Monte Carlo study of U(1) lattice gauge Higgs model of high-T_c superconductivity

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(Received 27 November 1990)

Using Monte Carlo simulations, we study the thermodynamics of a two-dimensional U(1) lattice gauge theory with Higgs scalar, which is derived from the t-J model of electrons as its Ginzburg-Landau theory. The U(1) gauge variables describe resonating valence bonds of spins, while the Higgs scalar represents the phase degrees of freedom of doped holes. Radial components of gauge variables are treated dynamically. We find a peak in the specific heat, which may be a precursor of a genuine superconducting phase transition that one would obtain when a weak three dimensionality is included.

To study phase transitions and critical phenomena, identification of their universality classes (symmetry, dimensionality, etc.) is essential. The exciting high-temperature superconducting phase transition of copper oxides[1] seems just to call for an analysis on this point. As a microscopic model for these materials, the t-J model,[2] originating from the Hubbard model with strong correlations, has acquired increasing interest. Its local U(1) gauge symmetry in the half-filled case (i.e., no holes) has been recognized in its Ginzburg-Landau (GL) theory in terms of resonating valence bonds (RVB).[3,4] With doped holes, the GL theory may be characterized as a U(1) *lattice gauge theory with Higgs scalar*.[5] The holes are interpreted there as a Higgs scalar, while the singlet spin pairs are described by U(1) lattice gauge variables. Its action can be represented solely in terms of complex gauge-invariant link variables that describe nearest-neighbor hole pairs and serve as an order parameter of superconductivity. However, being compared with the conventional U(1) lattice Higgs model[6] that has been studied in particle physics, the present model has a couple of features that may differentiate the universality class;[7] e.g., (i) it always contains an *even* number of link variables in the action, while the conventional theory has a single-link coupling, reflecting the kinetic and mass term $|D_\mu\phi|^2+m^2|\phi|^2$ and (ii) the radial components (i.e., amplitudes) of gauge variables are to be independent degrees of freedom, while they are set to unity in Ref. 6.

As the first step towards understanding this GL theory, Monte Carlo (MC) simulations have been done in Ref. 4 in a simplified system in which the amplitudes of link variables are fixed to be a constant determined by a mean-field theory (MFT) of the GL theory. Recently, Nakajima and Hori[8] also made MC simulations, using the amplitudes fixed by the MFT of Ref. 2 at half-filling, and including more interaction terms. Although these give some interesting features on the phase dynamics of GL theory, neglect of the dynamics of radial components leads one to miss certain important features: (a) In the half-filled case in two dimensions, it gives rise to a second-order phase transition by a condensation of amplitudes. It is spurious due partly to the MFT of amplitudes, since the system is equivalent to the antiferromagnetic (AF) Heisenberg model there and the Mermin-Wagner theorem[9] prohibits such a transition. (b) In the RVB picture, every spin belongs to a single RVB, as in a system of dimers. In a different context of a large-N analysis of the t-J model[10] the possibility of a dimer ground state at a certain parameter region has been pointed out. To allow for dimerlike configurations of hole pairs, it is essential to relax their radial components.

In this paper we report on the MC simulations performed for the GL theory, including the radial components of hole pairs. Concerning point (a) above, we find no genuine phase transition at half filling, now yielding a result consistent with general considerations. Concerning point (b), we compare the average value of the amplitude with its value in MFT, finding large fluctuations.

Let us summarize the model of Ref. 5. We start with the t-J Hamiltonian in the slave-boson and fermion representation,

$$\hat{H} = -t\sum_{x,\pm\mu}\hat{e}^\dagger_x\hat{a}^\dagger_{x\pm\mu}\hat{a}_x\hat{e}_{x\pm\mu} - \mu_c\sum_x(\hat{a}^\dagger\hat{a})_x + \frac{J}{4}\sum_{x,\mu}[(\hat{a}^\dagger\boldsymbol{\sigma}\hat{a})_x(\hat{a}^\dagger\boldsymbol{\sigma}\hat{a})_{x+\mu} - (\hat{a}^\dagger\hat{a})_x(\hat{a}^\dagger\hat{a})_{x+\mu}]. \quad (1)$$

x specifies a site on the d-dimensional lattice. The direction index μ runs from 1 to d. We use it also for the lattice unit vector; hence a nearest-neighbor (NN) link may be written as $(x, x+\mu)$. The original electron operator $\hat{C}_{x\sigma}$ has a spin index $\sigma = 1,2$ and is expressed as $\hat{e}^\dagger_x\hat{a}_{x\sigma}$, where $\hat{e}^\dagger_x$ is a canonical *boson* operator and creates the charged-hole state, while $\hat{a}^\dagger_{x\sigma}$ is a canonical *fermion* op-

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erator and creates the neutral spin state. Reflecting the completeness, they are constrained as $\hat{a}_x^\dagger \hat{a}_x + \hat{e}_x^\dagger \hat{e}_x = 1$. [We use the notation $(\hat{a}^\dagger \hat{a})_x \equiv \sum_\sigma \hat{a}_{x\sigma}^\dagger \hat{a}_{x\sigma}$, etc.; σ are Pauli matrices.] The chemical potential μ_c is to be chosen so that the electron density $\hat{n}_x = \sum_\sigma \hat{C}_{x\sigma}^\dagger \hat{C}_{x\sigma}$ satisfies $\langle \hat{n}_x \rangle = 1 - \delta$ $(0 \leq \delta \leq 1)$. The path-integral expression of the partition function $Z = \mathrm{Tr} \exp(-\beta \hat{H})$ is given by

$$Z = \int [d\lambda]_x [de\, da]_{x\tau} \exp\left(\int_0^\beta d\tau A \right),$$

$$A = -\sum_x [\bar{\omega}_x \dot{\omega}_x - i\beta^{-1} \lambda_x (\bar{\omega}_x \omega_x - 1)] - H, \tag{2}$$

where the three-component variable $\omega_x(\tau) = (a_{x1}, a_{x2}, e_x)(\tau)$ is a function of the imaginary time $\tau = (0, \beta)$ and describes classical paths. $\dot{\omega}_x$ stands for $\partial \omega_x / \partial \tau$. $a_{x\sigma}$ is a Grassmann number while e_x is a complex number. We denote their conjugates with overhead bars. H in the action A is obtained from $\hat{H}$ by substituting $(\hat{a}_{x\sigma}, \hat{e}_x)$ by ω_x. The λ integration ensures the constraint stated above. At the level of expectation values, it reads $\langle \bar{a}_x a_x + \bar{e}_x e_x \rangle = 1$. Since μ_c gives the condition $\langle \bar{a}_x a_x \rangle = 1 - \delta$, the hole concentration is determined as $\langle \bar{e}_x e_x \rangle = \delta$, as expected.

Below we respect the local constraints approximately, i.e., at the level of expectation values. So we write e_x as $e_x = \sqrt{\delta} \phi_x$, $\phi_x = \exp(i\varphi_x)$, with a τ-independent angle φ_x. Since the J term in A can be rewritten as $J \sum_{x,\mu} \bar{b}_{x\mu} b_{x\mu}$ in terms of the RVB variable $b_{x\mu} \equiv (a_{x+\mu,2} a_{x,1} - a_{x+\mu,1} a_{x,2})/\sqrt{2}$ sitting on $(x, x+\mu)$, one may introduce an independent complex link variable $B_{x\mu}$ for $b_{x\mu}$ through the Stratonovich-Hubbard transformation. Then Z becomes

$$Z = \int [d\phi]_x [da\, dB_\mu]_{x\tau} \exp\left(\int d\tau A' \right),$$

$$A' = -\sum_x [\bar{a}_x \dot{a}_x - t\delta \sum_{\pm\mu} \phi_{x\pm\mu} \bar{a}_{x\pm\mu} a_x \bar{\phi}_x - \mu_c (\bar{a}a)_x] - \sum_{x,\mu} [\bar{B}B - \sqrt{J}(\bar{B}b + \bar{b}B)]_{x\mu}. \tag{3}$$

To integrate over the spin field $a_{x\sigma}$ we write it as $a_{x\sigma} \equiv \phi_x a'_{x\sigma}$ introducing other Grassmann variables $a'_{x\sigma}$. Then ϕ_x appear only through the combinations $M_{x\mu} = \bar{\phi}_x B_{x\mu} \bar{\phi}_{x+\mu}$. Physically $M_{x\mu}$ (multiplied by δ) represents the hole-pair field. It carries the charge $2e$ and is invariant under the U(1) local gauge transformation; $B_{x\mu} \to \exp(i\theta_x) B_{x\mu} \exp(i\theta_{x+\mu})$, $(a_{x\sigma}, \phi_x) \to \exp(i\theta_x)(a_{x\sigma}, \phi_x)$ (with $a'_{x\sigma}$ unchanged). The model is now a U(1) gauge theory, since the measure $[da\, dB_\mu] = [da'\, dM_\mu]$ and the action themselves are invariant. The integration over $a'_{x\sigma}$ gives rise to the determinant of their quadratic kernel Γ. As before,[4] by expanding $\mathrm{Tr} \ln(\Gamma)$ with respect to $M_{x\mu}$ up to $O(M^4)$, and keeping only the static (τ-independent) modes of $M_{x\mu}$, we obtain the GL theory:

$$Z = \int [dM]_{x\mu} \exp(A_{\mathrm{GL}}),$$

$$A_{\mathrm{GL}} = A_0 + A_M,$$

$$A_0 = 2\beta\mu_c V(1-\delta) + 2\sum_{p_\mu} \ln\left\{ 1 + \exp\left[\beta \left(2t\delta \sum_\mu \cos p_\mu - \mu_c \right) \right] \right\},$$

$$A_M = c_2 \sum_{x,\mu} \bar{M}_{x\mu} M_{x\mu} + \Bigg(\sigma_1 \sum_{x,\mu\neq\nu} \bar{M}_{x+\nu,\mu} M_{x\mu} + \sigma_2 \sum_{x,\mu} \bar{M}_{x\mu} M_{x-\mu,\mu} + \sigma_3 \sum_{x,\mu<\nu} (\bar{M}_{x\mu} M_{x-\nu,\nu} + \bar{M}_{x-\mu,\mu} M_{x-\nu,\nu} + \bar{M}_{x\mu} M_{x\nu} + \bar{M}_{x-\mu,\mu} M_{x\nu}) + \mathrm{c.c.} \Bigg)$$

$$-\lambda \sum_{x,\mu} (\tfrac{1}{2} \rho_{x\mu}^4 + \rho_{x-\mu,\mu}^2 \rho_{x\mu}^2) - \lambda \sum_{x,\mu<\nu} (\rho_{x\mu}^2 \rho_{x\nu}^2 + \rho_{x-\mu,\mu}^2 \rho_{x\nu}^2 + \rho_{x\mu}^2 \rho_{x-\nu,\nu}^2 + \rho_{x-\mu,\mu}^2 \rho_{x-\nu,\nu}^2)$$

$$-\lambda \sum_{x,\mu<\nu} (M_{x\mu} \bar{M}_{x+\mu,\nu} M_{x+\nu,\mu} \bar{M}_{x\nu} + \mathrm{c.c.}), \tag{4}$$

where $\rho_{x\mu} \equiv |M_{x\mu}|$. ($V = L^d$ is the number of sites; $p_\mu = 2\pi k_\mu / L$, with $k_\mu = 1, 2, \ldots, L$.) Each term of A_M is illustrated in Fig. 1. The coefficients $c_2 = J(G_{00} + G_{11}) - \beta, \sigma_1 = JG_{11}, \sigma_2 = J(G_{11} + G_{02}), \sigma_3 = J(G_{11} + G_{03}), \lambda = J^2 G_{44}/2$ are defined here in terms of the thermal Green's functions G_{ij} (Ref. 11) given in Ref. 4.

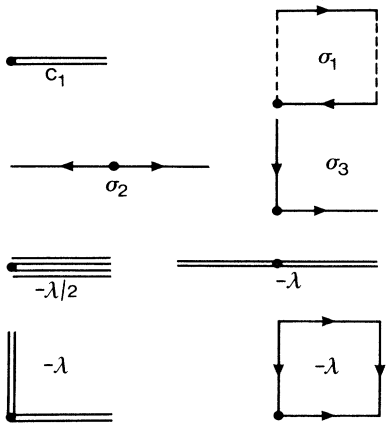

FIG. 1. Interaction terms in GL theory of Eq. (4). The segments express link variables $M_{x\mu}$ (with arrow) or $\rho_{x\mu} \equiv |M_{x\mu}|$ (without arrow). The solid circles locate the site x.

We performed MC simulations in two spatial dimensions. We think that simulations in pure two dimensions are worth doing because (i) the results are indispensable for an identification of the universality class, and (ii) the observed three dimensionality is actually very weak; a typical ratio α [$\equiv J_z/J_{x-y} = (t_z/t_{x-y})^2$] of interplane and intraplane electron hoppings in high-T_c material is estimated as $O(10^{-5})$.[12]

The Metropolis algorithm was used with typical sweeps of 10 000 times with six local hittings over a lattice of the size 20 × 20 with the periodic boundary condition. The GL coefficients were calculated numerically for infinite lattice and for $J = 0.1$ eV and $t = 0.3$ eV, using Matsubara Green functions and an expression of the density of states in terms of elliptic integrals. The system is frustrated since $\sigma_1, \lambda \geq 0$ by definition, and we found $\sigma_2 \geq 0$, $\sigma_3 \leq 0$. We have learned that the value of μ_c should be chosen carefully because, for $\langle \hat{n}_x \rangle = n_0 +$ n_M, the contribution n_M from A_M grows larger at lower temperatures. (Here n_0 denotes the contribution from A_0.) In Fig. 2, their typical behavior and a value of μ_c are shown.

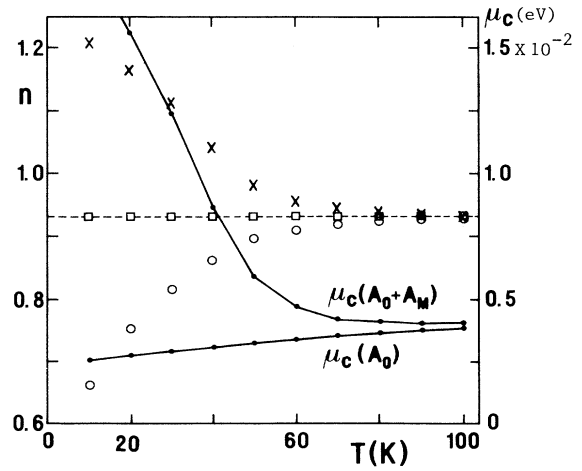

FIG. 2. $\mu_c(A_0 + A_M)$ plots the chemical potential for $\delta = 0.07$. The squares show the corresponding $\langle \hat{n}_x \rangle$ ($\equiv n_0 + n_M$), which is located at the desired value $1 - \delta = 0.93$ (dashed line). The crosses show n_0's. For reference, we plot the values $\mu_c = \mu_c(A_0)$ determined by using A_0 only. They give $n_0 + n_M$ shown by the circles.

In Fig. 3, curves of the specific heat per site C_v for T are plotted. At $\delta = 0$, we found no clear indications of a phase transition as previously stated. Already at $\delta = 0.02$, it has a clean peak at the temperature $T \simeq 17.5$ K. As δ increases, the peak height decreases and the peak location shifts to higher T. At $\delta = 0.07$, no peak remains any longer but the gradient of C_v with respect to T changes rather sharply at $T \simeq 50$ K, where the low-T branch (LTB) of C_v meets the high-T branch (HTB). For larger δ, globally speaking, the LTB becomes higher, while the HTB bocomes lower. They cross each other at $\delta \simeq 0.09$. At $\delta = 0.10$, the LTB is higher than the HTB.

We do not think these curves exhibit any signature of genuine phase transitions. Our guess is mainly based upon the following points: First, the argument given by Hohenberg *et al.*[9] allows us to expect no breakdown of global U(1) phase symmetry in the two dimensions (2D) also in our system. Second, we observed almost no size dependence of C_v. Simulations for smaller lattices such as 8 × 8 (for, say, $\delta = 0.04$, 0.07) give curves that look almost the same as those in Fig. 3. Rather, we think of these peaks and sharp changes of derivative as precursors of a genuine (second- or higher-order) phase transition into the superconducting phase, which the system

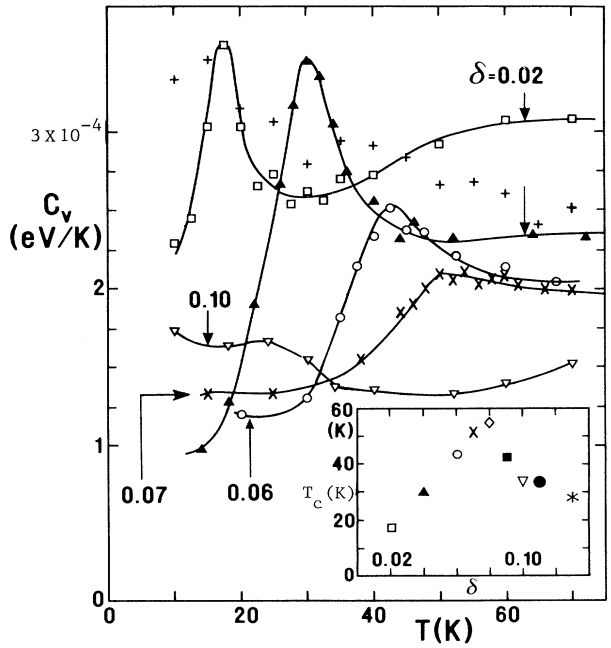

FIG. 3. Specific heat C_v vs temperature T. The lines are drawn as guides to the eye, respecting other data points measured for every step of ΔT=2–2.5 K. For $\delta = 0$ (marked by pluses), we found no sharp peaks up to $T = 400$ K. They approach the asymptotic value $\lim_{T\to\infty} C_v = k[2+(1-\delta)\ln([1-\delta]/[1+\delta])]$. In the inset, locations of peaks of C_v or sharp changes in dC_v/dT are marked. Results for $\delta = 0.08$, 0.09, 0.11, and 0.13 are included. T_c for $\delta = 0.16$ was below 20 K.

may exhibit when three dimensionality is included. It will be associated with the nonvanishing order parameter squared, $\lim_{|x-y|\to\infty}|\langle \bar{M}_{x\mu}M_{y\nu}\rangle|$. In the Higgs model of Ref. 6, a phase transition into the *Higgs* phase, in which gauge-invariant link variables have coherent phases and develop nonvanishing expectation values, is observed in three and four dimensions. So the expected superconducting phase may be characterized as a Higgs phase. Furthermore, for a very weak three dimensionality, the transition point may be located near these peaks and changes of derivative—the places where LTB and HTB meet. This expectation is suggested from the behavior of the classical XY model, which is realized as certain limiting cases of general gauge Higgs models, including the present one.[13] In the XY model, the C_v peak location and the Kosterlitz-Thouless (KT) transition point deviate by $\sim 20\%$ in 2D and the second-order transition point shifts from the KT point logarithmically with respect to small α.[14] In the inset of Fig. 3 the locations of such peaks and sharp changes of dC_v/dT are collected in the δ-T plane.

In Fig. 4, the fluctuations of ρ^2, $\langle\sum_{x,\mu}\rho_{x\mu}^2\rangle/dV$, are illustrated. In the MF treatment of Ref. 4, ρ^2 starts from a finite value (say, 1.88×10^{-3} for $\delta=0.07$) at low T and vanishes at finite T (153 K for $\delta=0.07$), while in the dynamical MC treatment it starts from a larger constant [the coefficients scale as $c_2,\sigma_i,\lambda = O(\beta)$ for small T] and increases as $\lim_{T\to\infty}\rho^2 = kT$, since $c_2\to-\beta$ dominates over $\sigma_{1,3},\lambda = O(\beta^4),\sigma_2 = O(\beta^6)$ at high T. The importance of fluctuations seems beyond doubt. However, it requires more study to judge whether a dimer phase takes place somewhere. For $\delta=0$, the coefficients are given as $c_2 = J\beta^2/4-\beta,\sigma_i=0,\lambda=J^2\beta^4/96$, and ρ^2 starts from zero at $T=0$. This difference is due to the extra local U(1) gauge invariance [under $M_{x\mu}\to\exp(i\theta_x)M_{x\mu}\exp(i\theta_{x+\mu})$] at $\delta=0$. There $M_{x\mu}$ fluctuate wildly and an expansion up to $O(M^4)$ might not be sufficient to describe AF transition even in three dimensions; Larger loops of $M_{x\mu}$'s might be relevant. For $\delta\neq0$ this U(1) symmetry is broken due to the t term of (1) and Eq. (4) is sufficient to describe a Higgs phase.

Finally we point out that, even though a powerful technique to study phase transitions, the GL theory is not a suitable tool to analyze the behavior of the system near $T\simeq0$, since (i) the effective expansion parameter $\beta^{1/2}\rho_{x\mu}$ may become quite large and (ii) modes other than the static one may become important. For this purpose, a generalized gap equation will be useful.

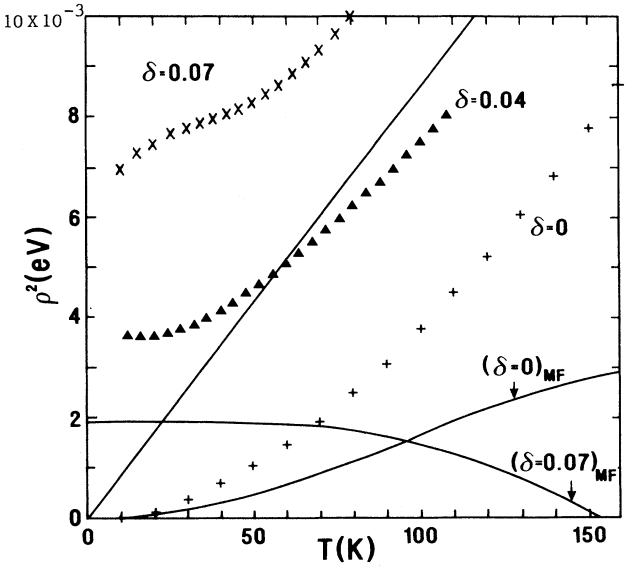

FIG. 4. $\rho^2\equiv\left\langle\sum_{x,\mu}\rho_{x\mu}^2/dV\right\rangle$ vs T. As $T\to\infty$, they approach kT (shown as the straight line), the leading term of the high-temperature expansion. Continuous curves with the suffix MF express the results of fixed $\rho_{x\mu}$ in the mean-field treatment up to $O(\rho^4)$ given in Ref. 4 (where the same values $t=0.3$ eV, $J=0.1$ eV were used). For $\delta=0$, ρ^2 is given by $96(-1+\beta J/4)/7J^2\beta^3$ and vanishes at $T=290$ K.

We would like to thank Tomo Munehisa for discussions and useful comments. One of the authors (T.M.) thanks Hidetoshi Fukuyama and Yasumasa Hasegawa for discussions and suggestions in the early stages of this work, and Christian Hege and Tilman Sauer for instructions in the use of the computer facilities. The numerical calculations have been done on the Hitachi HITAC S820 computer at the University of Tokyo and the Cray Research, Inc. X-MP/24 computer at Konrad Zuse Zentrum, Berlin.

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