Quantum Critical Phenomena in One-Dimensional Bose Systems

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(Received 5 June 1990)

We use quantum Monte Carlo techniques to study the critical properties of an interacting-boson model in one dimension. The phase diagram consists of a series of (Mott-) insulating phases at commensurate fillings and a superfluid phase. From the critical behavior of the superfluid density and the compressibility we measure the exponents ν and z, which agree with predictions based on a scaling analysis.

PACS numbers: 67.40.Db, 05.30.Jp, 05.70.Jk

The past few years have seen a major increase in activity in the field of strongly interacting fermionic systems. Besides high-temperature superconductivity, important issues are the identification of new exotic phases, the Mott-type metal-insulator transition,[1] and the role of disorder, which can localize the electrons.[2] The interplay of the two localization transitions is currently the subject of close scrutiny.[3] Our understanding of the corresponding phenomena in Bose systems in much less developed in spite of its quite general experimental relevance. Liquid ^{4}He and short-correlation-length superconductors are examples of the ordered case, while ^{4}He absorbed in porous media[4] and homogeneously disordered and granular[5] superconductors (where the Cooper pairs can be approximated as bosons) are natural realizations of the disordered case. The theoretical interest in these systems stems from the fact that their phase transitions are driven by quantum rather than thermal fluctuations. The analogs of the above Mott and Anderson transitions were only recently described by scaling theories.[6] However, these analytic approaches usually work with expansions around the upper critical dimension, so in low dimensions an approximation-free numerical analysis is very useful as an independent test of the results. Motivated by this, we report here on a quantum Monte Carlo study of the one-dimensional, strongly interacting Bose liquid.

We study the simplest model for interacting bosons on a one-dimensional lattice,[7]

$$\mathcal{H} = -t\sum_l (a_{l+1}^\dagger a_l + \text{H.c.}) + \sum_l (-\mu \hat{N}_l + V\hat{N}_l^2)\,. \quad (1)$$

$\hat{N}_l = a_l^\dagger a_l$ and a_l is the boson annihilation operator at site l. t is the hopping parameter, V is a boson repulsion, and μ is the chemical potential. The $T=0$ phase diagram can be sketched as follows.[6] At $t/V=0$ every site is occupied by an integer number n of bosons which minimizes the on-site energy: $\epsilon(n) = -\mu n + Vn^2$. Thus in the interval $2n-1 < \mu/V < 2n+1$, the density (occupation number per site) is pinned at the integer n. Inside this interval there is a finite gap in the one-particle spectrum and so the system is insulating. Correlations are localized with a finite correlation length ξ and the compressibility κ vanishes; i.e., these states are incompressible insulators. The gap decreases as t/V increases and eventually vanishes, giving the insulating phases lobelike shapes in the μ/V vs t/V plane.[6] At this critical value of t/V the kinetic energy overcomes the gap, the system becomes a conductive fluid, and this delocalization of the bosons leads to the formation of a superfluid state at zero temperature.

The phase transitions taking place at a generic point of the phase boundary belong to a different universality class from that at the tip of the lobes. This can be seen by performing a Hubbard-Stratonovich decoupling of the kinetic term and then performing a cumulant and a gradient expansion to obtain the effective action[6]

$$S = \int dk\, d\omega [\tfrac{1}{2}(k^2+\omega^2+r) + i\omega g] |\psi(k,\omega)|^2 + u\int dx\, d\tau |\psi|^4\,, \quad (2)$$

where g vanishes at the tips because of particle-hole symmetry. Therefore, when the transition occurs at integer densities, it belongs to the universality class of the (1+1)-dimensional XY model; i.e., it is a Kosterlitz-Thouless (KT) point. Here we do not analyze the multicritical aspects of this transition. On the insulating side, the inverse correlation length and consequently the gap are expected to vanish as $\xi^{-1} \approx E_g \approx \exp(-1/\sqrt{x-x_c})$, where $x = t/V$. In the delocalized phase, superfluid correlations decay as a power law with exponent K, where $(\pi K)^2 = (\rho_s \kappa t)^{-1}$, κ is the compressibility, and ρ_s is the superfluid density. Away from the commensurate values $g \neq 0$; thus the propagator acquires a special form and consequently when an ϵ expansion is developed around the upper critical dimension ($d_c = 2$), all of the poles lie in the upper half plane and so all the perturbative contributions vanish.[8] That means that the critical exponents assume their mean-field values and one expects the correlation length exponent $\nu = 0.5$ and the dynamical critical exponent $z = 2$. With these values the generalized Josephson relations yield for the superfluid density and compressibility exponents $\zeta = \alpha = \nu(z-1)$

=0.5, when expressed as a function of $\mu-\mu_c$. This new type of phase transition is driven by density fluctuations, as opposed to the XY transition, which is driven by phase fluctuations. We note that an explicitly one-dimensional formulation of this problem can be developed leading to an action very similar to the sine-Gordon model.[9] The periodic potential gives rise to one extra term containing the density of the bosons. So, it is quite natural to attempt a renormalization-group analysis directly in one dimension. Unfortunately, the density scales to strong coupling at a generic point of the phase boundary, thus preventing the extraction of the critical exponents. In what follows we determine the phase boundary and the above-mentioned exponents to test the reliability of the ϵ expansion.

We perform our Monte Carlo simulations using the "world-line" algorithm[10,11] on a one-dimensional chain of N sites with periodic boundary conditions. This involves rewriting the partition function and any operator expectation values of interest as a path integral by discretizing the imaginary time β into L subintervals of length $\tau=\beta/L$. We use the checkerboard decomposition[12] to evaluate the infinitesimal imaginary-time evolution operator $e^{-\tau H}$. This "Trotter approximation"[13,14] yields values for observables which differ from exact results by corrections of order τ^2. We have chosen τ so that these systematic effects are typically less than a few percent. We have also examined the effect of finite size by doing simulations on different size systems and comparing the observables. We have found that a 16-site chain does not suffer from any significant finite-size effects, and the only occasions where we had to use bigger systems were when we needed densities, $\rho=N_b/N$, that cannot be obtained on a 16-site system.

Our simulation works within an ensemble which conserves both particle (N_b) and winding numbers. However, by looking at the energy as a function of occupation, we can extract the chemical potential and make contact with grand-canonical formulations. Since nonzero-winding-number configurations are absent with free boundary conditions, their exclusion is not relevant in the thermodynamic limit.[10,15] We have verified our code against weak- and strong-coupling analytic calculations, and against exact diagonalization on small clusters in all regimes of temperature T, and couplings t and V. In the work reported below, unless otherwise indicated, we have chosen $t=1$, $V=20$. We have checked that the values of β are large enough to obtain ground-state properties by doing the simulation at various values and ensuring that averages of thermodynamic quantities did not change. Further details will be reported elsewhere.[16]

The effective one-particle transfer energy, $t_{\text{eff}}=t\times\langle a_{l+1}^\dagger a_l+a_l^\dagger a_{l+1}\rangle$, has been used in variational-wave-function studies of the Mott transition[17] and in Monte Carlo simulations to examine the interpolation between weak coupling and the strong-coupling Heisenberg regime in the Hubbard model.[18] In Fig. 1, we show this quantity as a function of boson occupation. The sharp minima at integer fillings corresponds to *incompressible insulating* phases as shown below. These cusps lead to discontinuities in the slope of the total energy E_N at integer fillings and hence to the opening of compressibility gaps. This can be seen by plotting (Fig. 2) the density ρ as a function of the chemical potential, $\mu=E_{N+1}-E_N$, which is evaluated numerically. The three plateaus correspond to the first three lobes of the Mott-insulating regions in the μ/V vs t/V phase diagram. For $t/V=0$, the gap is 2 and decreases as t/V increases. The $n=1$ lobe of the ground-state phase diagram is shown in Fig. 3. The cusp-shaped approach to the tricritical point is con-

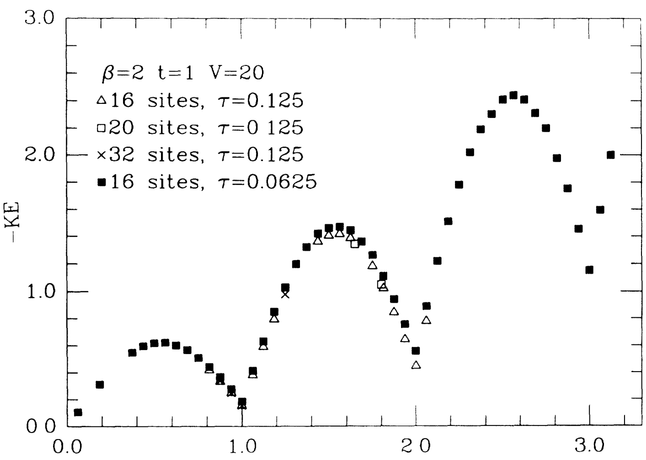

FIG. 1. The kinetic energy is shown as a function of occupation ρ for $t=1$, $V=20$. Different symbols represent various choices of lattice size and imaginary-time discretization length τ. Error bars are smaller than the data points.

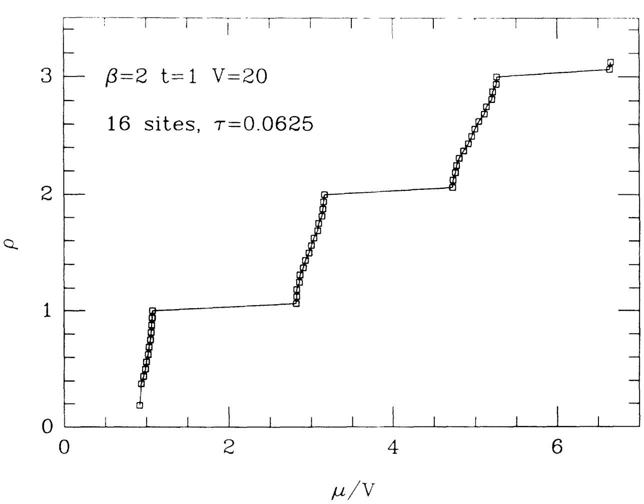

FIG. 2. The occupation (density) ρ as a function of chemical potential, $\mu=E_{N+1}-E_N$, going across the first three lobes of Mott-insulator regions. The solid line is to guide the eye.

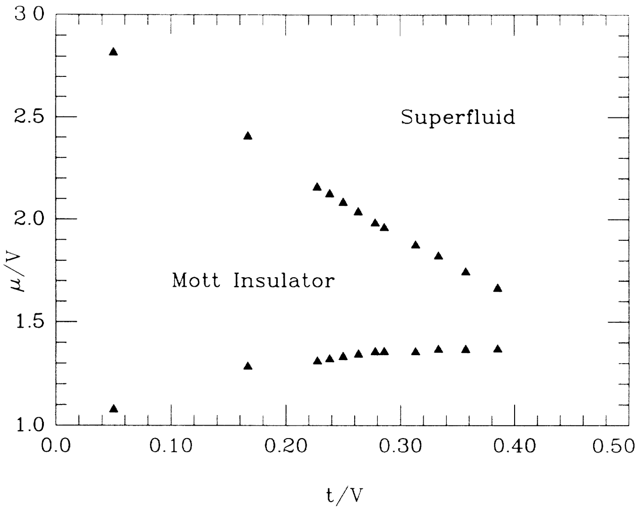

FIG. 3. The first lobe of the zero-temperature phase diagram.

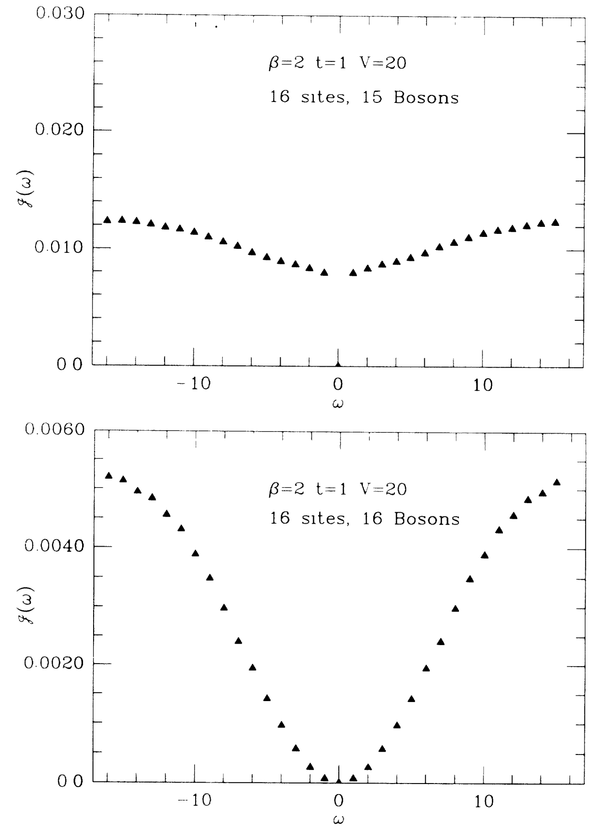

FIG. 4. $\tilde{\mathcal{J}}(\omega)$ is shown as a function of frequency on a $N=16$ site lattice for two different fillings, $N_b=15$ and 16.

sistent with the KT form for E_g discussed above. We find that the tip of the lobe is located at $t/V=0.43 \pm 0.02$. We bracket this critical value by extrapolating the gap to zero from the insulating side, and by studying the vanishing of ρ_s from the superfluid side. The superfluid density is expected to have a (nonuniversal) jump at the transition. However, at KT transitions the rapidly diverging correlation length usually leads to large finite-size rounding. We have not performed any detailed finite-size analysis at this point, but if we identify the location of the "jump" from the largest slope of ρ_s vs t/V, these two procedures yield values in agreement within the cited error bars. There are no exact theoretical predictions for this quantity.[19] Preliminary results indicate that the lobes at higher filling n terminate in a manner consistent with the $1/n$ mean-field prediction.

The slope in Fig. 2 gives the compressibility $\kappa=\partial\rho/\partial\mu$. It is seen that κ vanishes in the gaps and diverges at the boundaries. The evaluation of the corresponding critical exponent α requires data with exceedingly small statistical fluctuations as it involves two numerical differentiations. We obtained such data for the 16-site chain where the scaling region spanned half a decade and gave $\alpha \approx 0.52$. Using the hyperscaling relation[6] $\alpha=\nu(z-1)$, where ν is the correlation length critical exponent, and using $\nu z=1$ gives $\nu \approx 0.48$. This is consistent with the mean-field value $\nu=0.5$, in agreement with arguments suggesting that the lower critical dimension for this model is indeed $d_l=1$.

The superfluid density ρ_s satisfies[20] $\rho_s \propto \rho\langle W^2\rangle$, where W is the winding number. Defining

$$j(\tau)=\sum_{l=1}^{N_b}[x_l(\tau+1)-x_l(\tau)]\,, \qquad (3)$$

where $x_l(\tau)$ is the location of the lth boson at imaginary time τ, we see that the winding number satisfies

$$W=\frac{1}{N}\sum_{\tau=1}^{L} j(\tau)\,. \qquad (4)$$

This relation could be used to measure $\langle W^2\rangle$ if one were working in an ensemble that included nonzero-winding-number configurations. Alternatively, we can measure the correlation function $\mathcal{J}(\tau)=\langle j(\tau)j(0)\rangle$ for all τ, and perform a discrete Fourier transformation to obtain $\tilde{\mathcal{J}}(\omega)$. Because we are working in the $W=0$ sector, we always have $\tilde{\mathcal{J}}(0)=0$. However, the *extrapolation* of $\tilde{\mathcal{J}}(\omega)$ to $\omega=0$ can lead to a nonzero value which signals superfluidity.[10] The superfluid density is then $\rho_s \propto \rho\tilde{\mathcal{J}}(\omega\to 0)$. Figures 4(a) and 4(b) show $\tilde{\mathcal{J}}(\omega)$ as a function of ω for $N=16$ sites and $N_b=15$ and 16 and for V greater than its critical value. The behavior of $\tilde{\mathcal{J}}(\omega)$ shows that ρ_s goes from nonzero to zero as the occupation goes from noninteger to integer. For $N_b=17$, $\tilde{\mathcal{J}}(\omega)$ looks like the $N_b=15$ case, signaling a return to the superfluid phase. Combining this with our earlier results for κ, we conclude that the phase transition is from a compressible superfluid to the incompressible Mott insulator.

Finally, we can measure the critical exponents associated with the behavior of the superfluid fraction near the transition. In Fig. 5 we plot $\log_{10}[\tilde{\mathcal{J}}(\omega \to 0)]$ vs $\log_{10}(|\rho_c - \rho|)$. The critical density ρ_c takes integer values and is 1 at the first lobe. This yields a straight line with a slope ≈ 1.06. When the compressibility is singular at the transition, as is the case here, the superfluid density scales as[6] $\rho_s \sim |\rho_c - \rho|^{z-1}$. This gives $z = 2.06$ for the dynamic critical exponent, and since[6] $z\nu = 1$ we obtain $\nu = 0.49$. These values are consistent with the mean-field values $z_{\rm mf} = 2$ and $\nu_{\rm mf} = 0.5$, as well as the value for ν derived from the divergence of the compressibility.

In summary, for the density-driven Mott-insulator to superfluid transition at fixed V, we have obtained the critical exponents $\nu = 0.49$, $z = 2.06$, in good agreement with theoretical predictions. We have also studied κ and ρ_s for the first three lobes, and determined the phase boundary of the first lobe. We found its approach to the tricritical point to be in qualitative agreement with the form predicted by a KT transition. We are currently examining the effect of disorder in this model, in particular, the role it plays in the recently proposed "Bose-glass"[6] phase.

We would like to acknowledge very useful conversations with M. P. A. Fisher, C. Y. Young, F. D. M. Haldane, E. Y. Loh, Jr., D. Rokhsar, and R. L. Sugar. G.G.B.'s work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48. We acknowledge a "Grand Challenge" computing grant from the Department of Energy. G.T.Z. was partially supported by an Institutional Collaborative Research (INCOR) grant from LANL.

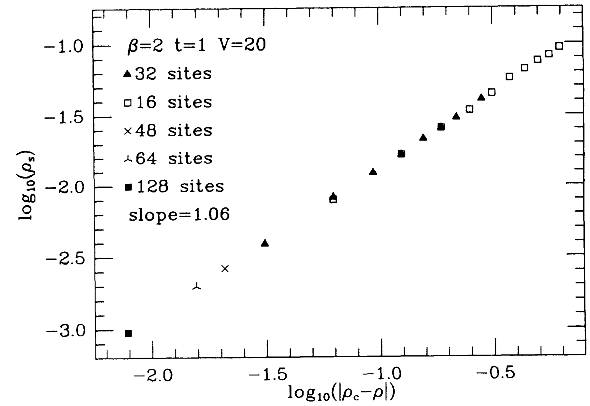

FIG. 5. A log-log plot of $\tilde{\mathcal{J}}(\omega \to 0)$ vs $|\rho_c - \rho|$. The slope is 1.06.

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