{N\theta}. \quad \text{(B3)}$$

The superfluid density ρ_S is defined with this twisted free energy $F_{N\theta}$ as

$$\rho_S \equiv \frac{1}{2\beta L^d(t/Z)}\left.\frac{\partial^2 F_{N\theta}}{\partial\theta^2}\right|_{\theta=0}. \quad \text{(B4)}$$

Next, we calculate ρ_S in the large-N limit. The partition function $Z_{N\theta}$ is obtained, as well as the nontwisted partition function (see Appendix A 1), as

$$Z_{N\theta} = Ae^{-(N\beta L^d/2)\bar{s}^2}[Z_{1\theta}(\bar{s})]^N, \quad \text{(B5)}$$

$$Z_{1\theta}(\bar{s}) = \prod_{\boldsymbol{k}}(1 - e^{-\beta\lambda_{\boldsymbol{k}\theta}})^{-1}, \quad \text{(B6)}$$

$$\lambda_{\boldsymbol{k}\theta} = -\mu - i\sqrt{U}\bar{s} - \frac{2t}{Z}\sum_{\delta=1}^{d-1}\cos k_\delta - \frac{2t}{Z}\cos(k_z+\theta). \quad \text{(B7)}$$

The derivation of the free energy is straightforward using this partition function. Then, we obtain the superfluid density as

$$\rho_S = \frac{1}{L^d}\sum_{\boldsymbol{k}}\frac{\cos k_z}{e^{\beta\lambda_{\boldsymbol{k}}} - 1} \quad \text{(B8)}$$

with $\lambda_{\boldsymbol{k}}$ defined in Eq. (A7). This superfluid density is lower than the total density of particles,

$$\rho \equiv -\frac{1}{L^d\beta}\frac{\partial F_{N\theta=0}}{\partial\mu}, = \frac{1}{L^d}\sum_{\boldsymbol{k}}\frac{1}{e^{\beta\lambda_{\boldsymbol{k}}} - 1}, \quad \text{(B9)}$$

and larger than the density of particles of $\boldsymbol{k}=0$,

$$\rho_0 = \frac{1}{L^d}\frac{1}{e^{\beta\chi^{-1}} - 1}. \quad \text{(B10)}$$

That is,

$$\rho_0 \le \rho_S \le \rho. \quad \text{(B11)}$$

As shown in Appendix A 2,

$$\rho = \rho_0 = \frac{\chi}{L^d\beta}, \quad \text{(B12)}$$

under the conditions $\beta t/L^2 \ge O(1)$, $d>2$, and $\beta t \to \infty$. Using inequality (B11), we obtain

$$\rho_S = \frac{\chi}{L^d\beta}. \quad \text{(B13)}$$

As shown in Sec. IV, we derive the MFSS form of ρ_S as

$$\rho_S = L^{-(d+2)/2}P_{\rho_S}^{UZ/t}\left(L^{(d+2/2)}Z\left(-\frac{\mu}{t} - 1\right), \frac{\beta t}{L^2 Z}\right), \quad \text{(B14)}$$

$$P_{\rho_S}^{u}(x,y) \equiv \frac{2y^{-1}}{x + \sqrt{x^2 + 4uy^{-1}}}. \quad \text{(B15)}$$

The applicability conditions of this MFSS form are $d>2$ and $\beta t/L^2 = O(1)$.

[1] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature (London) **415**, 39 (2002).
[2] Y. Kato, Q. Zhou, N. Kawashima, and N. Trivedi, Nat. Phys. **4**, 617 (2008).
[3] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
[4] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).
[5] B. Capogrosso-Sansone, N. V. Prokof'ev, and B. V. Svistunov, Phys. Rev. B **75**, 134302 (2007).
[6] N. Kawashima and Y. Kato, J. Phys.: Conf. Ser. **143**, 012012 (2009).
[7] K. Binder, M. Nauenberg, V. Privman, and A. P. Young, Phys. Rev. B **31**, 1498 (1985).
[8] J. G. Brankov, D. M. Danchev, and N. S. Tonchev, *Theory of Critical Phenomena in Finite-Size Systems Scaling and Quantum Effects* (World Scientific, Singapore, 2000), Chap. 6.
[9] E. Luijten, K. Binder, and H. W. J. Blöte, Eur. Phys. J. B **9**, 289 (1999).
[10] J. L. Jones and A. P. Young, Phys. Rev. B **71**, 174438 (2005).
[11] S. Singh and R. K. Pathria, Phys. Rev. B **38**, 2740 (1988).
[12] X. S. Chen and V. Dohm, Eur. Phys. J. B **5**, 529 (1998).
[13] J. Šmakov and E. Sørensen, Phys. Rev. Lett. **95**, 180603 (2005).
[14] J. Zhao, A. W. Sandvik, and K. Ueda, e-print arXiv:0806.3603.
[15] K. Binder and J.-S. Wang, J. Stat. Phys. **55**, 87 (1989).
[16] M. Zannetti, Phys. Rev. B **22**, 5267 (1980).
[17] L. D. Cesare, Nuovo Cimento D **1**, 289 (1982).
[18] Y. Kato, T. Suzuki, and N. Kawashima, Phys. Rev. E **75**, 066703 (2007).
[19] Y. Kato and N. Kawashima, Phys. Rev. E **79**, 021104 (2009).
[20] E. L. Pollock and D. M. Ceperley, Phys. Rev. B **36**, 8343 (1987).
[21] S. Singh and R. K. Pathria, Phys. Rev. B **34**, 2045 (1986).