Phase structure of lattice model of unconventional superconductors

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In this paper, we introduce a Ginzburg-Landau (GL) theory for the extended *s*- and *d*-wave superconductors (SC) in granular systems that is defined on a lattice. In contrast to the ordinary Abelian-Higgs model (AHM) that is a GL theory for the *s*-wave SC, Cooper-pair field (Higgs field) is put on links of the lattice in the present model. By means of Monte Carlo simulations, we study phase structure, gauge-boson mass (the inverse magnetic penetration depth) and density of instantons. In the ordinary noncompact U(1) AHM, there exists a second-order phase transition from the normal to SC states and the gauge-boson mass develops continuously from the phase transition point. In the present gauge system with link Higgs field, on the other hand, phase transition to the SC state is of first order at moderate coupling constants. The gauge-boson mass changes from vanishing to finite values discontinuously at the phase transition points.

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Ginzburg-Landau (GL) theory plays a very important role for study on superconducting (SC) phase transition. For conventional *s*-wave SC, it has a form of a noncompact U(1) lattice-gauge-Higgs model in which the order-parameter boson field sits on lattice sites.[1] In the last few decades, unconventional superconductors, whose order parameter of Bose condensation is not the usual *s*-wave, have been discovered.[2] In this paper we shall give and study a GL theory of unconventional SC like the $d_{x^2-y^2}$-wave SC in which the order-parameter field, the Cooper-pair wave function, changes its sign under a $\pi/2$ rotation of the real-space coordinates. Therefore in order to describe such an unconventional SC, the order-parameter field, Higgs boson field, must be put on lattice links instead of lattice sites.[3] On-site amplitude of the Cooper pair is vanishingly small because of, e.g., the strong on-site Coulomb repulsion.

We shall use the path-integral formalism, and define the model on a three-dimensional (3D) cubic lattice of system size L^3 with the periodic boundary condition. Before going into details of the extended model, let us first consider the ordinary *noncompact* Abelian-Higgs model (AHM) as a reference system, which is defined by the following action:

$$A_{\rm AHM} = \frac{1}{2}\left(\sum_{\rm pl} c_u F_{ij}^2(x) + \sum_{\rm link} \kappa \phi_{x+j} U_{x,j} \phi_x^\dagger\right), \qquad (1)$$

where $F_{ij}(x)=A_{x,i}-A_{x+j,i}+A_{x+i,j}-A_{x,j}$ $(i,j=1,2,3)$ and a gauge field $A_{x,i}$ on the link (x,i) is related to the electromagnetic vector potential $\vec{A}_i^{\rm em}$ as $A_{x,i}=\int_x^{x+i}\vec{A}^{\rm em}d\vec{\ell}$ and $U_{x,j}=e^{iA_{x,j}}$. ϕ_x is the Higgs field corresponding to the *s*-wave Cooper pair and in the London limit $\phi_x=e^{i\varphi_x}$ $(\varphi_x\in[-\pi,\pi])$. c_u^{-1} is the electric charge of the Cooper pair and κ is a parameter corresponding to the superfluid density and a decreasing function of the temperature (T). $A_{\rm AHM}$ is nothing but the 3D *XY* model coupled with the noncompact U(1) gauge field that describes the electromagnetic interactions.

We studied the phase structure of the model $A_{\rm AHM}$ by the Monte Carlo (MC) simulations calculating the internal energy $E=-\langle A_{\rm AHM}\rangle/L^3$ and the specific heat $C=\langle(A_{\rm AHM}-\langle A_{\rm AHM}\rangle)^2\rangle/L^3$. We found that there exists a second-order phase transition line[4] emanating from the 3D *XY* critical point at $(\kappa,c_u)=(0.46,\infty)$ (obtained in the system of size $L=24$). In Fig. 1(a), we show the specific heat as a function of κ with $c_u=1$. The specific heat exhibits a typical behavior of the second-order phase transition as the system size L^3 is increased from 8^3 to 24^3. This result is in sharp contrast to the *compact* AHM in the London limit in which no phase transitions occur and only the confinement phase exists.[5]

We also measured the gauge-invariant gauge-boson mass M_G which is defined through the correlation function of the operator $\sin[F_{ij}(x)]$. More precisely let us define the operator $O(x)$ as $O(x)=\Sigma_{i,j=1,2}\epsilon_{ij}\sin F_{ij}(x)$ $(\epsilon_{12}=-\epsilon_{21}=1)$, and its Fourier transformed operator in the 1-2 plane,

$$\tilde{O}(x_3) = \sum_{x_1,x_2} O(x) e^{ip_1x_1+ip_2x_2}. \qquad (2)$$

Then one can expect the following behavior;

$$\langle \tilde{O}(x_3)\tilde{O}(x_3+t)\rangle \propto e^{-\sqrt{p_1^2+p_2^2+M_G^2}\,t}. \qquad (3)$$

In Fig. 1(b), we show the result. We define the gauge-boson mass M_G from numerical results as $M_G={\rm sign}(\lambda^2-\vec{p}^2)\sqrt{\lambda^2-\vec{p}^2}$, where λ is the inverse correlation length of the Fourier transformed operator $\tilde{O}(x_3)$ with finite momentum $\vec{p}$[6]. The negative values for $\kappa<0.52$ in Fig. 1(b) come from the above definition of the mass M_G and it is considered as a finite-size effect.[6]

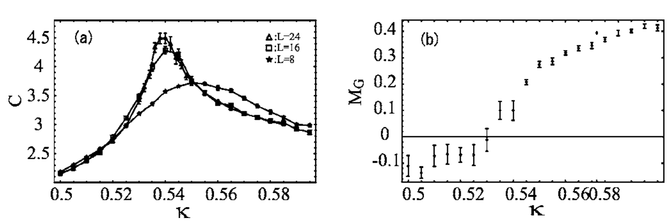

FIG. 1. Results of the MC simulations for the AHM with $c_u=1$. (a) Specific heat C as a function of κ. It indicates the existence of a second-order phase transition at $\kappa_c=0.538$ ($L=24$). (b) Gauge-boson mass M_G obtained from the correlation function of $\sin[F_{ij}(x)]$. The critical coupling is estimated as $\kappa_c=0.52$ ($L=16$).

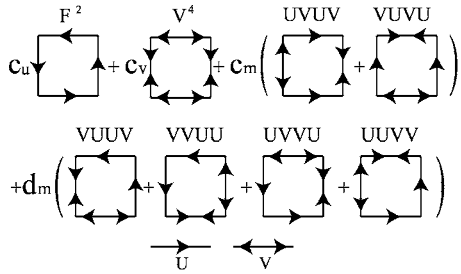

FIG. 2. Action $A_{\rm GL}$ of the GL theory (4).

From Fig. 1(b), we conclude that M_G is vanishing for $\kappa < 0.52$ and develops continuously as κ increases. This behavior obviously is consistent with the specific heat measurement in Fig. 1(a) and indicates the existence of a second-order phase transition from the normal to the Higgs-SC phases, though the value of the critical coupling κ_c obtained from M_G (κ_c=0.52 with L=16) is slightly different from that obtained by C (κ_c=0.54 with L=16). Similar phenomenon has been observed also in the previous studies on the U(1) gauge field coupled with the CP^1 fields.[7]

We applied the finite-size scaling to C as $C(\kappa,L) = L^{\sigma/\nu}\phi(L^{1/\nu}\epsilon)$, $\epsilon=(\kappa-\kappa_\infty)/\kappa_\infty$, where κ_∞ is the critical coupling at $L\to\infty$ and $\phi(x)$ is the scaling function. We found that κ_∞=0.534, ν=0.83, and σ=0.15.

Let us introduce the extended mode that is defined by the following action:

$$A_{\rm GL} = \frac{1}{2}\sum_{\rm pl}\,[c_u F_{ij}^2(x) + c_v V^4 + c_m(UVUV + VUVU) + d_m(UUVV + 3 \text{ cyclic permutations})], \qquad (4)$$

where $V_{x,j}$ is the spin-singlet Cooper-pair field on link that is related to electron operator $\psi_{x\sigma}(\sigma=\uparrow,\downarrow)$ as

$$V_{x,j} \propto \langle \psi_{x\uparrow}\psi_{x+j\downarrow} - \psi_{x\downarrow}\psi_{x+j\uparrow}\rangle. \qquad (5)$$

Because we shall mostly focus on the extended s-wave and $d_{x^2-y^2}$-wave SC's in the later discussion, we consider the only nearest-neighbor (NN) pair field $V_{x,j}$.[3] For example, in order to describe the d_{xy}-wave SC *simultaneously*, we must introduce a *next*-NN pair field in addition to $V_{x,j}$. Here it is interesting to notice that a GL theory for the spin-triplet p-wave superconductivity in ferromagnetic $ZrZn_2$ was proposed and it employs a SC order parameter similar to $V_{x,j}$.[8] Gradient terms of the GL theory for $ZrZn_2$ have a similar form to $A_{\rm GL}$ in Eq. (4).

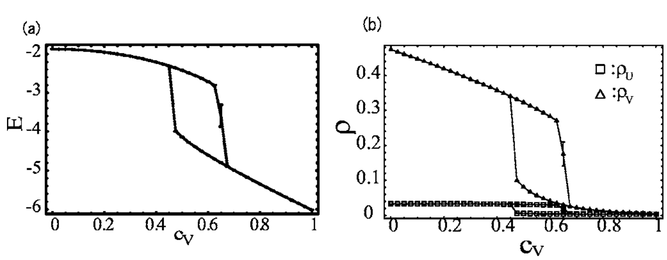

FIG. 3. Results for $A_{\rm GL}$ with c_m=1, d_m=0, c_u=0.5 (L=16). (a) Internal energy exhibiting hysteresis loop. (b) Densities of instanton. ρ_U (ρ_V) is the instanton density of the noncompact gauge field $A_{x,j}$ (compact gauge field $V_{x,j}$).

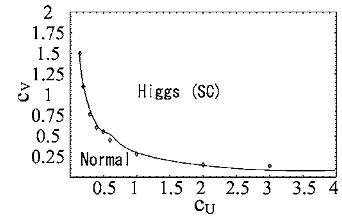

FIG. 4. Phase diagram of $A_{\rm GL}$ with c_m=1, d_m=0. Locations of the phase transition points are determined by those of center of the hysteresis loops. "Normal" phase denotes the Coulomb (confinement) phase of $U_{x,j}$ ($V_{x,j}$).

Hereafter we shall consider the London limit of $V_{x,j}$ and set $V_{x,j}=e^{i\theta_{xj}}$ ($\theta_{xj}\in[-\pi,\pi]$). Each term in $A_{\rm GL}$ is depicted in Fig. 2 where c_u, c_v etc., are coupling constants, and $A_{\rm GL}$ is constructed to be invariant under the following *noncompact* local gauge transformation:

$$A_{x,j} \to A_{x,j} + \alpha_{x+j} - \alpha_x, \quad V_{x,j} \to e^{i\alpha_{x+j}} V_{x,j} e^{i\alpha_x}. \qquad (6)$$

From Eq. (6), it is obvious that $V_{x,j}$ can be regarded as another gauge field dual to the electromagnetic gauge field.[9] We consider terms as local as possible for $A_{\rm GL}$, and the partition function Z is given as

$$Z = \int_{-\infty}^{\infty}[DA]\int_{-\pi}^{\pi}[D\theta]e^{A_{\rm GL}}. \qquad (7)$$

Compact U(1) version of the above $A_{\rm GL}$, in which $\Sigma_{\rm pl}F_{ij}^2(x)$ is replaced by $\Sigma_{\rm pl}U^4$, has been studied in the previous paper.[10] In the present paper, we study the noncompact U(1) gauge theory as a GL theory for the unconventional SC in which the gauge field $U_{x,j}$ describes the electromagnetic field.

There is credible evidence that the SC phase transition in the high-T_c cuprates is of second-order and furthermore it is in the 3D XY model universality class.[11] On the other hand, as explained above, the Cooper-pair field must sit on lattice links instead of sites in order to describe the $d_{x^2-y^2}$-wave SC state.[3] One of the simplest GL theory for the $d_{x^2-y^2}$-wave SC is $A_{\rm GL}$ given in (4). In the present paper, we shall study the phase structure and physical properties of $A_{\rm GL}$ by means of the MC simulations and compare the results with those of the noncompact AHM and the XY model.

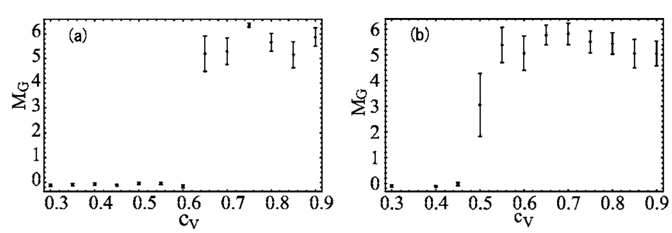

FIG. 5. Results for $A_{\rm GL}$ with c_m=1, d_m=0, c_u=0.5. (a) Gauge-boson mass (L=16) measured for increasing c_v. It exhibits a sharp discontinuity at c_v=0.6, the phase transition point. (b)Gauge-boson mass for decreasing c_v.

Let us first notice that for vanishing $c_m = d_m = 0$, the present system reduces to two independent decoupled gauge models, a noncompact U(1) gauge model of $A_{x,j}$ and a compact U(1) gauge model of $V_{x,j}$. Then it is obvious that there exist no phase transitions in that case. By giving finite values for c_m and/or d_m, we study phase structure in the c_u-c_v plane.

We first study the case $c_m = 1$, $d_m = 0$. It is instructive to consider the large-c_u limit in which configurations of the noncompact gauge field are restricted as $A_{x,j} \sim \varphi_{x+j} - \varphi_x$. Then the c_m terms in $A_{\rm GL}$ become as

$$\sum_{x,i,j} e^{-i\varphi_x} V_{x,i} e^{-i\varphi_{x+i}} e^{i\varphi_{x+j}} V^{\dagger}_{x+j,i} e^{i\varphi_{x+i+j}} + \text{c.c.} \tag{8}$$

We shall call the above term double Higgs coupling. As we explained above, the usual Higgs coupling of the compact gauge field $V_{x,j}$, $\sum_{x,j} e^{-i\varphi_x} V_{x,j} e^{-i\varphi_{x+j}}$, does *not* induce any phase transition. On the other hand, the doubly charged Higgs coupling, $e^{-i\varphi_x}(V_{x,i})^2 e^{-i\varphi_{x+i}}$, induces a phase transition from the confinement to Higgs phases.[12] Then it is interesting to study the extended model also from the viewpoint of the Higgs coupling and see if the Higgs phase transition occurs as the double Higgs coupling (8) is increased.

We studied the phase structure in the c_u-c_v plane by calculating E and C and found that there is a phase transition line. Typical behavior of E near phase transition points is shown in Fig. 3(a), which indicates that the transition is of first order. To see physical meaning of the phase transition, we measured the instanton densities of the gauge fields $U_{x,j}$ and $V_{x,j}$. We follow the definition of the instanton densities ρ_U and ρ_V given in Refs. 13 and 10. The result is shown in Fig. 3(b). As $U_{x,j}$ is the noncompact gauge field, the density of instanton ρ_U is vanishingly small. On the other hand, for $V_{x,j}$, ρ_V exhibits a hysteresis loop just like the internal energy E at the critical point. Vanishing of ρ_V for $c_v > 0.4(0.6)$ means that the observed phase transition is the normal to Higgs-SC phase transition. As in the compact U(1) gauge case,[10] adding small but finite positive d_m-term stabilizes the sign of $\langle UUVV\rangle$ as $\langle UUVV\rangle > 0$ in the Higgs-SC phase. This SC phase corresponds to the extended s-wave, because on-site amplitude of the Cooper pair is zero whereas *expectation values* of $V_{x,j}$ on links (x,j) $(j=1,2,3)$ have the same sign under the gauge-fixing condition $\varphi_x = 0$ in Eq. (8).[14]

In Fig. 4, we show the phase diagram obtained from the measurement of the internal energy. In Figs. 5(a) and 5(b), calculations of the mass of the gauge boson $A_{x,j}$ are given. Contrary to the AHM in Fig. 1, the gauge-boson mass exhibits a sharp discontinuity and acquires nonvanishing value at $c_v = 0.60(0.45)$.

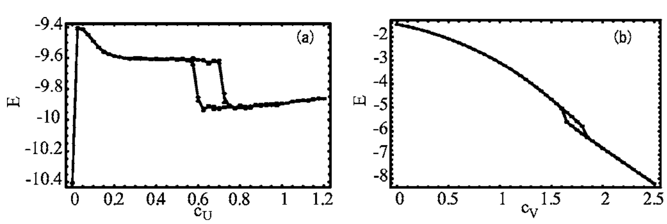

FIG. 6. Results for $A_{\rm GL}$ with $c_m = 0$, $d_m = -0.8$. (a) E as a function of c_u for $c_v = 3$. (b) E as a function of c_v for $c_u = 3$.

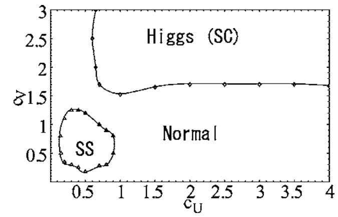

FIG. 7. Phase diagram for $c_m = 0$, $d_m = -0.8$. Locations of the phase transition points are determined by those of center of the hysteresis loops.

We also studied phase structure of the model with c_u, c_v fixed and c_m varied, and found that a first-order phase transition occurs at a critical coupling of c_m. Measurement of E and density of instantons exhibits similar behavior to those in Fig. 3.

Let us turn to the $d_m < 0$ case. In the large-c_u limit, $U_{x,j} \sim e^{i\varphi_{x+j}} e^{-i\varphi_x}$ and the d_m terms in $A_{\rm GL}$ prefer configurations like $\langle e^{-i\varphi_{x+i}} V_{x,i} V^{\dagger}_{x,j} e^{i\varphi_{x+j}}\rangle < 0$ $(i \neq j)$. Then under the gauge-fixing condition $\varphi_x = 0$, it is expected that the expectation value of the Cooper-pair field $\langle V_{x,i}\rangle$ changes its sign under a $\pi/2$ rotation in a plane. Though some of the d-wave SC materials have a layered structure, we first consider the three-dimensional (3D) isotropic case and set $d_m = -0.8$.

Phase structure was studied by means of the MC simulations as before and found that there exist phase transition lines. The internal energy E shows hysteresis loop at critical points as in the previous case. We show the calculations of E for certain places in the c_u-c_v plane in Fig. 6. Phase diagram obtained by the measurement of E and C is given in Fig. 7. The gauge-boson mass M_G exhibits a discontinuity at phase transition points as in the previous case.

Besides the normal and Higgs-SC phases, we found that there exists an exotic phase that we call staggered state (SS). Existence of a similar phase has been observed for the compact gauge model.[10] It stems from the fact that in 3D there are no configurations that satisfy $V_{x,i} V^{\dagger}_{x,j} < 0$ $(i \neq j)$ for *all* i and j simultaneously. In other words, the d_m terms cause frustrations. E and the instanton density exhibit the first-order phase transition at the boundary of the normal and SS states. In the SS, the translational symmetry with the unit lattice spacing is broken.[10] It is quite plausible that the SS is similar to the flux state considered by Affleck and Marston for quantum spin models.[15] We also found that as the system

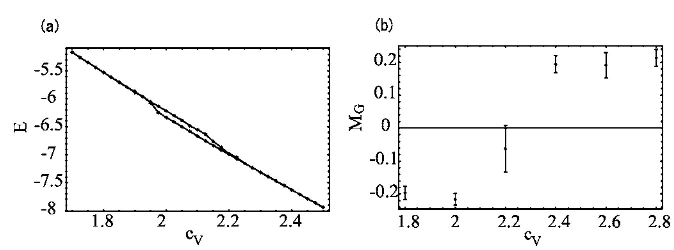

FIG. 8. Results for $A_{\rm GL}$ with $c_m = 0$, $d_m = -0.8(-0.4)$ for intralayer (interlayer) coupling and $c_u = 0.5$ $(L = 24)$. (a) E as a function of c_v for $c_u = 0.5$. (b) Measurement of M_G (average of M_G in three directions) as a function of c_v for increasing c_v. Values of M_G are much smaller than those in the 3D isotropic case.

size is getting larger, signal of the phase transition at the boundary is getting weaker.

Finally let us turn to anistropic cases and study how the phase structure changes due to the layered structure. To this end, we put different values for the interlayer and intralayer d_m's. Numerical results for $d_m=-0.8(-0.4)$ for the intralayer (interlayer) coupling with $c_u=0.5$ are given in Fig. 8. The SS, which exists in the isotropic case due to the frustration, is not observed in this case and the first-order phase transition to the Higgs-SC phase is observed instead. We also verified that the critical line of the normal-SC phase transition exists as in the isotropic case. However, discontinuity in the gauge-boson mass M_G at critical points becomes smaller than that in the isotropic case.

In conclusion, we studied the noncompact U(1) lattice gauge model with link Higgs field that is a GL theory for the unconventional SC including the extended *s*-, *d*-wave and also ferromagnetic *p*-wave SCs. By means of the MC simulations, we clarified the phase structure. There exist first-order phase transitions from the normal to Higgs-SC phases. We also observed that as the anisotropy of the layered structure is getting larger, signal of the first-order phase transition is getting weaker.

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