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Balabanyan, K; Prokof'ev, Nikolai; and Svistunov, Boris, "Superfluid-Insulator Transition in a Commensurate One-Dimensional Bosonic System with Off-Diagonal Disorder" (2005). *Physics Department Faculty Publication Series.* Paper 1154.
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arXiv:cond-mat/0301205v1 13 Jan 2003

Superfluid–Insulator Transition in Commensurate Disordered Bosonic Systems: Large-Scale Worm-Algorithm Simulations

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We report results of large-scale Monte Carlo simulations of superfluid–insulator transitions in commensurate 2D bosonic systems. In the case of off-diagonal disorder, we find that the transition is to a gapless incompressible insulator, and its dynamical critical exponent is $z = 1.65 \pm 0.2$. In the case of diagonal disorder, we prove the conjecture that rare statistical fluctuations are inseparable from critical fluctuations on the largest scales and ultimately result in the crossover to the generic universality class (apparently with $z = 2$). However, even at strong disorder, the universal behavior sets in only at very large space-time distances. This explains why previous studies of smaller clusters mimicked a direct superfluid–Mott-insulator transition.

PACS numbers: 03.75.Fi, 05.30.Jp, 67.40.-w

Quantum phase transitions in disordered systems remain a poorly understood phenomenon despite enormous interest in this field. The $T = 0$ transition between the superfluid (SF) and insulating (I) phases is believed to determine properties of various condensed matter systems: ^{4}He in porous media and aerogels [1, 2], ^{4}He on various substrates [1, 3, 4], thin superconducting films [5, 6, 7, 8, 9, 10, 11], Josephson-junction arrays [12], disordered magnets [13, 14], etc.

There are strong arguments that the basic Hamiltonian which captures all the essential physics of the SF-I transition is the bosonic Hubbard model with disordered chemical potential [15, 16, 17, 18]. In the limit of large occupation numbers, the bosonic Hubbard Hamiltonian is equivalent to the system of coupled Josephson junctions. Fermionic systems map to this Hamiltonian under the assumption that Cooper pairs are preformed at finite temperature, and the transition is driven only by quantum fluctuations of the phase of the complex order parameter. To deal with granular superconductors one may also introduce disorder to hopping amplitudes.

It was suggested in Ref. [16] that one has to consider only two competing insulating phases—the incompressible (gaped) Mott-insulator phase (MI), and the compressible gapless Bose glass (BG) phase. However, more recently it was argued that apart from the BG phase characterized as a compressible insulator with variable-range-hopping conductivity at finite temperature [16], there may exist other phases such as a Bose metal with finite conductivity in the $T \to 0$ limit [19] and an incompressible Mott glass with the conductivity pseudogap [20]. Theoretical calculations for the strongly coupled SF-I critical point are notoriously difficult and are not based on well controlled approximations since localization and interaction effects cannot be separated [21, 22]. Thus even the qualitative understanding of the phase diagram is still under debate. In particular, it was argued in [16, 17, 18, 23, 24] that MI and SF phases are always separated by the BG phase at any finite disorder. However experiments [1], most Monte Carlo simulations [25, 26, 27], and other theories [28, 29, 30] present evidence in favor of a direct transition between MI and SF phases (in the case of commensurate filling of the lattice and not so strong disorder). In $d = 1$ this contradiction was apparently resolved using arguments based on rare statistical fluctuations [24] (Lifshitz-Griffiths-McCoy singularities [31, 32, 33]), renormalization-group equations [34, 35], and quantum Monte Carlo simulations [36]).

In this Letter, we numerically address the problem of the SF-I transition in a disordered commensurate 2D system. Our large-scale simulations based on the classical Worm Algorithm [37] demonstrate the absence of the direct SF-MI transition. We clearly see, however, that—even at strong disorder—the universal asymptotic long-range behavior sets in only at large space-time distances. This result, on one hand, explains previous observations of the direct SF-MI transitions in simulations of much smaller clusters, and, on the other hand, implies that the superfluid stiffness and compressibility should obey generic scaling laws only in a very close vicinity of the phase transition point which may be hard to study experimentally.

The Worm algorithm (WA) [37] is a high-performance universal Monte Carlo scheme applicable to any model with the configuration space of continuous paths. The principle of WA is to work in an *extended* configuration space combining the physical closed-path sector and the broken-path sector with two path endpoints. *All* updates in the extended configuration space are through the motion of the endpoints (or even just one of them), so that the configuration evolution looks like a creeping worm. Though the WA updating strategy is based on local Metropolis moves (which is a key issue for its universality), it has a remarkable efficiency equivalent to that of the best cluster algorithms [38].

WA was introduced initially for the continuous-time path integral, or worldline, representation of lattice quantum systems [37]. More recently it was implemented within the Stochastic Series Expansion (SSE) method [39], and generalized to classical lattice systems in the

closed-path representations [38]. The optimal choice of WA depends on the problem being addressed; e.g. the quantum worldline scheme is best suited for *ab initio* simulations of bosons in optical lattices [40], while the SSE scheme has certain storage and computational advantages when simulating quantum models with a restricted Hilbert space, like spins and hard-core bosons [41, 42]. However, if one is interested in generic properties of quantum phase transitions, then the optimal choice is a $(d+1)$-dimensional *classical* scheme, which is algorithmically superior from all points of view. This approach was advocated in Ref. [18], and most recently, using WA, in Ref. [43].

The easiest way to derive the classical $(d+1)$-dimensional equivalent of the d-dimensional quantum model is to start from the lattice path integral for particle trajectories in imaginary time. The basic step is to "roughen" trajectories by replacing integrals over kink positions (particle jumps between lattice sites) in time by discrete sums. To this end one introduces a grid of imaginary times and requires that kinks occur only at time slices forming the grid. Bonds in the spatial direction of thus obtained $(d+1)$-dimensional lattice carry an integer charge—a spatial current equal to an algebraic sum of kinks associated with a given pair of sites and a time slice (the kink sign specifies its direction). The finite value of the time interval between slices, $\Delta\tau$, makes the roughening procedure, generally speaking, not unique. Only in the physical limit of $\Delta\tau \to 0$ the absolute values of spatial currents are either zero or unity. At strong roughening the constraint that the absolute value of the spatial bond charge is ≤ 1 is no longer necessary. The maximal value now depends on how we roughen the original trajectories with more than one kink between a given pair of sites during the time interval $\Delta\tau$—either as irrelevant rare events that are neglected, or by ascribing all such kinks to the same spatial bond of the $(d+1)$-dimensional lattice. Note, there is no *qualitative* difference between the two cases, and the choice is just a matter of convenience. Bonds in the temporal direction also carry an integer charge, equal to the occupation number of a given site between adjacent time slices. For the sake of symmetry, it is convenient to refer to the temporal-bond charges as temporal currents, so that each bond of the $(d+1)$-lattice carries an integer current, J. The conservation of the particle number imposes an obvious constraint on bond currents—the divergence of the $(d+1)$-current at any $(d+1)$-site is zero. Graphically, if one represents the bond currents by oriented lines (in accordance with the sign of J) then all contributions to the partition-function will have a form of closed-path configurations of such lines, while configurations for the Green-function will have two endpoints. WA simulates both quantities simultaneously, by switching between partition-function and Green-function sectors [37, 38].

Let us denote by $\{J_{\mathbf{x},\alpha}\}$ the bond current configuration where $\mathbf{x} = (\mathbf{r}, \tau)$ are discrete space-time coordinates, and index $\alpha = \hat{r}_1, \ldots, \hat{r}_d, \hat{\tau}$ stands for unit vectors of axis directions, so that $(\mathbf{x}, \alpha)$ defines a bond in the direction α, adjacent to the site $\mathbf{x}$. As usual, the configuration weight $W[\{J_{\mathbf{x},\alpha}\}]$ may be formally written as a Gibbs factor $\exp\{-H/T\}$ which for positive-definite W defines the classical bond Hamiltonian $H/T = -\ln W$. For models with on-site particle-particle interactions the configuration weight is simply given by the product of bond weights $W_{\mathbf{r}\alpha}(J_{\mathbf{x},\alpha})$, and, correspondingly,

$$H = \sum_{\mathbf{x}\alpha} H_{\mathbf{r}\alpha}(J_{\mathbf{x},\alpha}) \; . \tag{1}$$

The zero-divergence constraint can be written as $\sum_\alpha J_{\mathbf{x},\alpha} + \sum_\alpha J_{\mathbf{x},-\alpha} = 0$, where, by definition, the direction $-\alpha$ is understood as opposite to α and $J_{\mathbf{x},-\alpha} = -J_{\mathbf{x}-\alpha,\alpha}$.

In this paper, we are interested only in the universal critical behavior of the model (1), which is supposed to be insensitive to quantitative details of the Hamiltonian. This freedom may be used to make spatial and temporal directions symmetric with respect to each other. In the original quantum model, the temporal direction is not symmetric even with respect to its opposite because occupation numbers are always positive. Nevertheless, one may count them from some integer n_0, substitute $J_{\mathbf{x},\hat{\tau}} \to J_{\mathbf{x},\hat{\tau}} - n_0$, and formally consider $J_{\mathbf{x},\hat{\tau}} \in (-\infty, \infty)$. Alternatively, one may introduce a symmetric constraint, say, $|J| \leq 1$. The latter case, reminiscent of the mapping between bosonic and spin-1 systems, seems to be more natural and computationally economic. Historically, however, a model with $J \in (-\infty, \infty)$, motivated by its derivation from the Josephson-junction array Hamiltonian [18], was adopted. To retain the possibility of a direct comparison with previous numeric studies, we work with the same model [18]:

$$H/T = \sum_{\mathbf{x}\alpha} \left[\frac{1}{2} J^2_{\mathbf{x},\alpha} - \delta_{\alpha,\hat{\tau}} \mu_{\mathbf{r}} J_{\mathbf{x},\hat{\tau}} \right] / K \; . \tag{2}$$

In terms of the underlying bosonic system, K represents the particle hopping amplitude in units of the on-site repulsion, the discrete field $\mu_{\mathbf{r}} = \mu_0 + \tilde{\mu}_{\mathbf{r}}$ involves the chemical potential μ_0 and the white-noise diagonal disorder $\tilde{\mu}_{\mathbf{r}} \in [-\Delta, \Delta]$. In this study we are concerned with the commensurate filling of the lattice, i.e. $n = \langle\langle J_{\mathbf{x},\hat{\tau}} \rangle\rangle$ =integer, where $\langle\langle \ldots \rangle\rangle$ stands for the average over all lattice points, statistical and disorder fluctuations, and thus set $\mu_0 = 0$. [An accurate study of the half-integer n case has been reported recently by Alet and Sørensen [43]]. We also consider model (2) with the off-diagonal disorder introduced by letting the parameter K to be dependent on $\mathbf{r}$ and spatial direction, and confine ourselves to the case of a broken-bond disorder, where for some randomly chosen $\mathbf{r}$ and $\alpha' = \hat{r}_1, \ldots \hat{r}_d$ we set $K_{\mathbf{r}\tau\alpha'} \to 0$ (equivalent to a rigid constraint $J = 0$ on the corresponding bond). The phase diagram of the homogeneous system is shown in Fig. 1; the SF-I transition at the commensurate filling is located at $K_c^{(0)} = 0.33305(5)$

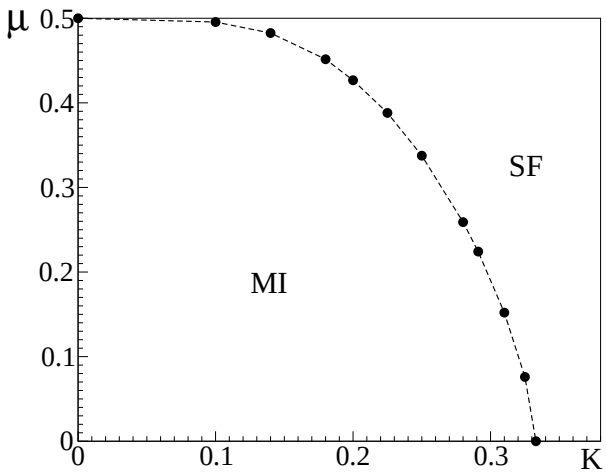

FIG. 1: The phase diagram of model (2) in the absence of disorder. Error bars are of order 10^{-3} and smaller than point size.

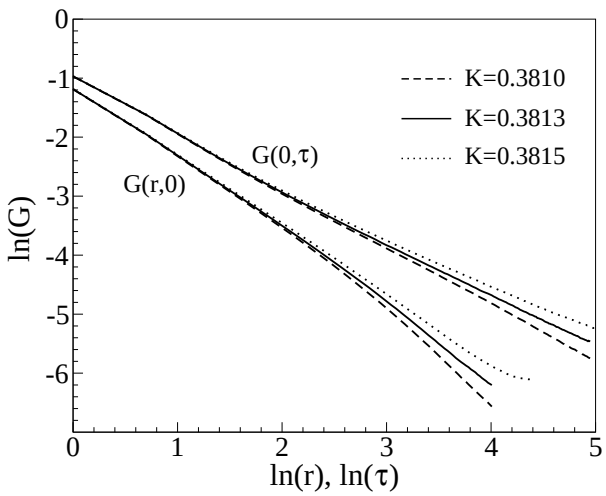

FIG. 2: Correlation functions $G(r,0)$ and $G(0,\tau)$ for $K = 0.3810,\ 0.3813,\ 0.3815$ and system size $L \times L \times L_\tau = 160 \times 160 \times 500$. Error bars are comparable to the line widths.

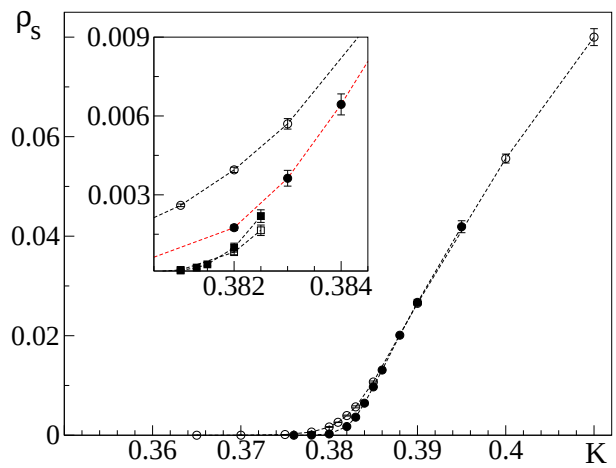

FIG. 3: Superfluid stiffness of the broken-bond model as a function of K at different system sizes; $40 \times 40 \times 40$ - open circles, $80 \times 80 \times 80$ - filled circles, $160 \times 160 \times 160$ - open squares, $160 \times 160 \times 500$ - filled squares.

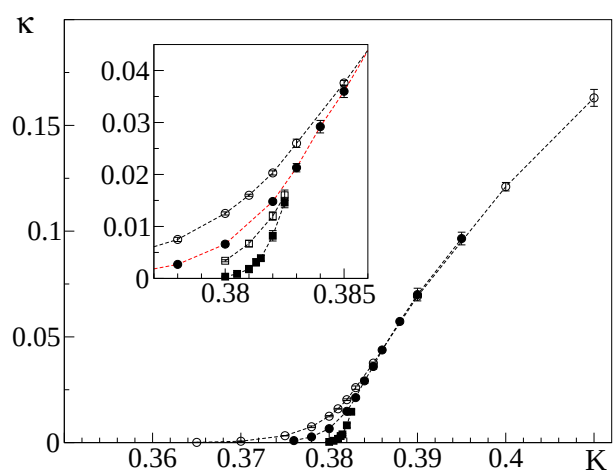

FIG. 4: Compressibility of the broken-bond model as a function of K at different system sizes; $40 \times 40 \times 40$ - open circles, $80 \times 80 \times 80$ - filled circles, $160 \times 160 \times 160$ - open squares, $160 \times 160 \times 500$ - filled squares.

[43]. The value of the MI gap is defined as half the difference between the critical values of the chemical potential in Fig. 1, i.e. $2E_{\rm gap}(K) = \mu_c^{(\rm up)} - \mu_c^{(\rm down)}$.

We start with the off-diagonal disorder case, and consider a system with a quarter of all bonds being broken. Typically, we include about 10^3 disorder realizations into the statistics for system sizes $L \leq 40$, and $4 \times 10^4/L$ for larger L. The critical point, K_c, and the dynamical exponent, z, may be obtained from the study of the Green function, $G(\mathbf{r},\tau)$, naturally evaluated within the WA approach [37]. At the critical point one should see a power-law decay: $G(r,0) \to r^{-(z+\eta)}$ as $r \to \infty$, and $G(0,\tau) \to \tau^{-(1+\eta/z)}$ as $\tau \to \infty$. This way we find (see Fig. 2, as well as Figs. 3, and 4)

$$K_c = 0.3813(2)\ , \tag{3}$$

$z + \eta = 1.37(8)$, $1 + \eta/z = 0.82(6)$, i.e.

$$z = 1.65(20)\ , \tag{4}$$

$$\eta = -0.3(1)\ . \tag{5}$$

It is clear in Fig. 2 that the asymptotic behavior of the correlation function sets in only at sufficiently large space-time distances > 10 lattice periods. Moreover, the short-range behavior of G mimics the critical point of the SF-MI transition in the regular system, where $z = 1$. This peculiar behavior implies that the curves for the superfluid stiffness, ρ_s, and compressibility, κ, will acquire their universal forms only in a very narrow region around the critical point. Away from this region, the form of $\rho_s(K - K_c)$ and $\kappa(K - K_c)$ curves should be essentially

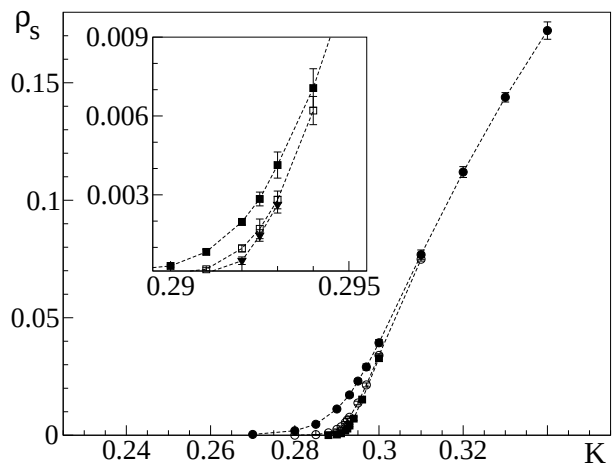

FIG. 5: Superfluid stiffness for the diagonal disorder case as a function of K at different system sizes; $10 \times 10 \times 20$ - filled circles, $20 \times 20 \times 49$ - open circles, $40 \times 40 \times 121$ - filled squares, $80 \times 80 \times 298$ - open squares, $160 \times 160 \times 733$ - triangle down

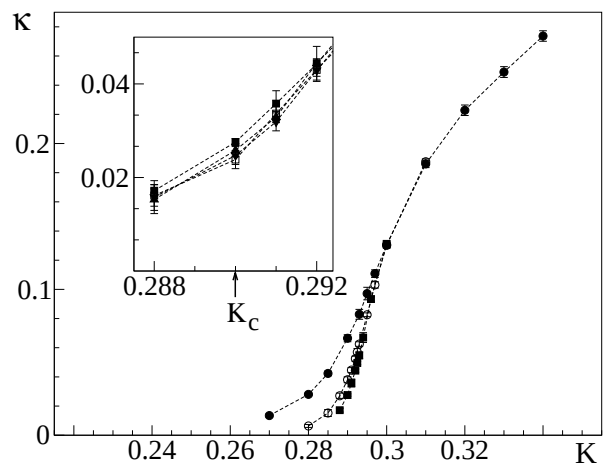

FIG. 6: Compressibility for the diagonal disorder case as a function of K at different system sizes; $10 \times 10 \times 20$ - filled circles, $20 \times 20 \times 49$ - open circles, $40 \times 40 \times 121$ - filled squares, $80 \times 80 \times 298$ - open squares, $160 \times 160 \times 733$ - triangle down, $160 \times 160 \times 160$ - triangle up. The data for $L \geq 80$ collapse on each other within the error bars.

different, as suggested by the extended transient evolution of z from ≈ 1 to its true critical value. In Figs. 3 and 4 we indeed observe such a behavior. The anomalously narrow critical region makes it virtually impossible—even with our large cluster sizes—to reliably determine the correlation radius critical exponent ν. Along with the dynamical exponent z it is supposed to determine the critical behavior of the compressibility, $\kappa \propto (K - K_c)^{\nu(2-z)}$ and superfluid stiffness, $\rho_s \propto (K - K_c)^{\nu z}$ [16]. The data in Figs. 3 and 4 at best guarantee only the inequalities $\nu(2 - z) < 1$ and $\nu z > 1$, but do not allow us to test the Harris criterion [44] $\nu > 2/d = 1$.

The finite-size scaling of the data for compressibility demonstrates no sign of saturation below K_c and thus strongly suggests that in the insulating state the compressibility vanishes. Though the insulating state is incompressible, it is easy to prove that it is *gapless* and thus is qualitatively different from the conventional Mott insulator and Bose Glass states. Indeed, in an infinite system it is always possible to find an arbitrarily large cluster that is nearly uniform (in the sense that fluctuations of K away from its cluster average value are arbitrarily small/rare). Taking into account that K_c in the disordered system is larger than the ideal-system critical value $K_c^{(0)}$, we conclude that such clusters are nothing else but finite-size *superfluid* lakes. Hence, the gap associated with adding one more particle to the cluster scales as $1/l^d$, where l is the cluster size. The absence of an upper bound on l immediately implies the absence of the global gap in the system spectrum and finite optical conductivity.

The diagonal-disorder case is different. Previously reported data [27] for small clusters $L \times L \leq 12 \times 12$ and disorder strength $\Delta = 0.2$ were interpreted as a direct SF-MI transition with $z = 1$. We extended the study of the $\Delta = 0.2$ case to system sizes $L \times L \leq 160 \times 160$ and did not find any deviations from the direct transition picture with vanishingly small compressibility below $K_c(\Delta = 0.2) = 0.325(1)$. However, the value of the MI gap in the ideal system is almost three times smaller than Δ at $K = K_c$, see Fig. 1. According to the argument/theorem of Refs. [16, 24], the state with $\Delta > E_{\rm gap}$ is a compressible (gapless) insulator, or BG, because in the infinite system one can always find arbitrary large regions with the chemical potential being nearly homogeneously shifted downwards or upwards by Δ (and thus they are doped with particles or holes). Since the distance between such regions is exponentially large for $\Delta \to 0$, their effect is simply undetectably small for $\Delta = 0.2$.

Even if the state right below K_c is a compressible insulator, the question remains whether Griffiths-McCoy singularities are inseparable from critical fluctuations and ultimately result in the crossover to the generic SF-BG transition, or they merely provide a regular background contribution to κ on which a singular contribution $\kappa_{\rm sing}$ is superimposed. The latter scenario implies a cusp on the compressibility curve, and criticality different from SF-BG. To answer this question we performed simulations for disorder strength $\Delta = 0.4$. As before, the ideal MI gap at the transition point $K_c = 0.2910(5)$ is about two times smaller than Δ, and κ has to be finite at K_c.

In Figs. 5 and 6 we show the data for the compressibility and superfluid stiffness which away from the critical point mimic the ideal-system behavior (with the correlation length exponent $\nu \approx 0.7$ and $z \approx 1$), but close to K_c show a spectacular crossover to another universality class. Strong finite-size corrections to κ for system sizes $L \leq 20$ saturate for $L > 20$, and the thermodynamic

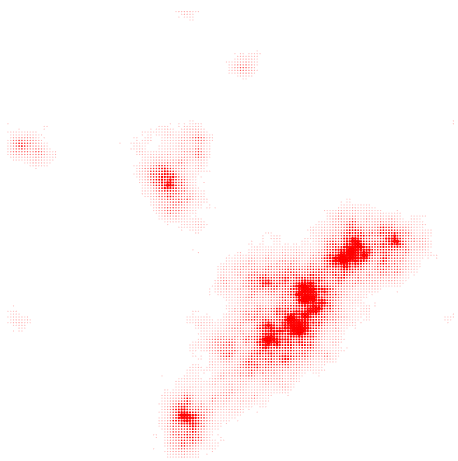

FIG. 7: A map of doped places slightly below K_c showing the picture of rare, well isolated regions. Point sizes are proportional to $\phi_N(\mathbf{r})$.

curve clearly demonstrates *finite*, and *non-singular* dependence $\kappa(K-K_c)$. At the same time, we observe a crossover in the $\rho_s(k-K_c)$ dependence, and see that ρ_s approaches zero with zero derivative, i.e. $\nu z > 1$. From the decay of the Green function at the critical point we obtain

$$z = 2.0(2) \,, \tag{6}$$

$$\eta = 0.11(2) \,. \tag{7}$$

Unfortunately, the large-scale crossover did not allow us to determine the critical exponent ν from this set of data. Recent data for half-integer n are best fit with $\nu = 1.15$, but they also suffer from large finite-size corrections [43]. Apparently, the best strategy in the future is to search for a classical model with the smallest crossover scale.

Within the WA approach one may directly visualize places where particles are added/removed at low temperature in a sample with a given disorder realization. The standard procedure of subtracting density maps obtained in canonical simulations $n(i,N) - n(i,N-1)$ is time consuming, and for large systems requires extremely high-precision data for $n(i,N)$. The new technique is based on the statistics of the Green function calculated at the chemical potential between the steps on the $N(\mu)$ curve, i.e. at $\mu = E_G(N) - E_G(N-1)$, where $E_G(N)$ is the ground state energy of the N-particle system. In the $T \to 0$ limit we write $G(N;\mathbf{r},\mathbf{r}',\tau=\beta/2) = F(N;\mathbf{r},\mathbf{r}')$ and notice that only ground states with $N-1$ and N particles contribute to the answer. Thus $F(N;\mathbf{r},\mathbf{r}') \approx \phi_N(\mathbf{r})\phi_N(\mathbf{r}')$ where $\phi_N(\mathbf{r})$ is given by the positive-definite groundstate-groundstate matrix element

$$\phi_N(\mathbf{r}) = \langle \Psi_G(N) | b^\dagger_{\mathbf{r}} | \Psi_G(N-1) \rangle \,, \tag{8}$$

and may be viewed as the added-particle "wavefunction". Its localization length diverges at the SF-I transition. The two important parameters which characterize the structure of the normalized wavefunction are the localization radius

$$\mathcal{R}^2 = \langle \, [\mathbf{r} - \langle \mathbf{r} \rangle]^2 \, \rangle = \sum_{\mathbf{r}} \, [\mathbf{r} - \langle \mathbf{r} \rangle]^2 \, \phi_N^2(\mathbf{r}) \,, \tag{9}$$

and the state "area", or the number of sites over which ϕ delocalizes,

$$\mathcal{A} = \frac{\sum_{\mathbf{r}} \phi_N^2(\mathbf{r})}{\sum_{\mathbf{r}} \phi_N^4(\mathbf{r})} \,. \tag{10}$$

The dependence of $\mathcal{A}$ on $\mathcal{R}$ gives the fractal dimension of the state. It is also important to monitor correlations in the overlaps between different states, $\sum_{\mathbf{r}} \phi_N(\mathbf{r})\phi_{N'}(\mathbf{r})$. For example, the percolation type scenario of the SF-I transition assumes large fractal superfluid "lakes" in the insulating phase; if so, then with the probability of order unity there must exist an almost complete overlap between a pair of states (ϕ_{N_a}, ϕ_{N_b}) with N_a, N_b from a narrow interval of width $\delta N \ll N$ around N.

In Fig. 7 we show a typical map of $\sum_{\mathbf{r}'} F(N=1;\mathbf{r},\mathbf{r}')$ for the insulating state at $K = 0.288$ and system size $L \times L \times L_\tau = 160 \times 160 \times 1000$. One can clearly see isolated regions doped with particles.

In summary, we have performed large-scale simulations of the superfluid–insulator transition in the $(2+1)$-dimensional classical analog of the commensurate disordered 2D bosonic system. For diagonal disorder, our results suggest that commensurability is not relevant in the long-range limit, and the universality class of the transition (superfluid–Bose-glass) is the same for all filling factors. In particular, we unambiguously resolved the finite compressibility at the critical point originating from rare statistical fluctuations and demonstrated that they are responsible for the crossover in critical behavior. We believe that our results rule out the earlier-reported direct superfluid–Mott-insulator transition in this model.

In the off-diagonal disorder case, the compressibility vanishes at the critical point. The incompressible insulating phase, however, is gapless, and its universality class is characterized by the dynamical critical exponent $z = 1.65 \pm 0.2$.

A general observation is that even for large diagonal and off-diagonal disorder, the universal asymptotic long-range behavior sets in only at large space-time distances (~ 20 lattice periods). This circumstance explains previous observations of the direct superfluid–Mott-insulator transition in small-size clusters and implies that the the superfluid stiffness and compressibility should obey generic scaling laws only in a very close vicinity of the phase transition point.

The authors are grateful to S. Sachdev for a fruitful discussion. This work was supported by the National Science Foundation under Grant DMR-0071767. BVS acknowledges a support from Russian Foundation for Basic Research under Grant 01-02-16508, from the Netherlands Organization for Scientific Research (NWO), and

from the European Community under Grant INTAS- 2001-2344.

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