Superfluid-Insulator Transition in Disordered Boson Systems

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We present results of path-integral Monte Carlo simulations of bosons on a two-dimensional square lattice in a random potential of average strength V and with on-site repulsion U. We find that the superfluid density ρ_s is enhanced by increasing V and U in certain regions of parameter space. By combining the results of ρ_s with the behavior of the density-density correlation function on lattices of size up to 10×10, we study the superfluid–to–Mott-insulator transition and the transition from a superfluid to a disorder-localized ("Bose-glass") phase.

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The localization problem for quantum systems has attracted a lot of attention over the years. There exists a scaling theory [1] for the metal-insulator transition of noninteracting electrons. However, experiments on doped semiconductors point toward the importance of including electron-electron interactions in addition to the random potential. While some progress has been made in understanding the behavior of the charge and spin degrees of freedom, this problem remains unsolved [2].

In this paper we study the localization problem for bosons. We present results of numerical simulations of strongly interacting bosons in a 2D random potential. This situation is realized experimentally in ^{4}He adsorbed in porous media [3] and may be used to understand the superconducting-insulating transition in granular [4] and homogeneously disordered films [5], at least near the critical point, and also possibly in short-coherence-length (e.g., high-T_c) superconductors [6].

We consider the following Hamiltonian:

$$H=-\tfrac{1}{2}t\sum_{\langle i,j\rangle}(a_i^\dagger a_j+\text{H.c.})+\sum_i V_i n_i+\tfrac{1}{2}U\sum_i n_i(n_i-1)\,, \tag{1}$$

where a_i ($a_i^\dagger$) is a boson annihilation (creation) operator at a site i on a 2D square lattice, $n_i=a_i^\dagger a_i$, t is the strength of the hopping between nearest neighbors, V_i is a uniformly distributed random variable at i in $[-V,V]$, and U is an on-site repulsive interaction between bosons.

Some universal features of this model have been studied previously using scaling techniques by Ma, Halperin, and Lee [7] and Fisher *et al.* [8], and by the renormalization-group method in 1D by Giamarchi and Schulz [9]. However, there are several questions regarding the nature of the phases and their characterization that remain open.

In this Letter, we report results for the disordered-boson Hamiltonian obtained by path-integral Monte Carlo (PIMC) techniques. In particular, we determine the superfluid density ρ_s and the spectrum of density excitations. We find indications of three phases: a superfluid phase (with $\rho_s>0$ and gapless excitations), a disorder-localized phase, often called the "Bose-glass" phase (with $\rho_s=0$ and gapless), and at a commensurate density $\rho=1$, a Mott phase (with $\rho_s=0$ and a finite gap). We also find unusual effects from the interplay between disorder V and interaction U. (i) In the disordered system, ρ_s is enhanced by increasing U, peaks for $U\approx V$, and then decreases. (ii) At an incommensurate density, for $V<V_c$, a critical amount of disorder, the system remains superfluid at large U; however, for $V>V_c$, it undergoes a transition to a disorder-localized phase at $U=U_c(V)$, which decreases with disorder. (iii) At a commensurate density $\rho=1$, we find strong support for a direct superfluid–to–Mott-insulator transition, without an intervening disorder-localized phase. The transition takes place at a critical value of $U=U_c(V)$ which *increases* with the disorder V.

Before we discuss these results in more detail, we present a brief description of the PIMC algorithm [10]. Our aim is to calculate the diagonal density matrix in the canonical ensemble $\rho(R,R;\beta)=\langle R|\exp(-\beta H)|R\rangle$, where $\beta=1/k_BT$. Upon inserting complete sets of states we obtain the path-integral expression,

$$\rho(R,R;\beta)=\frac{1}{N!}\sum_P\int\cdots\int dR_1\cdots dR_{M-1}\rho(R,R_1;\tau)\rho(R_1,R_2;\tau)\cdots\rho(R_{M-1},P(R);\tau)\,, \tag{2}$$

with $\tau=\beta/M$. In Eq. (2), R_m represents the ensemble of N particle coordinates on the mth (imaginary) time slice, $R_m=(\mathbf{r}_1^{(m)},\mathbf{r}_2^{(m)},\ldots,\mathbf{r}_N^{(m)})$, where $\mathbf{r}_j=(x_j,y_j)$ is the position of the jth particle in a periodic box of size $L\times L$. The density matrix for the Bose system is obtained by summing over permutations P of the particle coordinates.

The PIMC algorithm uses a high-temperature expansion for the density matrices $\rho(R_i,R_{i+1};\tau)$ and computes the sum over internal coordinates and permutations in Eq. (2) with a generalized Metropolis algorithm. The energy as well as quantities diagonal in the coordinates are then calculated as averages over the paths. The superfluid density is

determined from both the winding number [10,11] and the current autocorrelation function [12–14].

We have checked our PIMC results against exact diagonalization of small systems in 1D and performed extensive tests to verify that our results converge in the limits $\tau \to 0$ and $\beta \to \infty$. We have verified that for small systems the quantities of interest (e.g., ρ_s and the energies) seem to be self-averaging. In the superfluid and Mott phases they show small sample-to-sample variations, as seen by averaging over ≈ 20 samples. In the disorder-localized phase, as discussed later, we find strong dependence on the choice of initial conditions [15].

In our simulations, the insulating phases are generally indicated by the vanishing of ρ_s. In order to further characterize the insulating phases we calculate the spectrum of low-lying *density* excitations in the Feynman-Bijl approximation, i.e., under the assumption that there is only one low-lying mode accessible to the system at each wavelength. Consider the trial state created by the density operator $\rho_k = \sum_j \exp(ikr_j)$ and orthogonal to the normalized ground state $|\Psi_0\rangle$:

$$|\Psi_k\rangle = \rho_k|\Psi_0\rangle - \langle\Psi_0|\rho_k|\Psi_0\rangle|\Psi_0\rangle . \quad (3)$$

The variational energy of this trial state is given by a generalization of the lattice f-sum rule [16] to disordered systems by

$$\omega_k \equiv E_k - E_0 = \epsilon_k |K|/S(k) \geq E_{\rm gap} , \quad (4)$$

where ϵ_k is the single-particle (band) energy, K is the total kinetic energy, and $S(k) = (1/N)[\langle\rho_k\rho_{-k}\rangle - |\langle\rho_k\rangle|^2]$ is the structure factor. The insulating phases are distinguished by the long-wavelength behavior of the structure factor as discussed below.

The Hamiltonian in Eq. (1) simplifies in several limits. For *noninteracting* bosons ($U=0$) the particles condense at zero temperature into the lowest one-particle eigenstate, which, for an infinite lattice at nonzero V, is localized. Therefore, ρ_s vanishes for any choice of the disorder. For a periodic 10×10 lattice we have calculated ρ_s from the shift in the energy of the lowest eigenvalue with a change of the boundary conditions [12] and find it to be $\rho_s/\rho \sim 2\times10^{-4} \ll 1$ at $V/t=4$. This also indicates that the system size is much larger than the localization length of the noninteracting system. Another limit amenable to analysis is the *classical* state ($t=0$ with U and V finite). At a commensurate density for $U > 2V$ the classical solution is a Mott insulator, with the density at each site $\langle n_i\rangle = \rho$ (an integer) and a gap to excitations $\Delta E = U - 2V$. It can be easily seen that the gap decreases with disorder. At other densities the classical ground state can also be computed and is seen to be gapless. Finally, for interacting bosons in *zero disorder* ($V=0$) our numerical simulations [11] have determined the transition between the superfluid state and the Mott insulator to be $U/t \sim 8.5$ in the commensurate case ($\rho=1$), and found no transition for incommensurate densities. Similar properties were found in 1D [13].

Incommensurate density of bosons $\rho=0.75$.—The behavior of ρ_s as a function of U is shown in Fig. 1. In the clean system, ρ_s/ρ is unity for $U=0$ and decreases monotonically with increasing U, finally saturating at a finite value. For a finite V, in the noninteracting limit ρ_s vanishes for the infinite system, and is close to zero on our finite system. We can see clearly that an increase in U leads to an *enhancement* of ρ_s for small U, as the interaction term prohibits an extensive number of bosons from occupying the one-particle localized ground state. Therefore, the interaction term screens the randomness and effectively delocalizes the system. ρ_s peaks when $U \approx V$ and then decreases for larger U. ρ_s in the disordered system, even though nonmonotonic as a function of U, is always less than that in the clean system, as might be expected. It appears from Fig. 1 that for small disorder $V < V_c$ the system remains superfluid at large values of U. We believe this behavior should persist at arbitrarily large U; however, further calculations are needed to pin down the behavior of ρ_s in this region. This is different from the scenario presented in Ref. [8], where a Bose-glass phase appeared for any disorder in the hard-core limit.

We next calculate the density-density correlation function and find that in the superfluid phase $S(k) \sim k$. Since $\epsilon_k \sim k^2$, this confirms, from Eq. (4), the existence of phonon modes with a dispersion $\omega_k = ck$, where the sound velocity c decreases with disorder.

The incommensurate case is of particular interest for large values of the disorder for which the insulating disorder-localized (the so-called Bose-glass) phase is expected to exist. To probe this state, it may seem natural to do simulations at large values of the disorder and determine the excitation spectrum. However, this is not feasible, at least with our present algorithm. At large disorder, our simulations get trapped in a local minimum, which depends on the initial conditions. We are thus unable to effectively move the system through configuration

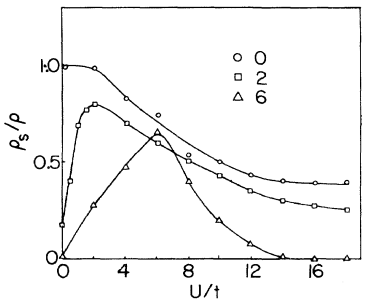

FIG. 1. Superfluid density ρ_s/ρ vs interaction strength U/t in a 6×6 system of density $\rho=0.75$ and $\beta t=4$. The values of the disorder parameter are $V/t=0$ (circles), 2 (squares), and 6 (triangles).

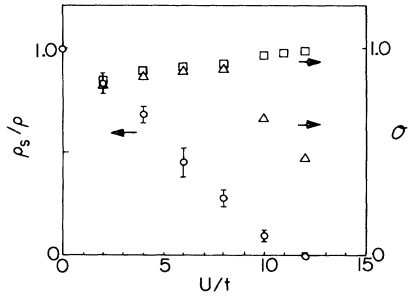

FIG. 2. Superfluid density ρ_s/ρ as a function of U/t at a constant ratio of $V/U=1$ (circles) in a 10×10 system of density $\rho=0.75$ and $\beta t=4$. Also shown is the overlap function of the density with the classical density O vs U/t for simulations starting in the classical state (squares) and in a random state (triangles).

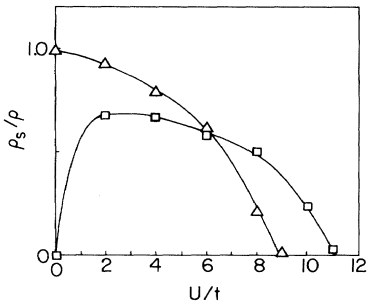

FIG. 3. Superfluid density ρ_s/ρ vs interaction strength U/t in a 10×10 system of density $\rho=1$ and $\beta t=4$. The values of the disorder parameter are $V/t=0$ (triangles) and 2 (squares).

space. However, we *are* able to demonstrate convergence of our simulations in the superfluid phase, even for small values of ρ_s (at large V). This allows us to approach the transition from the superfluid side. To quantify the notion of a local minimum, we define an overlap function O of the density with the classical density $n_i^{\rm cl}$ at site i given by $O=\sum_i \delta n_i \delta n_i^{\rm cl}/[\sum_i (\delta n_i)^2 \sum_j (\delta n_j^{\rm cl})^2]^{1/2}$, where $\delta n_i = n_i - \rho$. $O=1$ if the density at each site coincides with the classical density. We show the behavior of O and ρ_s in Fig. 2 for a system with $\rho=0.75$ and $U=V$ as a function of U/t for two different initial conditions, one of them the classical ground state. In the superfluid phase, both simulations converge to a unique state, independent of the starting configuration. The linear behavior of ρ_s/ρ as a function of U/t is consistent with scaling theory [8]. By extrapolating to $\rho_s=0$ we obtain the approximate location of the phase transition to be $U_c/t\sim10$. Near the transition the density in the ground state is extremely close to that in the classical state since $O\sim1$. This suggests a description of the superfluid state near the transition obtained by including quantum phase fluctuations around the classical solution.

Commensurate density of bosons $\rho=1$.—There are important differences from the incommensurate case, pointing to some unusual effects at commensuration as seen from the behavior of ρ_s as a function of U in Fig. 3. In particular, we find that in the range $6\lesssim U/t\lesssim 8.5$, ρ_s in the disordered system $V/t=4$ is *higher* than in the clean system. By studying the behavior of the structure factor, we find that disorder *enhances* the density fluctuations at large interaction at a commensurate density. For $8.5\lesssim U/t\lesssim 11$, the disordered system continues to be superfluid, while the clean system is already in a Mott phase.

Beyond $U/t\gtrsim 11$, the disordered system also enters a Mott phase as indicated by the following: (a) The average single-particle density at each point in the lattice is closely pinned to 1. (b) The correlation of the density with the underlying random disorder $\langle n_i V_i\rangle$ is vanishingly small. (c) The structure factor $S(k)\sim k^2$, and from Eq. (4) this implies that a Mott gap opens up in the excitation spectrum as shown in Fig. 4. At $U/t=14$, for example, both the disordered system with $V/t=4$ and the clean one with $V=0$ show the opening of a Mott gap that is *smaller* in the disordered case. For comparison at $U/t=6$, on the other hand, the spectrum is gapless in both cases and ρ_s is finite. Extensive simulations [14] seem to give no indication of a disorder-localized phase sandwiched between the superfluid and the Mott insulator as conjectured by Fisher *et al.* [8]. The Bose glass would unmistakably show up as a phase in which $\rho_s=0$, $\langle n_i V_i\rangle\neq0$, and with no gap. This has not been observed. Our numerical evidence favor instead a direct transition from the superfluid into the insulator at a critical value of the interaction which *increases* with the disorder. Our results in the superfluid and Mott phases do not depend on the choice of the initial conditions. Quite spectacularly, in the Mott phase, even close to the onset of superfluidity, a random initial condition evolves into a state with a completely uniform density.

In conclusion, we have performed the first simulations of interacting bosons in a disordered medium in two dimensions. Our simulations support the existence of (at least) three phases: a superfluid phase, a disorder-local-

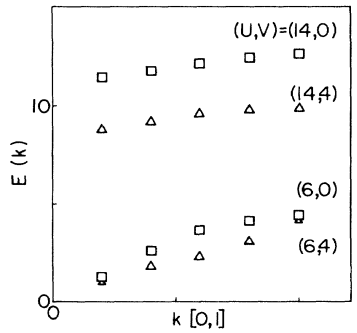

FIG. 4. Energy of density excitations along [0,1] at $\rho=1.0$. For $U/t=6$ (lower triangles) and $U/t=14$ (upper triangles) in the disordered system $V/t=4$. For the clean system with $U/t=6$ (lower squares) and $U/t=14$ (upper squares).

ized (Bose-glass) phase, and a Mott insulating phase for commensurate densities. At a commensurate density, the system seems to undergo a direct transition from the superfluid phase to a Mott insulating phase without an intervening disorder-localized phase. This occurs at an interaction strength $U=U_c$ for any disorder V, where U_c is found to *increase* with increasing V.

In future numerical work on this problem, we are planning to modify our algorithm, by including global moves of clusters of particles, in order to allow simulations directly in the disorder-localized phase. One promising avenue for further analytical and numerical work on the superfluid to Bose-glass transition is to exploit the strong correlation of the quantum-mechanical ground state near the transition with the classical state, a feature which emerges from our simulations.

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Note added.— After this work was submitted we became aware of a similar study in 1D by Scalettar, Batrouni, and Zimanyi [17].

[1] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979); P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).

[2] D. Belitz and T. R. Kirkpatrick, Phys. Rev. Lett. **63**, 1296 (1989); M. Milovanovic, S. Sachdev, and R. N. Bhatt, Phys. Rev. Lett. **63**, 82 (1989).

[3] M. H. W. Chan, K. I. Blum, S. Q. Murphy, G. K. S. Wong, and J. D. Reppy, Phys. Rev. Lett. **61**, 1950 (1988).

[4] H. M. Jaeger, D. B. Haviland, B. G. Orr, and A. M. Goldman, Phys. Rev. B **40**, 182 (1989).

[5] D. B. Haviland, Y. Liu, and A. M. Goldman, Phys. Rev. Lett. **62**, 2180 (1989); D. B. Haviland, Y. Liu, T. Wang, and A. M. Goldman (to be published).

[6] M. Randeria, J. M. Duan, and L. Y. Shieh, Phys. Rev. Lett. **62**, 981 (1989); Phys. Rev. B **41**, 327 (1990).

[7] M. Ma, B. I. Halperin, and P. A. Lee. Phys. Rev. B **34**, 3136 (1986).

[8] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).

[9] T. Giamarchi and H. J. Schulz, Europhys. Lett. **3**, 1287 (1987); Phys. Rev. B **37**, 325 (1988).

[10] D. M. Ceperley and E. L. Pollock, Phys. Rev. B **30**, 2555 (1984); E. L. Pollock and D. M. Ceperley, Phys. Rev. B **36**, 8343 (1987); D. M. Ceperley and E. L. Pollock (to be published).

[11] W. Krauth and N. Trivedi, Europhys. Lett. **14**, 627 (1991).

[12] A. J. Leggett, Phys. Fennica **8**, 125 (1973).

[13] G. G. Batrouni, R. T. Scalettar, and G. T. Zimanyi, Phys. Rev. Lett. **65**, 1765 (1990).

[14] W. Krauth and N. Trivedi (to be published).

[15] Presently, the simulations (which take on the order of 10^8 iterations per sample) are too complex to allow a true disorder average on larger systems in order to provide a definitive test of the hypothesis of self-averaging.

[16] N. Trivedi and D. M. Ceperley, Phys. Rev. B **40**, 2737 (1989); **41**, 4552 (1990).

[17] R. T. Scalettar, G. G. Batrouni, and G. T. Zimanyi, Phys. Rev. Lett. **66**, 3144 (1991).