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Numerical study of the onset of superfluidity in two-dimensional, disordered, hard-core bosons

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The ground-state of hard-core bosons in a random one-body potential is studied numerically to observe the transition from superfluid to insulating "Bose glass" phase. Finite-size scaling analyses are performed to estimate the transition point and critical exponents. The dynamical critical exponent is $z=1.95\pm0.25$ and is consistent with the prediction of Fisher *et al.* [Phys. Rev. B **40**, 546 (1989)]. Values for other exponents and preliminary results regarding the universal conductivity are presented.

There has been much recent interest in the zero-temperature, onset-of-superfluidity phase transition in interacting Bose systems.[1-6] In this phenomenon the ground-state superfluidity is destroyed by sufficiently strong disorder that tends to "localize" the bosons. The transition is believed to be continuous, occurring at a critical value of disorder strength, and near this point scaling laws for thermodynamical variables should hold.[1] The insulating state has been called the "Bose glass."[1] Recent experiments involving ^{4}He in Vycor and silica gels have attempted to observe and characterize the phase transition.[7] Granular superconductors and disordered superconducting films[8] are also expected to act similarly with the electron Cooper pairs behaving approximately as bosons.

I have studied a simple model believed to undergo the onset of superfluidity transition, namely, a two-dimensional lattice of hard-core bosons in the presence of a random one-body potential (with rms deviation Δ). As is well known, hard-core bosons can be mapped onto a spin-$\frac{1}{2}$ *XY* ferromagnet, and, for the case considered here, the quenched disorder appears as a random magnetic field along z at each site. This paper reports a finite-size scaling analysis of the critical point. From the numerical study of small systems ($4\leq N\leq 25$), I have determined the location of the transition Δ_c and the values of critical exponents with an accuracy of 10–20%. Although the uncertainties are somewhat large, these results provide a useful characterization of the phase transition. It appears the prediction of Fisher *et al.*[1] that the dynamical critical exponent z is equal to the spatial dimensionality d holds for the case studied here. The compressibility computed in this work is found to be finite through the transition, which also strongly suggests[1] that $z=d$. Estimates of exponents for which there are no predictions are presented below.

The Hamiltonian for hard-core bosons in a random potential is taken as

$$H=-\frac{J}{2}\sum_{\langle ij\rangle}(a_i^\dagger a_j+a_j^\dagger a_i)+\sum_{i=1}^{N}h_i(2n_i-1)+V_{\rm hc} \quad (1)$$

where $\langle ij\rangle$ denotes a sum over nearest neighbors of the $N=L^2$ lattice sites. $a_i^\dagger$ (a_i) is the Bose creation (annihilation) operator at site i and $n_i=a_i^\dagger a_i$. The hard-core term $V_{\rm hc}$ restricts $n_i\leq 1$. The first term in H is the quantum lattice-gas kinetic energy,[9] and the second represents a random external potential, yielding energies $\pm h_i$ when a boson is present at site i or not. In the magnetic language,[9] H is expressed exactly as

$$-J\sum_{\langle ij\rangle}(S_i^xS_j^x+S_i^yS_j^y)+2\sum_i h_iS_i^z$$

where S_i^x, S_i^y, S_i^z are spin-$\frac{1}{2}$ operators. J will be the unit of energy. The fields at different lattice sites are independent, sampled from a uniform probability distribution $P(h_i)$ with $\langle h_i\rangle=0$ and $\langle h_i^2\rangle\equiv\Delta^2$. The calculations are performed in the fixed boson density $\rho=N_b/N$ sectors. For each of the 100 to 500 system realizations of disorder the ground-state eigenvector ψ_0 is computed by the Lanczos algorithm or by an accelerated power method.[10]

The soft-core boson Hubbard model (with an energy $\sim U$ for multiple occupancy) has been studied recently both with and without disorder.[1-6,11,12] For commensurate boson densities ($\rho=1,2,\ldots$) there is a special Mott insulator to superfluid (MISF) transformation in the *pure* system as U is varied. It is predicted[1] to be in the universality class of the $d+1$ dimensional classical *XY* model. For sufficiently small U, particles can hop on top of each other and the excess particles and holes then Bose condense to form a superfluid. For large U such fluctuations become improbable, and the system is an insulator. This special transition, of course, is not present in the hard-core system since $U=\infty$.[13] However, one can easily show[14] that the pure system, *generic* ($\rho\to 1^-$) MISF critical scaling laws are reproduced by the hard-core system. For the *disordered* system, the Bose glass to superfluid transition is believed to be in the same universality class as the finite U disordered boson Hubbard model. This view should certainly be correct in $d\geq 2$ where particles can move around each other and with bounded disorder satisfying $U\gtrsim\Delta$. Then, it should not be crucial whether or not bosons can pile up at the same site. In recent Monte Carlo simulations[4,6] of the disordered soft-core boson Hubbard model the small U regime has been explored. There it has been found that increasing repulsion U actually increases ρ_s (thus, repulsion *de*localizes the particles). It has been speculated[4] that in this regime the Bose glass that results from increasing disorder may actually be a different phase from the Bose glass obtained at large U. The present work does not address this interesting question, being limited to $U=\infty$. Below I show that the Monte Carlo results of Krauth, Trivedi, and Ceperley[6] are suggestive of a superfluid to Bose glass transformation at large U and $\rho=\frac{3}{4}$. The mechanism that drives the transition in this case hinges on whether or not the hopping term $\sim J$ can overcome the tendency to localize a boson $\sim\Delta$.

The thermodynamic and structural properties are computed as follows. The chemical potential $\mu=\partial E/\partial N_b$ and compressibility $\kappa^{-1}=N\partial^2E/\partial N_b^2$ are derived from finite differences with $N_b\pm 1$. The superfluid density ρ_s is computed via the helicity modulus,[9] $\Upsilon=(\hbar^2/m)\rho_s$, where $\Upsilon\equiv(1/L^{d-2})\partial^2E/\partial\theta^2$. The phase twist θ is achieved from terms $e^{i\theta}a_i^\dagger a_j+e^{-i\theta}a_j^\dagger a_i$ in H whenever the bond i-j penetrates the periodic boundary along $\hat{\mathbf{x}}$.

Off-diagonal long-range order is measured for bosons by the $\mathbf{k}=0$ condensate fraction, n_0, that is the square of the order parameter:

$$n_0\equiv\frac{1}{N}\langle\psi_0|a_0^\dagger a_0|\psi_0\rangle=\frac{1}{N^2}\langle\psi_0|\sum_{i,j}S_i^+S_j^-|\psi_0\rangle\,. \qquad (2)$$

In the spin language, with $M_a\equiv\sum_i S_i^a/N$ $(a=x,y,z)$ and $M_{xy}^2\equiv M_x^2+M_y^2$, one has $n_0=M_{xy}^2+(\rho-1/2)/N$, and, hence, n_0 measures long-ranged xy spin correlations. At $T=0$, both ρ_s and n_0 are driven to zero for sufficiently large disorder that localizes the bosons and breaks up superfluid coherence.

The above thermodynamic functions are singular at Δ_c and are expected to obey scaling laws. I simply list the results that are discussed at length in Ref. 1. Setting $\delta\equiv\Delta-\Delta_c$, the superfluid density and condensate fraction (in the infinite system) vanish as $\rho_s\sim|\delta|^\zeta$ and $n_0\sim|\delta|^{2\beta}$ for $\delta<0$ and are zero for $\delta>0$. The superfluid correlation function $\Gamma(\mathbf{r})=\langle a(\mathbf{r})a^\dagger(0)\rangle$ is long ranged for $\Delta<\Delta_c$ and decays exponentially to zero above the transition. Near the transition the correlation length ξ diverges as $|\delta|^{-\nu}$. At Δ_c, $\Gamma(\mathbf{r})$ behaves as a power law $\Gamma(\mathbf{r})\sim r^{-(d+z-2+\eta)}$ (defining η). z is the *dynamical* critical exponent that describes how temporal correlations diverge via $\xi_\tau\sim\xi^z$. Lastly, the singular part of the compressibility and the *total* compressibility go, respectively, as

$$\kappa_s\sim|\delta|^{-\alpha}\equiv|\delta|^{\nu(d+z)-2},\quad \kappa\sim|\delta|^{\nu(d-z)}\,. \qquad (3)$$

Figure 1 shows the ρ_s data for $L=2$, 3, 4 and $\rho=\frac{1}{2}$ ($L=3$ has been interpolated to $\rho=\frac{1}{2}$). At small Δ, ρ_s tends toward a nonzero value, while for large Δ it extrapolates to zero. It is natural to suspect that a phase transition occurs in between. To compare with the previous Monte Carlo work, calculations were performed at $\rho=\frac{3}{4}$ and $\Delta=0.0$, 0.6, 1.7. These disorder strengths correspond to the ones reported in Fig. 1(a) of Krauth, Trivedi, and Ceperley[6] for a 6×6 lattice (note that $V=\sqrt{12}\Delta$ where V is the disorder parameter of Ref. 6). The values computed here, $\rho_s/\rho=0.27$, 0.15, and 0.02 for increasing Δ are in good accord with the large U trend in Ref. 6 (note that there appears to be a discrepancy between the data in Fig. 4 of Ref. 5 and the pure system data in Ref. 6). It will be shown below that the critical disorder strength for the hard-core system is about $\Delta_c\approx1.4$. Thus, the large U results of Krauth, Trivedi, and Ceperley[6] are consistent with the hard-core boson scenario found here, namely, the system is superfluid for $\Delta=0.0$, 0.6 but not so for $\Delta=1.7$. One-dimensional diagonalizations were performed to

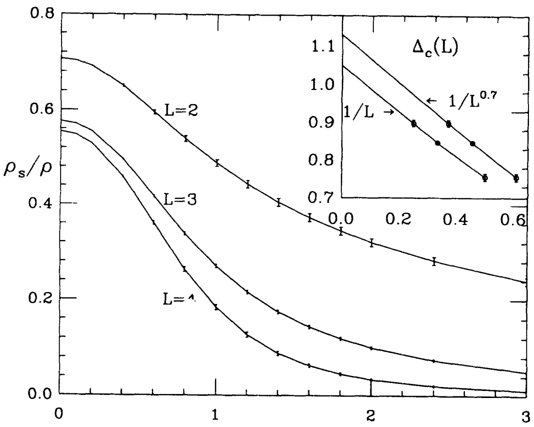

FIG. 1. Superfluid density ρ_s as a function of disorder strength Δ at density $\rho=\frac{1}{2}$. The inset shows the extrapolation of the point of maximum slope of $\rho_s^{1/6}$ (see text) to infinite system size using both $1/L$ and $1/L^{1/\nu}$ with $\nu=1.4$.

compare with the large U, $\rho<1$ results of Batrouni, Scalettar, and Zimanyi.[3,4] For the pure system, I find good agreement ($\approx5\%$) between the one-dimensional (1D) hard-core boson results[15] and the $U=20$ kinetic energy, chemical potential, and ρ_s, in Figs. 1, 2, and 5, respectively, of Ref. 3. For the 1D disordered case, the trend $\rho_s\to0$ as $U\to\infty$ in Fig. 4 of Scalettar, Batrouni, and Zimanyi[4] is consistent with the fact that any disorder localizes the spinless, noninteracting fermions of the Jordan-Wigner transformed spin-$\frac{1}{2}$ XY model. Exact diagonalizations of the disordered 1D case will be published elsewhere.

Several techniques were used to analyze the 2D disordered hard-core boson data. The first method used here to find the critical point examines the position of maximum slope $\Delta_c(L)$ of $[\rho_s(\Delta,L)]^{1/n}$ vs Δ. The nth root is taken since it is expected[1] that ρ_s vanishes faster than linearly as $\delta\to0^-$. Finite-size scaling predicts[16] that $\Delta_c(L)-\Delta_c\sim L^{-1/\nu}$. The inset to Fig. 1 shows the extrapolation to $L=\infty$ using the value of ν found below and $n=6$, and suggests that $\Delta_c\approx1.15$.

The second technique to estimate the Bose glass to superfluid transition point uses the finite-size scaling moment ratio[17,18] $g_L(\Delta)\equiv\langle(M^2)^2\rangle/\langle M^2\rangle^2$, where M^2 is either M_x^2 or M_{xy}^2. A very useful property found to hold for a wide variety of critical phenomena is that the different L curves tend to cross at Δ_c with relatively small finite-size corrections.[17,18] Figure 2 displays the $g_L(\Delta)$ curves derived from M_x. To remove some of the finite-size error, the "self-correlation" terms [those in Eq. (2) with $i=j$] have been subtracted from M^2. From the finite-size scaling ansatz, g_L is a function of the combination $L^{1/\nu}\delta$. To estimate ν one may adjust it until the g_L vs $L^{1/\nu}\delta$ curves overlap. The choice $\nu=1.4$ and $\Delta_c=1.25$ is displayed in the inset to Fig. 2. The relation[17,18] $\partial g_L/\partial\Delta\propto L^{1/\nu}$ at Δ_c may also be used to estimate ν. Either method suggests $\nu=1.4\pm0.3$. The value is consistent with the bound $\nu\geq2/d$ derived by Chayes *et al.*,[19] and is also consistent with the recent prediction ($\nu=1.4$) of Zhang and Ma[20] using a real-space renormalization group.

In Barber and Selke's generalization of Nightingale's[21]

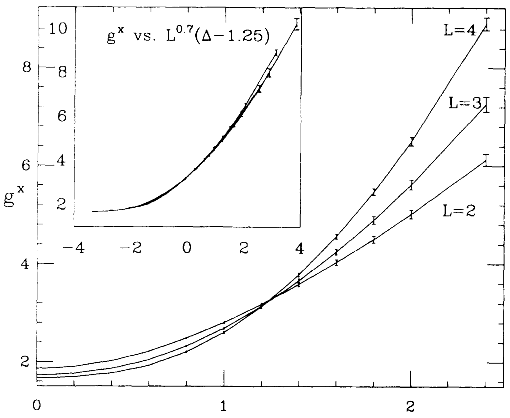

FIG. 2. Moment ratio location of the critical point Δ_c using M_x at $\rho=\frac{1}{2}$. The inset shows the scaling plot assuming $\nu=1.4$ and $\Delta_c=1.25$.

phenomenological renormalization group one defines the function

$$\Xi(\Delta,L,L')\equiv\frac{\ln[P(\Delta,L)/P(\Delta,L')]}{\ln(L/L')} \tag{4}$$

for all pairs of system sizes L and L' studied. P is a singular quantity with critical exponent γ, and so behaves[16-18] as $L^{\gamma/\nu}\bar{P}(L^{1/\nu}\delta)$ near the transition. The Ξ curves tend to cross[21] at Δ_c, at which point they take on the value γ/ν. The functions Ξ derived from ρ_s and from M_{xy}^2 are plotted in Fig. 3, and indicate a transition point close to that found by the two previous schemes.

The above methods place Δ_c in the range 1.1–1.3. The scaling with L at Δ_c can be used to deduce the critical exponents. After applying a correction to scaling extrapolation suggested by Binder,[17,18] I obtain $\zeta/\nu=1.95\pm0.25$ and $2\beta/\nu=1.4\pm0.3$. Using the generalized Josephson relation[1] $\zeta/\nu=(d+z-2)=z$, one sees that the value computed here is in agreement with the prediction $z=d$ of Ref. 1. The exponent $\zeta\approx2.8$ and implies the superfluid density is a markedly flat function of Δ near the transition (as opposed to the familiar temperature-driven λ transition in $d=2$ or 3).

A consequence of $z=d$ is that the total compressibility is finite (and nonzero) at the transition [Eq. (3)]. The data for κ plotted in Fig. 4 are consistent with finite $\kappa(\Delta_c)$. Also shown is the exact $L=\infty$ result for $\Delta\gg J$ (i.e., $\kappa=0.145/\Delta$) which strongly suggests there is no dramatic size dependence to κ over the entire range of Δ. The *singular* part of the compressibility goes as $\kappa_s\sim|\delta|^{-\alpha}$ and from Eq. (3) one has $\alpha=-3.6\pm1.0$. A singularity of such high order would be difficult to observe directly.

From the generalized hyperscaling relation[1] $2\beta/\nu=(d+z-2+\eta)$, I extract $\eta=-0.55\pm0.15$ which is consistent with the bounds derived in Ref. 1 of $2-d-z\le\eta\le2-d$, based on certain "continuity" requirements on the single-particle density of states. The value also agrees with that obtained directly from the power-law decay of the $L=4$ correlation function $\langle a(\mathbf{r})a^\dagger(0)\rangle$ at criticality.

The above calculations were repeated at $\rho=\frac{1}{5}$ for $L=3$, 4, and 5. The $L=3$, 4 results were interpolated to $\rho=\frac{1}{5}$. The transition appears to occur at $\Delta_c=1.4\pm0.1$ with values of the critical exponents in agreement with those computed at $\rho=\frac{1}{2}$. The apparently weak dependence of Δ_c on ρ may be partially due to the fact that (from particle-hole symmetry) $\Delta_c(\rho)$ is even about $\rho=\frac{1}{2}$.

Turning to the conductivity, it has been conjectured[1] that precisely *at* the transition the system is metallic. Furthermore, the value of conductivity should be universal, as has been discussed for the $d=1$ case and also for the $d=2$ pure system MISF transition.[11,12] At Δ_c the ground-state conductivity has been computed here by the Kubo formula,

$$\mathrm{Re}\sigma(\omega)=\frac{1}{\hbar\omega}\frac{1}{L^2}\mathrm{Re}\left[\int_0^\infty dt e^{i\omega t}\langle\psi_0|[\hat{J}_x(t),\hat{J}_x(0)]|\psi_0\rangle\right], \tag{5}$$

with the current operator $\hat{J}_x=(ie^*J/2\hbar)\sum_{j,\delta}\delta_x a_{j+\delta}^\dagger a_j$. e^* is the charge carried by one boson ($e^*=2e$ for Cooper

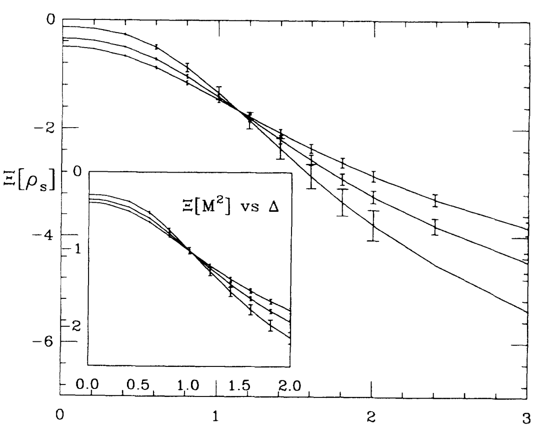

FIG. 3. Phenomenological renormalization-group function Ξ vs disorder strength for all pairs of $L=2$, 3, 4 for the superfluid density ρ_s and M_{xy}^2 (inset).

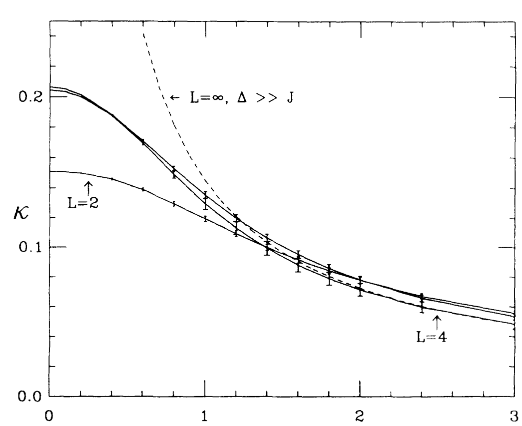

FIG. 4. Compressibility as a function of disorder strength for $L=2$, 3, 4 at $\rho=\frac{1}{2}$. The dashed line indicates the infinite system, exact result from ignoring the hopping term.

pairs). The current-current time correlation function in the integral was computed by repeated application of the operator $\exp(iHdt/\hbar)$ to $\hat{J}_x|\psi_0\rangle$ using a Trotter breakup[22] and averaging over disorder. The $L=3$ data for $\sigma(\omega)$ suggest a low (but not zero) frequency value of $\sigma/\sigma_Q \approx 0.055$ and for $L=4$, $\sigma/\sigma_Q \approx 0.105$. $\sigma_Q \equiv e^{*2}/h$. Assuming a $1/L^2$ correction implies an infinite system value of $\sigma_c/\sigma_Q \approx 0.17 \pm 0.01$. A $1/L$ correction yields $\sigma_c/\sigma_Q \approx 0.25 \pm 0.02$. It is not clear what is the exact form of the correction, indeed, a more careful finite-size scaling analysis needs be performed before a reliable value can be deduced. A heuristic argument can be given in favor of a $1/L^2$ correction: the integral[23] $\int_0^\infty d\omega \, \mathrm{Re}\sigma(\omega)$ is equal to $\pi^2\sigma_Q(\langle -T_x\rangle - \rho_s)$, where T_x is the kinetic energy per site in the x direction. All of the data computed here obey this sum rule. Numerically, I find the corrections to $\langle T_x\rangle$ and ρ_s are $1/L^2$ (i.e., $1/L^z$). Now, *assuming* the correction to $\mathrm{Re}\sigma(\omega)$ comes from an overall rescaling factor at most ω (as the data suggests), then there should be a $1/L^2$ correction for $\mathrm{Re}\sigma(\omega)$ at small ω. The conductivities computed at $\rho=\frac{1}{5}$ are consistent with a $1/L^2$ behavior, and extrapolate to a value $\sigma_c/\sigma_Q \approx 0.15 \pm 0.01$.

The value $\sigma_c/\sigma_Q \sim 0.15-0.17$ is not unreasonable, as Cha *et al.*[11] have found in $d=1$ that an appropriately defined universal conductance for the Bose glass to superfluid transition is 25% *lower* than that for the MISF transition, and, for the $d=2$ MISF case they find $\sigma_c/\sigma_Q = 0.285 \pm 0.02$. The lower value at the Bose glass to superfluid transition suggested by the present data is, therefore, consistent with the $d=1$ trend.

In summary, I have reported a finite-size scaling study of the $d=2$, $T=0$, Bose glass to superfluid phase transition in which the critical exponents ζ, β, η, z, and ν and the universal conductivity have been computed. z is found close to 2, in agreement with the prediction of Ref. 1. One may argue that the system sizes ($L=2$, 3, 4) are too small to study the critical phenomenon reliably. It is possible that the results reported here may be biased due to the small lattices considered. This would certainly be the case if large or rare domains of disorder or a long crossover or localization length play a crucial role in the transition. The most likely scenario seems, however, that the true exponents are close to those reported here since nothing unexpected happened in the finite-size scaling analysis. Present work on 5×5 lattice with $N_b=12$ should allow one to address more carefully the magnitude of corrections to scaling for this system.

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[15]In fact, in one dimension one has the exact results for the spin-$\frac{1}{2}$ XY model: $E/N = -(1/\pi)\sin(\pi\rho)$, $\mu = -\cos(\pi\rho)$, $\pi\kappa = 1/(1-\mu^2)^{1/2}$, $\rho_s/\rho = \sin(\pi\rho)/\pi\rho$. These results may be extracted from E. Lieb, Ann. Phys. (N.Y.) **16**, 407 (1961). The scaling exponents of these quantities as $\rho \rightarrow 1^-$ are precisely the mean-field ones discussed in Refs. 1 and 3.

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