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Ginzburg-Landau theory of resonating valence bonds and its U(1) phase dynamics

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We formulate a Ginzburg-Landau theory for the resonating-valence-bond model of antiferromagnetism and high-T_c superconductivity, the order parameters of which are complex link variables. We investigate the dynamics of their phase part using the Monte Carlo method and obtain an indication of a transition to a superconducting phase. When the doping parameter is zero, the theory becomes equivalent to a U(1) lattice gauge theory in two dimensions.

The discovery of high-T_c superconductivity and the subsequent active experimental analyses have posed the challenging theoretical problem of clarifying its mechanism. It is widely believed that superconductivity occurs predominantly in two-dimensional planes. There is growing suspicion that the mechanism may involve antiferromagnetism rather than the conventional electron-phonon exchange.[1-4] Among many other theoretical approaches there is much interest in Anderson's resonating-valence-bond (RVB) model,[2-4] which was originally proposed to describe the ground-state of antiferromagnetism.[5]

When we recall the success of Ginzburg-Landau (GL) theory in describing the Bardeen-Cooper-Schrieffer (BCS) model, it is appealing to construct a similar theory for the RVB model. Since the RVB model is based on the concept of valence bonds and spin-singlet pairs of nearest-neighbor electrons, one needs to introduce in GL theory order parameters which are capable of describing these bonds. This is in contrast with the conventional BCS model. There the order parameter is chosen to be a complex scalar field, and the corresponding GL theory contains relatively simple dynamics of the XY-model type. In Ref. 4 Anderson, Baskaran, Zou, and Hsu pointed out the importance of the phase degrees of freedom among the order parameters. In this paper, we formulate a GL theory for the RVB model and study its phase dynamics beyond mean-field theories by using the Monte Carlo method.

Our starting model Hamiltonian is that of Baskaran, Zou, and Anderson[3] (BZA),

$$H_{\mathrm{BZA}}(C^{\dagger},C) = -t\delta\sum_{x,i,\sigma}(C^{\dagger}_{x,\sigma}C_{x+i,\sigma}+\mathrm{H.c.}) - J\sum_{x,i}b^{\dagger}_{x,i}b_{x,i}-\mu\sum_{x,\sigma}n_{x,\sigma}\ , \tag{1}$$

where $C^{\dagger}_{x,\sigma}$ is a creation operator of an electron of spin σ at site x on a two-dimensional square lattice,

$$b^{\dagger}_{x,i}=(C^{\dagger}_{x,\uparrow}C^{\dagger}_{x+i,\downarrow}-C^{\dagger}_{x,\downarrow}C^{\dagger}_{x+i,\uparrow})/\sqrt{2}$$

is a creation operator of a valence bond on the link $(x,x+i)$ $(i=1,2)$ and $n_{x,\sigma}=C^{\dagger}_{x,\sigma}C_{x,\sigma}$. The parameters t and J have their origin in the Hubbard model with on-site electron repulsion $(U>0)$.[3,6] We include the chemical potential to guarantee the relation $\langle n_{x,\uparrow}+n_{x,\downarrow}\rangle=1-\delta$ for the doping parameter δ. We consider the partition function $Z=\mathrm{Tr}\exp(-\beta H_{\mathrm{BZA}})$ and write it in a path-integral form over Grassmann variables:[7]

$$Z=\lim_{N\to\infty}\prod_{\tau=1}^{N}\prod_{x,\sigma}\int d\psi^{*}_{\sigma}(x,\tau)d\psi_{\sigma}(x,\tau)\exp\left[-\sum_{\tau=1}^{N}\left[\sum_{x,\sigma}\psi^{*}_{\sigma}(x,\tau)[\psi_{\sigma}(x,\tau+1)-\psi_{\sigma}(x,\tau)]+\Delta\beta\mathcal{H}(\tau)\right]\right]\ , \tag{2}$$

where $\mathcal{H}(\tau)=H_{\mathrm{BZA}}[\psi^{*}_{\sigma}(x,\tau),\ \psi_{\sigma}(x,\tau)]$, and $\Delta\beta=\beta/N$. We introduce the auxiliary collective fields $B_i(x)$ to describe the valence-bond operators $b_{x,i}$. By putting a complex variable $B_i(x)$ on the link $(x,x+i)$ with Gaussian measure, the four-fermi interaction in (2) is converted into the form of $-B^{*}_{i}(x)B_i(x)+J^{1/2}[b^{\dagger}_{x,i}B_i(x)+\mathrm{H.c.}]$. A Berezin integral over electron variables then generates a determinant for the full quadratic kernel

$$(\psi^{*}_{\uparrow},\psi_{\downarrow})(x,\tau)\Gamma(x,\tau;x',\tau')(\psi_{\uparrow},\psi^{*}_{\downarrow})^{t}(x',\tau')\ .$$

The effective theory in terms of $B_i(x,\tau)$ reads

$$Z=\int\prod_{x,\tau,i}dB^{*}_{i}(x,\tau)dB_i(x,\tau)\det\Gamma\exp\left[-\Delta\beta\sum_{x,i,\tau}B^{*}_{i}(x,\tau)B_i(x,\tau)\right]\ . \tag{3}$$

The block elements of the matrix Γ have the following representations:

$$\Gamma_{11}=\delta_{xx'}[(\delta_{\tau',\tau+1}-\delta_{\tau',\tau})/\Delta\beta-\mu\delta_{\tau',\tau}]-(t\delta)\delta_{\tau,\tau'}\sum_{\pm i}\delta_{x',x\pm i}\ ,$$

$$\Gamma_{12}=-\sqrt{J/2}\delta_{\tau\tau'}\sum_{\pm i}B_{\pm i}(x,\tau)\delta_{x',x\pm i}\ ,$$

and $\Gamma_{22}=-\Gamma_{11}(\tau\leftrightarrow\tau')$, $\Gamma_{21}=\Gamma^{*}_{12}$, where $B_{-i}(x,\tau)=B_i(x-i,\tau)$. In order to get GL theory, we now perform the follow-

ing procedures on (3). First, we consider only the static (zero Matsubara frequency) mode in $B_i(x,\tau)$, which we call $B_i(x)$. Second, we expand $\mathrm{Tr}\ln\Gamma$ up to the order of B^4. Third, we retain only the terms that have the short-range interactions (accessible within the second-order hopping expansion with respect to $t\delta$). The similar procedures are employed in deriving GL theory from the BCS model.[8] Here we divide $B_i(x)$ into its radial and phase parts, $B_i(x)=\rho_i(x)U_i(x)$ [$U_i(x)\in \mathrm{U}(1)$]. We neglect the fluctuation of the radial part and replace it by a constant ρ.[9] The GL theory then takes the form

$$Z=\int\prod_{x,i}dU_i(x)e^{A}\ , \tag{4}$$

where $A=A_0+A_\rho+A_U$. A_0 is an action which does not include B:

$$A_0=2\sum_p \ln\{1+\exp[\beta\mu+2\beta t\delta(\cos p_1+\cos p_2)]\}\ ,$$

where the momenta are given by $p_i=2\pi n_i/L (n_i=1,2,\ldots,L)$. A_ρ is a coherent term, $A_\rho/V=C_2\rho^2+C_4\rho^4$, where $V=L^2$, $C_2=-2\beta+2J(G_{00}+G_{11})$, and $C_4=-7J^2G_{44}/2$. A_U is responsible for the U(1) phase dynamics (see Fig. 1),

$$A_U=\sum_x\Big(-\lambda U_{x,2}U^*_{x+2,1}U_{x+1,2}U^*_{x,1}+\sigma_1(U_{x+2,1}U^*_{x,1}+U_{x+1,2}U^*_{x,2})+\sigma_2\sum_i U_{x-i,i}U^*_{x,i}$$
$$+\sigma_3(U_{x,2}U^*_{x,1}+U_{x,2}U^*_{x-1,1}+U_{x-2,2}U^*_{x-1,1}+U_{x-2,2}U^*_{x,1})+\text{c.c.}\Big)\ ,$$

where

$$\lambda=J^2\rho^4G_{44}/2;\ \sigma_1=J\rho^2G_{11};\ \sigma_2=J\rho^2(G_{02}+G_{11});\ \sigma_3=J\rho^2(G_{03}+G_{11})\ .$$

The G_{ij} are sums of products of Green's function,

$$g(x)=\frac{\Delta\beta}{V}\sum_p \exp(ipx)/\left[\exp(i\theta_n)-1-\Delta\beta\left(\mu+2t\delta\sum_i\cos p_i\right)\right]\ ,$$

over Matsubara frequencies $\theta_n=\pi(2n-1)/N$ ($n=1,2,\ldots,N$), and given by

$$G_{00}=\sum g(0)g(0)^*,\ G_{11}=\sum g(1)g(1)^*,$$
$$G_{02}=\sum g(0)g(2)^*,\ G_{03}=\sum g(0)g(1+i)^*,\ G_{44}=\sum[g(0)g(0)^*]^2\ .$$

When δ is zero, the RVB model is known to describe antiferromagnetic quantum Heisenberg spins.[3] At this point, only λ survives in A_U and our GL theory becomes (after the conjugate transformation of half of the U's) equivalent to a U(1) lattice gauge theory, which is exactly solvable in two dimensions. This four-body term generates resonance (flip-flop) of valence bonds. As δ increases, the two-body interactions become important. They describe the hopping of valence bonds and violate the U(1) gauge symmetry at $\delta=0$.

In order to determine ρ and μ as functions of T and δ,

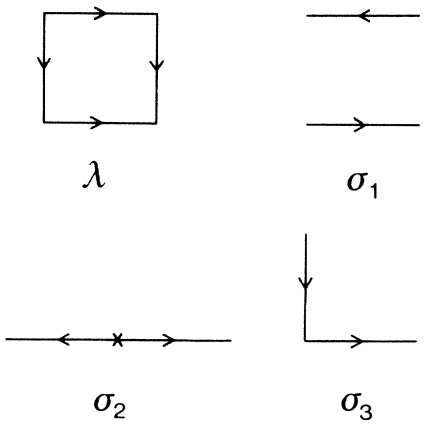

FIG. 1. Schematic diagrams of A_U in Eq. (4). A segment with an arrow represents U or U^*. The λ term ($-\lambda UU^*UU^*$) has a different structure and the opposite sign ($\lambda>0$) from the plaquette term ($g^{-2}UUU^*U^*$) in lattice gauge theory.

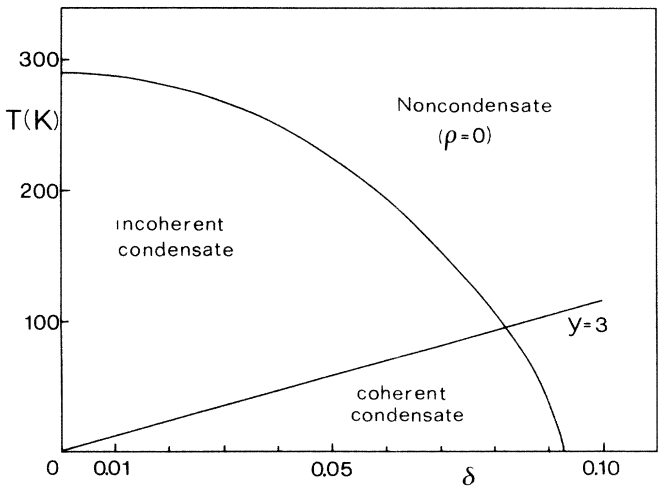

FIG. 2. Phase structure in the δ-T plane. The line of $y=3$ is shown to distinguish the incoherent condensate and the coherent condensate, the latter should be identified as a superconducting state.

we use two conditions: (i) imposing $\langle n \rangle = 1 - \delta$, and (ii) minimizing the effective action $-\ln Z$ with respect to ρ. This is a complicated coupled problem because one needs to calculate U(1) dynamics also. We use only the U-independent action $A_0 + A_\rho$ to calculate $\langle n \rangle$ and minimize it. This procedure is found to be a good approximation after a numerical study of A_U. One can show that for each set of (μ,ρ) at (δ,T) there is associated a solution $(-\mu,\rho)$ at $(-\delta,T)$. Therefore, we consider only positive δ. We have chosen $J = 0.1$ eV and $t = 0.3$ eV (see Refs. 1-4). In Fig. 2 the line of $\rho = 0$ is given, across which the system exhibits a second-order phase transition and the condensate starts to develop. We have calculated some other $\rho = 0$ curves with different sets of J and t. They look rather similar to each other, when plotted in the $t\delta - J^{-1}T$ plane. The intercept at the $\delta = 0$ line is always given by $T = J/(4k)$.

We used a 20×20 lattice to calculate the coefficients in A_U. We observed that the finite-size effects become strong for very low temperatures. Then we calculate several kinds of U correlations for the U(1) system of (4) by the standard heat-bath Monte Carlo method.[10]

The results on a 20^2 lattice are presented in Figs. 3, 4, and 5. The data are classified according to the different values of $y = \beta t \delta$, each of which represents a straight line in the δ-T plane. For the plaquette expectation values, we observe no significant change up to $y = 10.0$ (the maximum value in our simulation). Parallel and perpendicular UU^* correlations in Figs. 4 and 5, in contrast, take almost negligible values up to $y = 3.0$,[11] but then suddenly increase. Therefore, the region of condensate in the δ-T plane may be partitioned according to the magnitudes of two-body correlations. We draw in Fig. 2 the line of $y = 3.0$ as a possible borderline.

Due to the finite size of the lattice, we cannot conclude that this sharp change demonstrates a phase transition, but it is tempting to regard it as an indication of a phase transition from the antiferromagnetic insulator phase to the superconducting phase. They are characterized according to whether the bonds localize or move. The two-body hopping correlations should be sensitive to this transition. In Fig. 2 we observe that the highest possible tem-

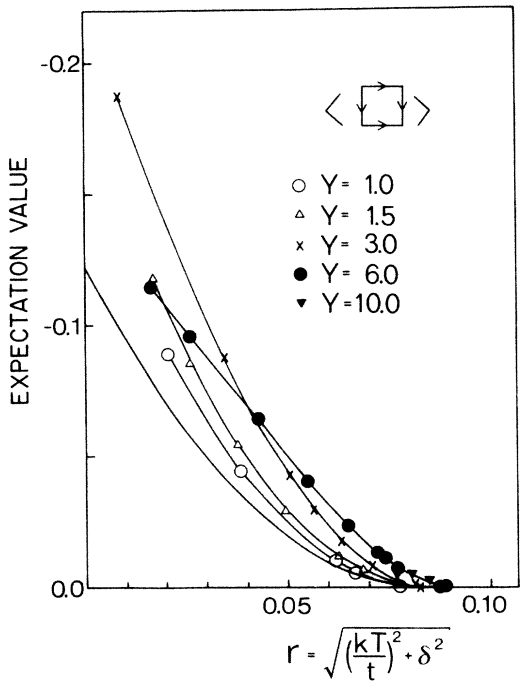

FIG. 3. Expectation values of the palquette term plotted along constant y's vs $r \equiv [(kT/t)^2 + \delta^2]^{1/2}$. The case of $y = 0$ allows for an exact solution and is depicted by a line without markers.

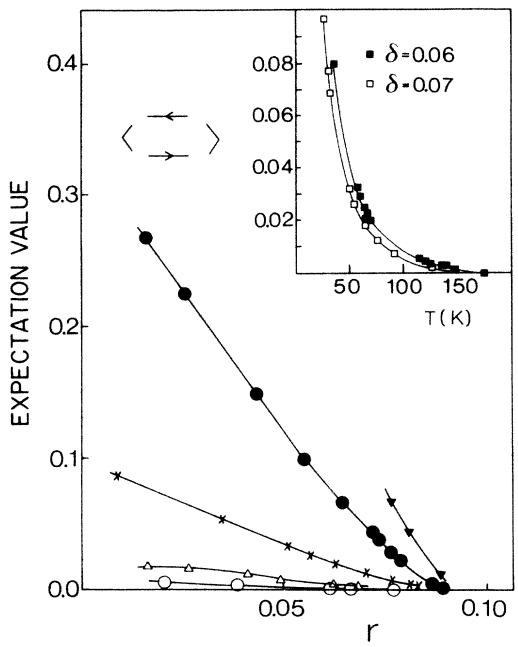

FIG. 4. Expectation values of parallel bond-hopping term vs r. The inset shows cross sections at $\delta = 0.06$ and 0.07.

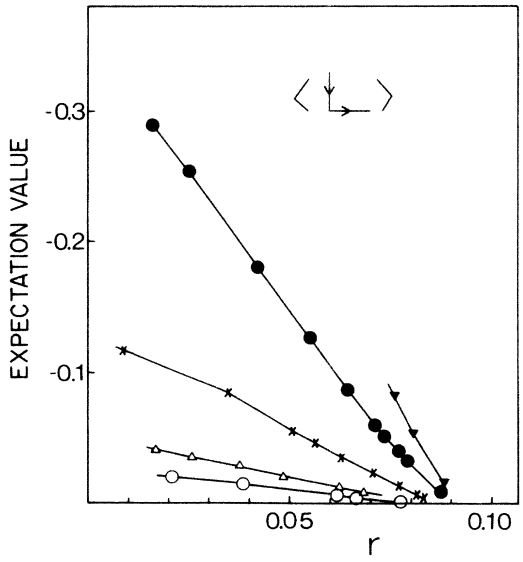

FIG. 5. Expectation values of perpendicular bond-hopping term vs r.

perature in this "superconducting phase" is more or less 100 K.

Our straightforward GL theory describes two different mechanisms: (i) ρ condensation or noncondensation, and (ii) U(1) phase coherence or incoherence. From the above argument, one may characterize these cases by (i) super or normal, and (ii) metal or insulator, respectively. For example, a superconductor is a coherent condensate, and an antiferromagnetic insulator is an incoherent condensate.[12]

In conclusion, to derive GL theory and explain high-T_c superconductivity from the RVB model, we have used assumptions and techniques similar to those in BCS-GL theory, and get different kinds of order parameters (site versus link variables) and phase dynamics [XY type versus U(1) gauge + UU^* hopping]. Although our U(1) dynamics are more complicated due to the competing interactions, it can still be handled by a standard Monte Carlo method in lattice gauge theories. We hope this effective theory will prove itself useful in describing high-T_c superconductivity, just as the standard GL theory has in the case of BCS-type superconductivity.

Note added. After submission of the paper, we became aware of work by Baskaran and Anderson.[13] They have also described a RVB model in terms of U(1) lattice gauge theory, but did not do Monte Carlo calculations.

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[1]J. E. Hirsch, Phys. Rev. B **35**, 8726 (1987); V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987); J. E. Hirsch, *ibid.* **59**, 228 (1987); R. H. Parmenter, *ibid.* **59**, 923 (1987).

[2]P. W. Anderson, Science **235**, 1196 (1987); S. A. Kivelson, D. S. Rokhsar, and J. P. Sethna, Phys. Rev. B **35**, 8865 (1987); M. H. Cohen and D. H. Douglass, *ibid.* **35**, 8720 (1987); A. E. Ruckenstein, P. J. Hirschfeld, and J. Appel, *ibid.* **36**, 857 (1987).

[3]G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987).

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[5]P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973).

[6]In addition to Eq.(1), the effective Hamiltonian of the Hubbard model at large U contains also a pair hopping term $\propto J\delta\sum b^{\dagger}_{x,i}b_{x+i,j}$. We neglect it for simplicity and due to the suppression of order δ.

[7]F. A. Berezin, *The Method of Second Quantization* (Academic, New York, 1966); Y. Ohnuki and T. Kashiwa, Prog. Theor. Phys. **60**, 548 (1978).

[8]See, e.g., B. Sakita, *Quantum Theory of Many Variable Systems and Fields,* Lecture Notes on Physics, Vol. 1 (World Scientific, Singapore, 1985); H. Kleinert, Fortschr. Phys. **26**, 565 (1978). One may doubt the validity of GL theory in two dimensions because of the strong infrared fluctuations. However, the fluctuations of our system will be milder because of antiferromagnetic couplings (e.g., at $\delta=0$, the model is equivalent to $H_{\rm AF}=J\sum S_xS_{x+i}$). The Goldstone mode may have the dispersion of the form $|k|$ instead of k^2, which gives rise to the convergent k integral. See Ref. 4 and P. W. Anderson, Phys. Rev. **86**, 694 (1952). This observation is consistent with our Monte Carlo results.

[9]The fluctuation of $\rho_l(x)$ is massive and will play a less relevant role than the U fluctuation.

[10]See, for example, K. J. M. Moriarty, Phys. Rev. D **25**, 2185 (1982).

[11]At $y=0$, the expectations of two-body bond hoppings vanish because of the gauge symmetry at $\delta=0$.

[12]The other two cases (normal coherence and normal incoherence) may characterize a normal metal and a paramagnetic insulator, respectively. In order to discuss Mott-type metal-insulator transition between these two states, it will be necessary to include the fluctuation in $\rho_l(x)$.

[13]G. Baskaran and P. W. Anderson, Phys. Rev. B **37**, 580 (1988).