Monte Carlo simulation of hard-core bosons on a three-dimensional lattice

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A model of hard-core bosons on a three-dimensional (3D) lattice has been studied using both quantum Monte Carlo and classical Monte Carlo techniques. We have calculated the transition temperature for Bose-Einstein condensation, the zero-temperature penetration depth and the specific-heat critical amplitude, and have explored the hyperuniversal scaling relationship between these quantities pertaining to the expected 3D XY critical point. As a conclusion we draw a phenomenological analogy between the model studied and extreme type-II superconductors.

I. INTRODUCTION

In recent years, model systems with strong electron correlations have been extensively studied with the aim of deepening our understanding of cuprate superconductors. A particularly prominent model system is the Hubbard model, with its conceptual simplicity but rather nontrivial physical properties. In this paper we concentrate on the three-dimensional (3D) attractive Hubbard model which exhibits a crossover from a BCS-type superconductivity to Bose-Einstein condensation as coupling strength increases. In the strong coupling regime it can be mapped to a model of interacting local pairs undergoing Bose-Einstein condensation. In this coupling regime the attractive electron interaction leads to preformed local pairs moving by dissociation.[1] Because the pairs undergo Bose-Einstein condensation to a superfluid state, it is of interest to investigate the phase transition, including the critical-point behavior and the dependence of these properties on pair concentration.

We present and discuss the following results of quantum Monte Carlo (QMC) simulations: the transition temperature and zero-temperature superfluid density as a function of pair density. Using the classical Monte Carlo technique we estimate the critical amplitude of the specific heat. Then, using the universal scaling relations for the 3D XY critical point, we assess the consistency of our estimates of the transition temperature with those of the superfluid density and the critical amplitude of the specific heat.

Motivated by the experimental observation of critical behavior analogous to that of a neutral superfluid in extreme type-II superconductors, we conclude by discussing certain similarities between the results presented here and the properties of the cuprate superconductors.

In the limit of strong attraction, second-order degenerate perturbation theory maps the attractive Hubbard model to a model of hard-core bosons

$$\mathscr{H}=-\sum_{\langle i,j\rangle} t_{ij}b_i^\dagger b_j+U\sum_{\langle i,j\rangle} n_i n_j-\mu_B\sum_i n_i, \qquad (1)$$

where the sums are taken over nearest neighbors, $n_i=b_i^\dagger b_i$ is the number operator, t_{ij} is the hopping matrix, and U is the nearest-neighbor interaction. The terms b and $b^\dagger$ are hard-core boson operators

$$[b_i,b_{j\neq i}^\dagger]=0,\quad \{b_i,b_i^\dagger\}=1,$$
$$[b_i,b_j]=0,\quad [b_i^\dagger,b_j^\dagger]=0, \qquad (2)$$

where the anticommutator on equal sites inhibits double occupancy.

The mapping from the attractive Hubbard model formally yields $t=U$, but an obvious extension is to soften this condition, allowing U/t to vary. In this paper we will consider only $U=0$ and $U=t$, because these choices prevent the occurrence of mixed phases. Indeed, for larger U the model will exhibit charge density wave phases as well as metal-insulator transitions, which will complicate matters. Previously, the phase diagram of the 2D and 3D model has been studied for various values of U in terms of a mapping to a classical spin model.[2] QMC simulations have been performed by Onogi and Murayama[3] on the 2D model to investigate the Kosterlitz-Thouless transition in the presence of disorder. Finally, Schneider *et al.* [4] investigated the 3D model using the random-phase approximation (RPA), BCS, and exact diagonalization.

II. MONTE CARLO RESULTS

For our QMC simulations we used a worldline algorithm and checkerboard decomposition with the Suzuki-Trotter formula having periodic boundary conditions and winding number updates.[5] For a detailed description of the path-integral decomposition we refer to the paper by Blaer and Han.[6]

In accordance with the Suzuki-Trotter decomposition we write the partition function as $Z=\mathrm{Tr}e^{-\beta H}=\mathrm{Tr}(e^{-\Delta\tau H_1}e^{-\Delta\tau H_2})^{\beta/\Delta\tau}+\mathscr{O}(\Delta\tau^2)$, where the Hamiltonian is decomposed into two nonoverlapping parts $H=H_1+H_2$. In the following we have set $\Delta\tau=1/4$ and performed 50 000 thermalization updates followed by 100 000 measurements. We have studied lattice sizes of $4\times4\times4$ and $6\times6\times6$; $2\times2\times2$ was found to be too small to yield useful results.

The transition temperature has been estimated as a function of filling for the two cases $U=0$ and $U=t$. To find the transition temperature we computed the specific heat as a function of temperature. The specific heat has a well-defined peak at the phase transition, which is broadened for our system sizes but still allows reliable estimates of T_c. According to scaling theory[7] the transition temperature in the thermo-

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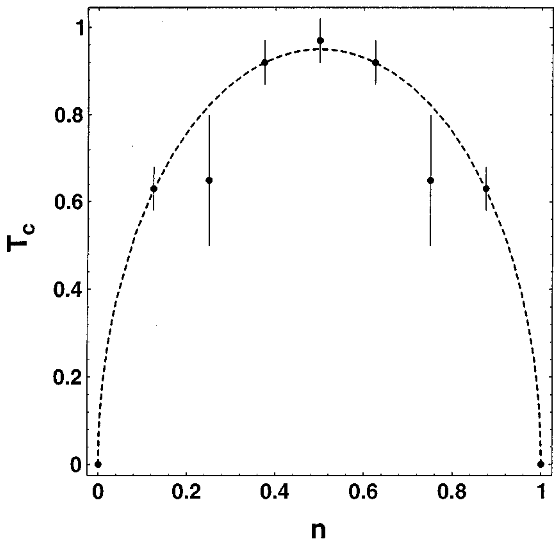

FIG. 1. The transition temperature after finite size scaling vs carrier density for $U=0$. The dashed line is the phenomenological formula $T_c \propto [n(1-n)]^{1/2}$.

dynamic limit is related to the peak position, T_p, for a finite system of linear size L by $T_p = T_c + \alpha/L^{1/\nu}$. To estimate the thermodynamic T_c we have used the scaling relation $\nu = 2/3$. This provides an estimate at best, because our numerics allowed us to obtain reliable data for only two system sizes.

Figures 1 and 2 show our estimates for the transition temperatures obtained from finite size scaling as a function of pair filling. The points for $0.5 < n < 1$ have been obtained from the data for $0 < n < 0.5$ by using particle-hole symmetry. For comparison we included the result of the RPA treatment by Schneider *et al.*[4] and Micnas *et al.*,[1] given by

$$(2n-1)^{-1} = \frac{1}{N}\sum_k \coth\left(\frac{\epsilon_0 - \epsilon_k}{2k_B T_c}(2n-1)\right), \tag{3}$$

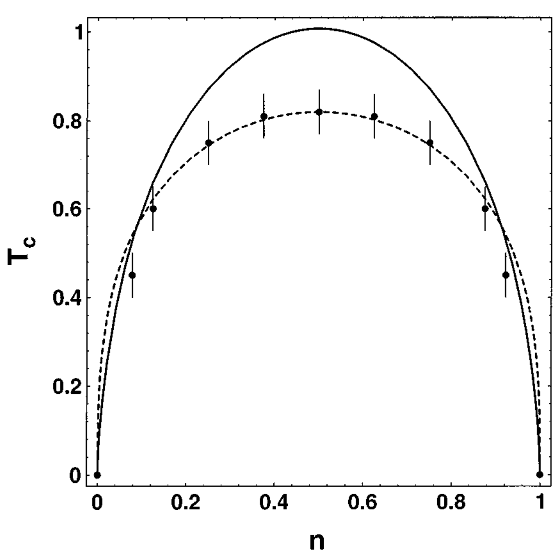

FIG. 2. The transition temperature after finite size scaling vs carrier density for $U=t$. The dashed line is the phenomenological formula $T_c \propto [n(1-n)]^{1/3}$. The solid line shows the RPA result of Schneider *et al.* (Ref. 4).

where ϵ_k is the boson dispersion. One sees (solid line) that the RPA appears to overestimate the transition temperature somewhat.

In the limit $n \to 0$ we expect the system to behave like that of a dilute Bose gas, where $T_c \propto n^{2/3}$. Although this is indeed compatible with the data, we observe for higher fillings that we can fit the overall behavior quite well with two phenomenological formulas: $T_c \propto [n(1-n)]^{1/3}$ for $U=0$ and $T_c \propto [n(1-n)]^{1/2}$ for $U=t$ (dashed curves).

At half-filling, the two cases $U=0$ and $U=t$ can be mapped to the XY model and the Heisenberg model, respectively. Here analytical estimates for T_c exists from high-temperature series expansion (HTSE). For $U=0$, the HTSE result is $T_c = 1.01t \pm 0.01$,[8] and for $U=t$ it is $T_c = 0.84t$,[9] compared with $0.97t$ and $0.82t$, respectively. This is well within the error bars of the results of our simulations.

In Eq. (1) we presume that the pairs are heavily screened, so long-range Coulomb forces can be neglected. However, the presence of charge will still lead to electrodynamic effects. In a magnetic field the hopping term will be changed to contain the usual Peierls phase factor $\exp[i(2\pi/\phi_0)\int_i^j \underline{A}d\underline{l}]$. It has been shown by Schafroth[10] that, for a condensed ideal Bose gas, this leads to the London expression for the penetration depth, which is again related to the superfluid density.

Here we find the helicity modulus, Υ,[11] by using a winding number algorithm. The helicity modulus is related to the London penetration depth

$$\frac{1}{\lambda^2} = 4\pi\left(\frac{2e}{\hbar c}\right)^2 \Upsilon. \tag{4}$$

Another quantity is the muon-spin relaxation rate which is related to the zero-temperature London penetration depth by

$$\sigma(0) = \left(\frac{2754B}{\lambda(0)}\right)^2 \propto \Upsilon, \tag{5}$$

where $B = 0.813$ in sintered materials and $B=1$ in single crystals.

The temperature dependence of the superfluid density (proportional to Υ) was calculated by QMC and the zero-temperature superfluid density estimated by extrapolating to zero temperature. In Fig. 3 we have shown $n_s(0)$ vs filling for $U=0$. The error bars in the figure result from the extrapolation to zero temperature. We have shown results only for $U=0$, because results for $U=t$ are identical within the error bars. The resulting curve is seen to be fitted quite well with the mean-field result $n_s(0) = n(1-n)$ (solid line). We remark that similar results have been obtained by Onogi and Murayama[3] for the 2D model.

In the critical region around T_c the heat capacity peak is thought to be dominated by thermal fluctuations, and quantum effects are considered negligible except for their influence on the location of T_c. Thus, to study the critical amplitude of the heat capacity peak we made a classical Monte Carlo simulation to be able to obtain larger systems than with QMC in order to better resolve the heat capacity peak.

The Bose-Hubbard model can be mapped to a spin model with the transformation

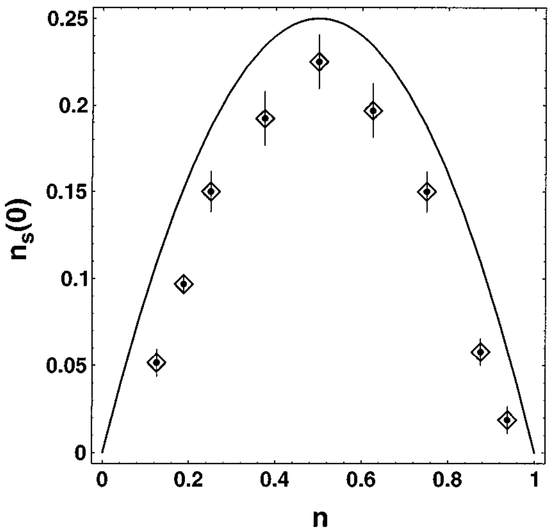

FIG. 3. The zero-temperature superfluid density vs boson density. The solid line shows the mean-field result, $n_s(0)=n(1-n)$.

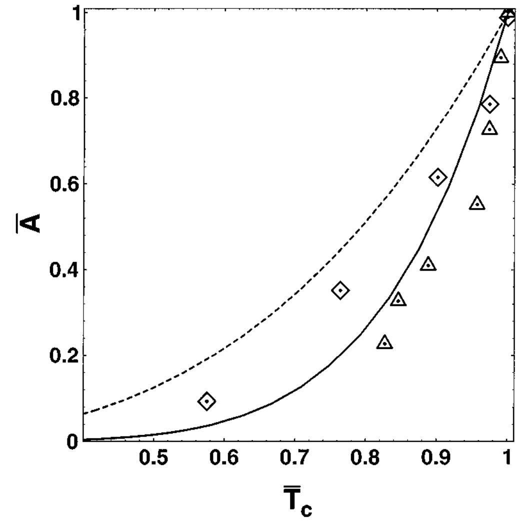

FIG. 4. The critical amplitude of the heat capacity scaled as a function of the critical temperature scaled. Squares denote MC data ($U=0$), triangles experimental data from YBCO (Ref. 12). The solid line is T_c^6, the dashed line T_c^3.

$$b_j^\dagger = S_j^x + iS_j^y, \tag{6}$$

$$b_j = S_j^x - iS_j^y, \tag{7}$$

$$n = \frac{1}{2} + \frac{1}{N}\sum_j \langle S_j^z \rangle, \tag{8}$$

where the spin variables are spin 1/2.

The Hamiltonian then becomes

$$\mathscr{H} = -t\sum_{\langle i,j\rangle} (S_i^x S_j^x + S_i^y S_j^y) + U\sum_{\langle i,j\rangle} S_i^z S_j^z - m\sum_i S_i^z, \tag{9}$$

where the sum is taken over nearest neighbors. Here the external magnetic field m has the role of a chemical potential. Thus, to keep the pair density fixed in a grand canonical simulation, we must vary the magnetic field such that we have a fixed magnetization. We emphasize that in the presence of a field, fluctuations in the z direction are massive, and the model is in the 3D XY universality class and not in the Heisenberg universality class (3D XYZ) as one might naively think.

All simulations were performed with classical spins on a $16\times16\times16$ lattice having 5000 thermalization sweeps and 10 000 averaging sweeps using the metropolis algorithm and restricted to $U=0$. The resulting specific heats display a very well-defined lambda-shaped peak, as expected for a neutral superfluid.

Following Ghiron *et al.*[12] the resulting curves for $\langle C\rangle$ vs T were fitted with the function

$$\frac{C}{T} = -A\ln(t_r^2+t_0^2) + B\left(1-\tanh\frac{t_r}{t_0}\right) + D, \tag{10}$$

where the reduced temperature is $t_r=(T-T_c)/T$, t_0 models the fact that the heat capacity peak is not divergent for a finite system and the tanh term models the mean-field-like step behavior. In Fig. 4 the resulting estimates for the critical amplitudes, A, are shown as a function of T_c together with the experimental data from Ghiron *et al.*[12]

For a 3D XY critical point, the three quantities, penetration depth, transition temperature, and specific heat critical amplitude are not independent of one another, but related by the hyperuniversal scaling relations[13]

$$k_B T_c = \frac{\Phi_0}{16\pi^3}\frac{\xi_0^\phi}{\lambda_0^2}, \tag{11}$$

$$R_\xi = A(\xi_0^\phi)^d, \tag{12}$$

where $R_\xi=0.3$, Φ_0 is the flux quantum, λ_0 is the penetration-depth-critical amplitude, and A is the heat-capacity-critical amplitude. If we now assume that the zero-temperature penetration depth is proportional to the critical amplitude, $\lambda_0\propto\lambda(0)$, the hyperuniversal relations together with the QMC results predict $A\propto T_c^6$ and $A\propto T_c^3$ for $U=0,t$, respectively. A fit to this law is shown in Fig. 4, and is seen to be in reasonable agreement with the simulation results and experimental data. The assumption that λ_0 is related to $\lambda(0)$ is further corroborated by recent experiments on $La_{2-x}Sr_xCuO_4$.[14]

Thus, it is seen that the Bose-Hubbard model, Eq. (1), agrees qualitatively rather well with the predictions of the 3D XY hyperuniversal scaling relation concerning its dependence on filling.

III. RELATION WITH CUPRATE SUPERCONDUCTORS

As there is a growing number of experiments showing the importance of fluctuations and a 3D XY critical point in high-T_c superconductors,[13] it is of interest to investigate to what extent the properties of the hard pair model treated here agree with the experimental findings on cuprate superconductors. First we note that the T_c vs filling curve we obtained in Figs. 1 and 2 behaves similarly to the bell-shaped curves found in experiments, assuming a linear relation between boson filling and electron concentration. Here one must keep in mind that the relation between the boson filling fraction and the electron doping is nontrivial.[15]

Another issue is the relation between the zero-temperature penetration depth and the critical amplitude of the penetration depth. Experiments on $La_{2-x}Sr_xCuO_4$ have shown that the ratio of these quantities is nearly constant.[14] This is consistent with the findings in this paper owing to the hyperuniversal scaling relation, Eq. (11). The dependence of the measured zero-temperature penetration depth on doping[14] is also in agreement with our estimates shown in Fig. 3. Third, the behavior of the specific-heat critical amplitude depicted in Fig. 4 is in qualitative agreement with experimental data of YBCO.[12] Finally we find $T_c \propto [n(1-n)]^{1/3} \propto \sigma(0)^{1/3}$, where $\sigma(0)^{1/3} \propto 1/\lambda(0)^2 \propto n_s(0)/M$ and M is the boson mass. Thus, in the underdoped regime, T_c increases with doping and, in the overdoped regime, T_c shows reverse evolution. In Fig. 5 this behavior is compared with the experimental data of a large number of cuprate superconductors. For most materials the data collapses more or less on a curve in accordance with the QMC prediction. However, some materials follow more closely the outline of a fly's wing, as observed for $Tl_2Ba_2CuO_{6+\delta}$.[16,17] This effect might be attributed to the breaking of particle-hole symmetry. One way to break particle-hole symmetry is to imagine bosons of finite extensions, occupying more than one site. This will introduce a topological difference between particles and holes, thus breaking particle-hole symmetry, as well as make superconductivity vanish at a filling smaller than 1, like in cuprates where superconductivity vanishes at a filling around $n=0.27$ electrons per unit cell. Phenomenologically we study this result by exploring the effect of using a nonsymmetrical interpolation formula for T_c vs n, such as

$$T_c \propto n^{2/3}\left(1-\frac{2}{5}n\right). \tag{13}$$

This kind of formula gives rise to a curve that resembles the outline of a fly's wing as shown in Fig. 5.

In conclusion we have studied some scaling properties of the superconducting phase transition of the 3D Bose-Hubbard model. Although the theoretical problem of high-temperature superconductivity in its full complexity is much beyond this model system, we find intriguing similarities. This might indicate that the phase transition in cuprates is closer to Bose-Einstein condensation of preformed or fluctuating pairs than to a BCS-type of Fermi-surface instability.

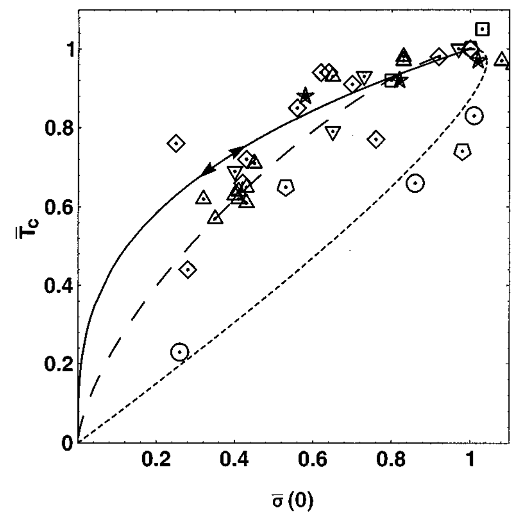

FIG. 5. Transition temperature vs zero-temperature superfluid density. Dotted line for the case of particle-hole symmetry and solid and dashed lines for broken symmetry in the underdoped and overdoped regime as obtained from QMC. Data taken from Ref. 13: ⊡, $Tl_2Ba_2Ca_2Cu_3O_{10}$, $Tl_{0.5}Pb_{0.5}Sr_2Ca_2Cu_3O_9$; $Bi_{2-x}Pb_xSr_2Ca_2Cu_3O_{16}$; ◇, $Y_{1-x}Pr_xBa_2Cu_3O_{6.97}$; △, $YBa_2Cu_3O_x$, ▽, $La_{2-x}Sr_xCuO_4$; ⋆, $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+\delta}$, ⊙, $Tl_2Ba_2CuO_{6+\delta}$; (pentagon), $Ca_{1-x}Y_xSr_2Tl_{0.5}Pb_{0.5}Cu_2O_7$.

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