Phase Diagram of a Disordered Boson Hubbard Model in Two Dimensions

Ji-Woo Lee,[1] Min-Chul Cha,[2] and Doochul Kim[1]

[1]*School of Physics and Center for Theoretical Physics, Seoul National University, Seoul 151-742, Korea*

[2]*Department of Physics, Hanyang University, Kyunggi-do, Ansan 425-791, Korea*

(Received 29 May 2001; published 26 November 2001)

We study the zero-temperature phase transition of a two-dimensional disordered boson Hubbard model. The phase diagram is constructed in terms of the disorder strength and the chemical potential. Via Monte Carlo simulations, we find a multicritical line separating the weak-disorder regime, where the Mott-insulator-to-superfluid transition occurs, from the strong-disorder regime, where the Bose-glass-to-superfluid transition occurs. On the multicritical line, the insulator-to-superfluid transition has the dynamical critical exponent $z = 1.35 \pm 0.05$ and the correlation length critical exponent $\nu = 0.67 \pm 0.03$. We suggest that the proliferation of the particle-hole pairs screens out the weak-disorder effects.

DOI: 10.1103/PhysRevLett.87.247006 PACS numbers: 74.20.De, 73.43.Nq, 74.40.+k

The boson localization due to a random potential has continuously attracted significant attention as a paradigm of the zero-temperature quantum phase transition [1]. The superconductor-insulator transition has been believed to be a manifestation of the boson localization transition. Two-dimensional realization of this transition may be found in disordered thin-film superconductors [2], Josephson-junction arrays [3], and ^{4}He films adsorbed in porous media [4]. An interacting boson model, called the boson Hubbard model, has been proposed [5] to describe the transition between an insulator and a superfluid (SF). In the disorder-free case, the insulating ground state is a Mott insulator (MI), which has commensurate boson density and a finite Mott gap which suppresses the excitations of freely moving particles or holes. As the gap vanishes the system becomes a superfluid. In the presence of disorder, even with a vanishing energy gap, particles or holes excited can be localized by a random potential, resulting in a Bose glass (BG) insulator.

The interplay of interaction and disorder has attracted considerable interest in this model. It has been argued that in the presence of disorder the transition from the insulating to the superfluid state occurs only through the BG phase on the assumption that arbitrarily weak disorder is always relevant in two dimensions [5]. Recently, however, quantum Monte Carlo studies of the boson Hubbard model in the Villain representation have shown that transitions at [6] or near [7] the tip of the MI lobes, the points with the particle-hole symmetry, are most likely direct from the MI state to the SF state for weak disorder. Path-integral quantum Monte Carlo simulations [8] and real-space renormalization calculations [9,10] of the boson Hubbard model support the scenario of the direct MI-SF transition at the tips. A simple scaling argument combined with renormalization calculation at the mean-field level predicts [11] that the direct MI-SF is possible around the tip of the MI lobe in high dimensions ($d > 4$) while it is possible only at the tip in low dimensions ($2 \leq d < 4$). Field-theoretical renormalization group studies at the tip, on the other hand, show that disorder is always relevant in two dimensions [12,13]. Strong-expansion studies suggest that the direct transition is always unlikely to occur in the presence of disorder [14]. Similar problems in one dimension have also attracted considerable interest recently [15]. Here, it appears that a direct MI-SF transition is not supported.

In this work, we investigate the onset of the superfluidity in a two-dimensional boson Hubbard model in the presence of disorder via quantum Monte Carlo simulations which employ a (2 + 1)-dimensional classical action. We find that a multicritical line exists, separating the weak-disorder regime from the strong-disorder regime, and on the line, the insulator-to-superfluid transition is associated with novel values of the critical exponents: i.e., $z = 1.35 \pm 0.05$ and $\nu = 0.67 \pm 0.03$, where z and ν are the dynamical and the correlation length critical exponents, respectively. These results are summarized in Fig. 1. It shows that the direct MI-SF transition survives around the

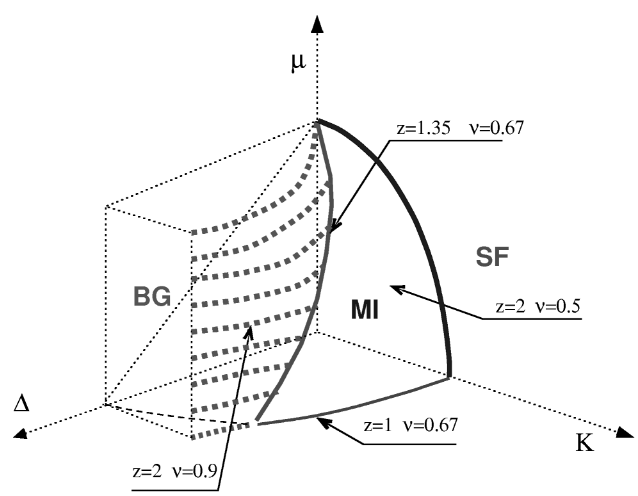

FIG. 1. Schematic phase diagram of a disordered boson Hubbard model. Here μ is the chemical potential, Δ is the strength of disorder, and K is the parameter characterizing the hopping of bosons. The particle-hole symmetry is defined by the condition $\mu = 0$. The multicritical line separates the critical surface into the direct MI-SF transition region and the BG-SF transition region.

tip of the MI lobe for weak disorder. This means that the weak disorder is irrelevant for the localization transition in two-dimensional interacting boson systems that have near integer fillings. Strong disorder changes the nature of the transition to that of the BG-SF transition.

We consider a boson Hubbard model on the two-dimensional square lattice, given by the Hamiltonian

$$H = \frac{1}{2}\sum_i U n_i^2 - \sum_i \mu_i n_i - \frac{t}{2}\sum_{\langle i,j\rangle}(b_i b_j^\dagger + b_i^\dagger b_j), \tag{1}$$

where $b_i^\dagger$ (b_i) denotes the boson creation (destruction) operator at site i ($n_i \equiv b_i^\dagger b_i$), μ_i denotes the local chemical potentials, U denotes the on-site repulsion energy, t denotes the hopping strength to the nearest neighbors, and finally the last sum is over nearest neighbor pairs. The disorder effect is embedded in local chemical potential as $\mu_i = \mu + v_i$, where v_i are random variables independently and uniformly distributed in the range $[-\Delta, \Delta]$. Thus Δ characterizes the strength of disorder.

To perform Monte Carlo simulations, we follow the standard procedure [16] to transform the two-dimensional Hamiltonian in Eq. (1) to the (2 + 1)-dimensional classical action

$$S = \frac{1}{2K}\sum_{(x,y,\tau)}^{\nabla\cdot\vec{J}=0}[\vec{J}^2(x,y,\tau) - 2(\mu + v_i)J^\tau(x,y,\tau)], \tag{2}$$

where x and y are spatial coordinates and τ is the imaginary-temporal coordinate. Here $K \sim \sqrt{t/U}$, analogous to the temperature in classical systems, and $\vec{J}(x,y,\tau)$ is the integer current vectors which measure the fluctuations along the corresponding direction of the components. In the transformation from Eq. (1) to Eq. (2) one assumes that superfluidity is destroyed only by phase fluctuations.

We are interested in the phase diagram of Eq. (2) in the space of (K, μ, Δ). The transition described by the classical action is studied by Monte Carlo simulations. We perform the simulations on the lattice of various sizes, denoted by $L \times L \times L_\tau$, where L and L_τ are sizes of the systems along a spatial and the imaginary-temporal axis, respectively. The periodic boundary conditions are adopted. In order to extract the critical properties of the transition, we analyze the data using the finite-size scaling theory. An important quantity which indicates the onset of the superfluidity is the superfluid stiffness, which is measured by the formula

$$\rho = \frac{1}{L_\tau}[\langle n_x^2\rangle]_{\mathrm{av}}, \tag{3}$$

where $n_x = (1/L)\sum_{(x,y,\tau)} J^x(x,y,\tau)$ is the winding number along the x direction. Here $[\ldots]_{\mathrm{av}}$ denotes the average over different realizations of disorder. The finite-size scaling behavior of the superfluid stiffness is given by [17]

$$\rho = L^{-(d+z-2)}\tilde{\rho}(L^{1/\nu}\delta, L_\tau/L^z), \tag{4}$$

where $\delta = (K - K_c)$ is the distance from the critical point K_c for each Δ and μ, $\tilde{\rho}$ is a scaling function, and d is the spatial dimension. Throughout this work, we set $d = 2$. Another useful quantity is the compressibility, which directly shows whether the Mott gap vanishes at the transition. It is given by the formula

$$\kappa = \frac{L_\tau}{L^d}[\langle n_\tau^2\rangle - \langle n_\tau\rangle^2]_{\mathrm{av}} \tag{5}$$

with $n_\tau = (1/L_\tau)\sum_{(x,y,\tau)} J^\tau(x,y,\tau)$, and is assumed to take the scaling form

$$\kappa = L^{z-d}\tilde{\kappa}(L^{1/\nu}\delta, L_\tau/L^z) \tag{6}$$

with another scaling function $\tilde{\kappa}$.

In order to investigate the scaling behavior of the superfluid stiffness and the compressibility, one must specify the dynamical critical exponent, z, in advance so as to fix the aspect ratio L_τ/L^z throughout the simulations. We have tried various values of z and have chosen the one which gives the best scaling behavior satisfying Eq. (4). For lattices with noninteger L_τ, the superfluid stiffness is obtained by a simple interpolation of the two values measured in the lattices of nearby integer sizes.

The effect of disorder at various strengths is investigated on the $\mu = 0$ plane. For strong disorder, say for $\Delta > 0.45$, the onset of superfluidity follows the BG-SF transition behavior with $z = 2$ and $\nu = 0.9$, and the compressibility is finite at the transition as suggested by the scaling argument [5] and confirmed by subsequent numerical simulations [16]. For $\Delta < 0.35$, however, the transitions take the signature of the direct MI-SF transition with $z = 1$ and $\nu = 0.67$, as reported in the recent simulations [6], while the compressibility vanishes at the transition. At the intermediate strength of disorder, naive scaling analysis using either $z = 1$ or $z = 2$ fails. In this work, we take a different approach and allow the possibility of intermediate values of z by varying the aspect ratio L_τ/L^z until the scaling plots collapse onto a single curve.

A new scaling behavior emerges, at the intermediate strength of disorder, which has $z = 1.35 \pm 0.05$ and $\nu = 0.67 \pm 0.03$. This scaling behavior is shown in Fig. 2. We observe the best scaling when $z = 1.35$. In addition, with this value of z, K_c's obtained from the scaling behavior of the superfluid stiffness and the compressibility data curves are consistent with each other. The compressibility vanishes at the transition as expected for $z < d$ [see Fig. 2(b)]. Kisker and Rieger reported [6] $z \approx 1.4$ for the intermediate strength of disorder, $\Delta = 0.4$. However, they interpreted the result as simply measuring an effective exponent. As we can see in Fig. 2, the robust finite-size scaling behavior for various sizes strongly suggests that the transition truly has new values of the critical exponents. In order to rule out the possibility that we are disguised by finite-size effects, we have performed simulations adopting

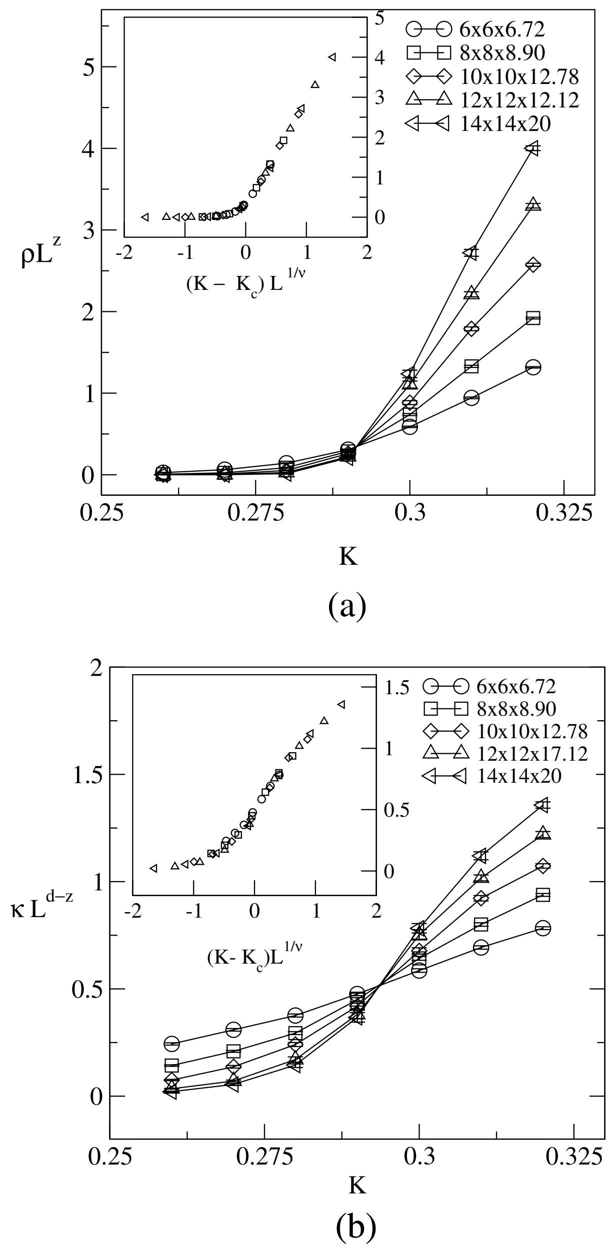

FIG. 2. The finite-size scaling behavior of (a) the superfluid stiffness and (b) the compressibility at the tip of the MI lobe ($\mu = 0$) with $\Delta = 0.40$. We set $z = 1.35$. The curves cross at $K_c = 0.292$. The insets show the scaled data along the K direction with $\nu = 0.67$.

a different aspect ratio and find the same critical exponents. The value of the correlation length critical exponent happens to be the same as the pure transition at the tip.

This behavior persists even off the tip ($\mu \neq 0$). The off-tip transition of the pure case, usually called the generic transition, is of a mean-field type, so that $z = 2$ and $\nu = 1/2$ for the MI-SF transition. If disorder is relevant, we expect in general that the correlation length critical exponent has a different value [18]. Thus, we can numerically identify the BG-SF transition from the MI-SF transition by measuring ν as well as by observing the compressibility. Previously Park *et al.* have reported [7] that even in the presence of weak disorder, the generic transition survives near the tip. As Δ increases, the generic MI-SF transition ends at the critical value, $\Delta_c(\mu)$, above which the BG-SF transition occurs.

The critical strength of disorder, $\Delta_c(\mu)$, therefore defines a multicritical line, separating the critical surface $K_c(\mu, \Delta)$ into the two regions: the strong-disorder region and the weak-disorder one. Figure 3 is the measured $\Delta_c(\mu)$. Numerically we find good scaling behaviors using the above exponents for a range of parameters (see Fig. 3 inset). The error bars in Fig. 3 show such ranges. We believe that, in larger systems, the finite range should shrink to a point. Otherwise, the existence of an incompressible localized phase other than the BG phase is required, which is unreasonable.

The existence of the multicriticality strongly suggests that in the presence of disorder two different universality classes exist, in one of which disorder is irrelevant. The irrelevance of weak disorder may be understood from the abundance of the particle-hole pairs excited. At the tips, the proliferation of particle-hole pairs near the transition modifies the particle propagation to yield $z = 1$ (otherwise $z = 2$) in the pure case. These particle-hole pairs may screen the disorder effects. In order to directly check the possibility that the proliferation of particle-hole pairs may screen out the weak-disorder effects, we have repeated Monte Carlo simulations of the classical model

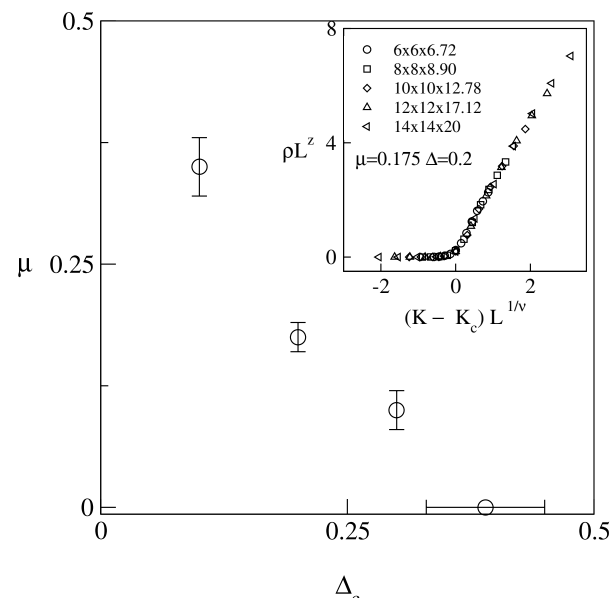

FIG. 3. The critical strength of disorder, $\Delta_c(\mu)$, as a function of the chemical potential μ. At the tip ($\mu = 0$), we have tuned the value of Δ to find the critical one. The error bar indicates the range in which the scaling plots show the behavior expected on the multicritical point. Off the tip μ is tuned instead, while Δ is fixed. Inset: the superfluid stiffness scaling curves away from the tip ($\mu = 0.175$) at $\Delta = 0.2$ with $z = 1.35$ and $\nu = 0.67$.

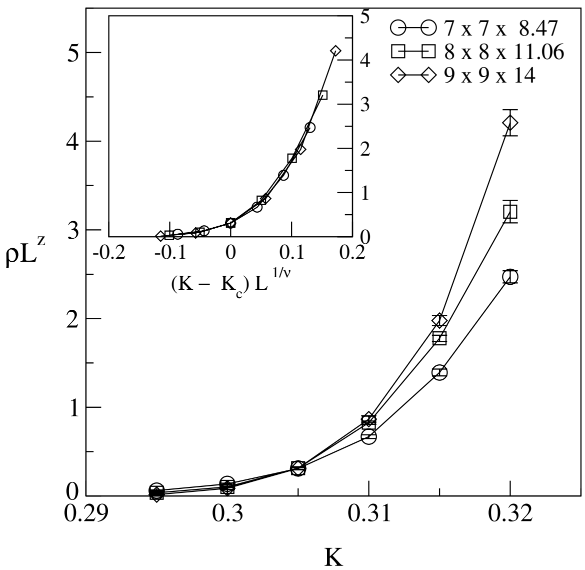

FIG. 4. The finite-size scaling behavior of the superfluid stiffness at $\Delta = 0.3$ ($\mu = 0$) for the systems in which the particle-hole pair fluctuations are completely suppressed. We set $z = 2$. The inset shows the scaled data along the K direction with $\nu = 0.9$. These exponents indicate that the nature of the transition is of the BG-SF one.

given by Eq. (2) under the condition that the background particle-hole fluctuations are completely suppressed. For simulations of the system governed by the action of Eq. (2), one should generate all possible current configurations $\{\vec{J}(x, y, \tau)\}$ [16]. The suppression of the particle-hole fluctuations is realized by disallowing any Monte Carlo updating which generates local particle-hole current loops. In the spatial planes, however, all possible current configurations are allowed as usual. Thus the allowed current configurations, if they are not restricted in a spatial plane, percolate in the τ direction (the imaginary temporal direction).

Figure 4 shows the scaling behavior of the superfluid stiffness when the particle-hole fluctuations are suppressed at the tip ($\mu = 0$) for relatively weak disorder ($\Delta = 0.3$). The scaling shows that the critical exponents are $z = 2$ and $\nu = 0.9$, indicating the BG-SF transition occurs. Note that, with the particle-hole fluctuations, the transition has the behavior of the MI-SF transition [6,7] at this strength of disorder. This simulation result, therefore, is consistent with the argument that the particle-hole pair fluctuations make the weak disorder irrelevant to the transition.

Now one may question how the particle-hole fluctuations screen the disorder. In the mean-field picture, ignoring the particle-hole fluctuations, particles (holes) are localized by arbitrarily weak disorder due to the coherent impurity backscattering. However, the proliferation of the particle-hole pairs could hinder the coherent backscattering. A particle propagating could be captured and destroyed by holes, and a new particle starts to propagate. A phase shift which accompanies such a particle-exchange process may destroy the coherent backscattering of the particle. As a result, this effect could screen out a weak random potential, making it irrelevant. Slightly off the tip, there are still abundant particle-hole pairs fluctuating. Thus this screening effect will survive even off the tip.

In summary, via quantum Monte Carlo simulations of the phase-only model of a disordered boson Hubbard model, we have found that there is a multicritical line which divides the universality of this model into the weak-disorder regime and the strong-disorder regime. In the weak-disorder regime, disorder is irrelevant for the insulator-to-superfluid transition. On the multicritical line, the dynamical critical exponent $z = 1.35 \pm 0.05$ and the correlation exponent $\nu = 0.67 \pm 0.03$ are obtained. Our result strongly suggests the direct MI-SF transition survives for weak disorder. We argue that the particle-hole pairs fluctuating near the tip will screen out disorder to make a weak random potential irrelevant.

The work of M. C. C. has been supported by Korea Research Foundation Grant No. KRF2000-041-D00125.

[1] S. L. Sondhi, S. M. Girvin, J. P. Carini, and D. Sahar, Rev. Mod. Phys. **69**, 315 (1997).
[2] N. Marković, C. Christiansen, A. M. Mack, W. H. Huber, and A. M. Goldman, Phys. Rev. B **60**, 4320 (1999).
[3] H. S. J. van der Zant *et al.,* Phys. Rev. B **54**, 10 081 (1996).
[4] P. A. Crowell, F. W. Van Keuls, and J. D. Reppy, Phys. Rev. Lett. **75**, 1106 (1995); Phys. Rev. B **55**, 12 620 (1997).
[5] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).
[6] J. Kisker and H. Rieger, Phys. Rev. B **55**, R11 981 (1997); Physica (Amsterdam) **246A**, 348 (1997).
[7] S. Y. Park *et al.,* Phys. Rev. B **59**, 8420 (1999).
[8] W. Krauth, N. Trivedi, and D. Ceperley, Phys. Rev. Lett. **67**, 2307 (1991).
[9] L. Zhang and M. Ma, Phys. Rev. B **45**, 4855 (1992).
[10] K. G. Singh and D. S. Rokhsar, Phys. Rev. B **46**, 3002 (1992).
[11] F. Pázmándi and G. T. Zimányi, Phys. Rev. B **57**, 5044 (1998).
[12] I. F. Herbut, Phys. Rev. B **57**, 13 729 (1998).
[13] Y. B. Kim and X. G. Wen, Phys. Rev. B **49**, 4043 (1994).
[14] J. K. Freericks and H. Monien, Phys. Rev. B **53**, 2691 (1996).
[15] S. Rapsch, U. Schollwöck, and W. Zwerger, Europhys. Lett. **46**, 559 (1999); R. V. Pai, R. Pandit, H. R. Krishnamurthy, and S. Ramasesha, Phys. Rev. Lett. **76**, 2937 (1996); N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. **80**, 4355 (1998)
[16] M. Wallin, E. S. Sørensen, S. M. Girvin, and A. P. Young, Phys. Rev. B **49**, 12 115 (1994).
[17] M.-C. Cha *et al.,* Phys. Rev. B **44**, 6883 (1991).
[18] For discussions, see, for example, J. T. Chayes, L. Chayes, D. S. Fisher, and T. Spencer, Phys. Rev. Lett. **57**, 2999 (1986); F. Pázmánd, R. T. Scalettar, and G. T. Zimányi, Phys. Rev. Lett. **79**, 5130 (1997); I. F. Herbut, Phys. Rev. B **61**, 14 723 (2000).