Strong fluctuation effects in phase-frustrated multiband superconductors

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We compare the phase-diagram of an effective theory of a three-dimensional multi-band superconductor obtained within standard and cluster mean-field theories, and in large-scale Monte Carlo simulations. The system features three phases, namely a superconducting state with broken chiral symmetry, a normal metallic phase, and an unusual metallic state with broken $\mathbb{Z}_2$ time-reversal symmetry. Surprisingly, in three dimensions mean field theory not only fails in locating correctly the positions of the phase transitions, as well as the character of the transitions between the different states, it also does not identify the unusual metallic state. The large fluctuation effects are due to strong frustration originating with interband Josephson-couplings.

Strong fluctuation effects in condensed matter systems are typically manifested in low dimensions at any nonzero temperature, where fundamental theorems [1–3] prevent the breaking of continuous symmetries, such as the loss of translational, rotational, as well as local and global $U(1)$ symmetries. The first is relevant for freezing of liquids into crystals with long-range order, the second is relevant for ordering in magnets, while the last two give rise to superconductivity and superfluidity. In three dimensions, mean-field theories where fluctuation effects are ignored have often met with much success, notably in low-temperature superconductors arising out of good metals [4]. The dominant fluctuations in a strong type-II superconductor/superfluid are phase fluctuations of the order parameter [5–8]. The phase-stiffness is governed by the inverse square of the magnetic penetration length, which in good metals often are quite large. On the other hand, in superconductors such as the high-$T_c$ cuprates or the superconducting pnictides, phase-fluctuations may be significant. This is quite typical of superconductors with a large Ginzburg-Landau parameter $\kappa$ [5–8].

In this paper, we identify another source of strong fluctuation effects other than low dimensionality, which is particular to superconductors with three or more energy-bands on which superconductivity can reside. Examples of such system are heavy fermion and iron pnictide superconductors.[9, 10] Comparing the phase diagram of a model of these systems as obtained in standard as well as cluster [11, 12] mean-field theories, with results obtained in large-scale Monte-Carlo simulations of the same model, we conclude that standard mean-field theories are not capable of capturing even the correct structure of the phase diagram in such system in three dimensions. The principle mechanism driving these large fluctuation effects, is frustration of the phases of the superconducting order parameter originating with interband Josephson couplings [13–15].

The London model for an $n$-band superconductor is given by [16–18]

$$ F = \sum_{\alpha=1}^{n} \left( \frac{1}{2} (\nabla \theta_\alpha - e B) \right) + \sum_{\alpha,\alpha' > \alpha} \eta_{\alpha \alpha'} |\psi_\alpha| |\psi_{\alpha'}| \cos(\theta_\alpha - \theta_{\alpha'}) + \frac{1}{2} (\nabla \times B)^2. $$ (1)

Here, $|\psi_\alpha| e^{i \theta_\alpha}$ denote the superconducting condensate components in different bands labeled by $\alpha \in \{1, \ldots, n\}$, while the second term represents interband Josephson couplings of strength $\eta_{\alpha \alpha'}$. The field $B$ is the magnetic vector potential that couples minimally to the charged condensate matter fields. By collecting gradient terms for phase differences, Eq. (1) can also be cast in the form

$$ F = \frac{1}{2} g^2 \left( \sum_\alpha |\psi_\alpha|^2 \nabla \theta_\alpha - e g A \right)^2 + \frac{1}{2} (\nabla \times A)^2 + \sum_{\alpha,\alpha' > \alpha} \frac{|\psi_\alpha|^2 |\psi_{\alpha'}|^2}{2 g^2} |\nabla \theta_{\alpha'}|^2 + \eta_{\alpha \alpha'} |\psi_\alpha| |\psi_{\alpha'}| \cos(\theta_\alpha - \theta_{\alpha'}), $$ (2)

where $g^2 = \sum_\alpha |\psi_\alpha|^2$. Thus, the vector potential is coupled to the $U(1)$ sector of the model, but not to phase
London limit is given by [15, 23]

\[
H = -\sum_{\langle i,j \rangle, \alpha} a_{\alpha} \cos(\theta_{\alpha,i} - \theta_{\alpha,j} - A_{ij}) \\
+ \sum_{i, \alpha' > \alpha} g_{\alpha \alpha'} \cos(\theta_{\alpha,i} - \theta_{\alpha',i}) \\
+ q \sum_{i, \lambda} \left( \sum_{\mu, \nu} \epsilon_{\lambda \mu \nu} \Delta_\mu A_{i,i+\nu} \right)^2.
\]  

(3)

Here, \( i, j \in \{1, 2, \ldots, N = L^3 \} \) denote sites on a lattice of size \( L \times L \times L \), and \( (i, j) \) indicates pairs of nearest neighbor lattice sites (assuming periodic boundary conditions). We may, without loss of generality, choose \( a_1 = 1, \quad a_{\alpha} \in (0, 1], \quad \alpha > 1 \), where \( g_{\alpha \alpha'} \) are interband Josephson couplings. We have rescaled the gauge field \( A \leftrightarrow eA \) and introduced \( q \equiv 1/(2e^2) \). In these units, \( q \) parametrizes the London penetration depth of the superconductor.

In the limit \( e \to 0 \leftrightarrow q \to \infty \), where fluctuations in the gauge field may be neglected, the model is reduced to

\[
H = -\sum_{\langle i,j \rangle, \alpha} a_{\alpha} \cos(\theta_{\alpha,i} - \theta_{\alpha,j}) \\
+ \sum_{i, \alpha' > \alpha} g_{\alpha \alpha'} \cos(\theta_{\alpha,i} - \theta_{\alpha',i}).
\]  

(4)

By letting \( g_{\alpha \alpha'} \to \infty \) in the lattice London model such that the ratio \( g_{\alpha \alpha'}/g_{\beta \beta'} \) is finite, we may derive a “reduced” version of the model given by Eqs. (3) and (4), for which the intercomponent phase fluctuations are suppressed. Namely, the “phase star” of a lattice site locks into one of the two possible \( Z_2 \) configurations minimizing the contribution from the Josephson term in the Hamiltonian. That is, in this approximation the phase differences can have only two values. The \( Z_2 \) domain wall then represents a change of the phase difference over one lattice spacing.

For the case without a fluctuating gauge-field, the reduced lattice London model is given by a rather unusual coupled Ising-XY type of model [15],

\[
H = -\sum_{\langle i,j \rangle} \left[ (1 + K_1 \sigma_i \sigma_j) \cos(\theta_i - \theta_j) \\
+ K_2 (\sigma_i - \sigma_j) \sin(\theta_i - \theta_j) \right].
\]  

(5)

Here \( \sigma_i \in \{-1,+1\} \) denotes the \( Z_2 \) chirality of the “phase star”, \( \theta_i \equiv \theta_{\alpha,i} \), and

\[
K_1 \equiv \frac{2}{\sum_{\alpha > 1} a_{\alpha} [1 - \cos(2\phi_{\alpha})]}, \quad K_2 \equiv \frac{2}{\sum_{\alpha > 1} a_{\alpha} [1 + \cos(2\phi_{\alpha})]},
\]  

(6)

The lattice version of an \( n \)-band superconductor in the
The angles $\phi_{\alpha} \equiv \theta_{\alpha,i} - \theta_{\beta,i}, \alpha > 1$ are determined by the ratios $g_{\alpha\alpha}/g_{3\beta}$ of the Josephson-couplings. For site-independent Josephson-couplings, the $\phi_{\alpha}$’s are also site-independent. If $K_1$ and $K_2$ are treated as free parameters, the model Eq. (5) in principle allows a uniform as well as staggered ordering of the $\mathbb{Z}_2$ $\sigma_i$-variables on the lattice, in addition to the disordered state. A uniform ordering means that the phases illustrated in Fig. 1a have the same chirality throughout the lattice, while a staggered ordering means that the chirality alternates from lattice site to lattice site. We will refer to the former as “ferromagnetic” ordering in the $\mathbb{Z}_2$ sector, while the latter will be referred to as “antiferromagnetic”.

Up to an overall scaling factor, the model may also be written on a somewhat more familiar form of a coupled Ising-XY model,

$$H = -\sum_{\langle i,j \rangle} (1 + J \sigma_i \sigma_j) \cos(\theta_i - \theta_j - \alpha(\sigma_i, \sigma_j))$$

(8)

where $J = \frac{W}{1 + \sqrt{1 - W^2}}$, $W \equiv \frac{2(K_1 - K_2^2)}{1 + K_1^2 + 2K_2^2}$, and

$$\alpha(\sigma_i, \sigma_j) \equiv \begin{cases} 0 & \sigma_i = \sigma_j \\ \pm \arctan \left( \frac{2K_2}{1 - K_1} \right) & \sigma_i = -\sigma_j = \pm 1 \end{cases}$$

(9)

A reduced model including electric charge is obtained by replacing $\theta_i - \theta_j$ by $\theta_i - \theta_j - A_{ij}$ in Eq. (5) or Eq. (8) and adding a Maxwell term $q \sum_{i,\lambda} (\sum_{\mu,\nu} \lambda_{\mu\nu} \Delta_\mu A_{i,i+\nu})^2$ to the Hamiltonian.

The free energy density of the reduced model in the mean-field approximation is given by (see supplementary material)

$$f = M \left[ r \frac{I_1(\beta r)}{I_0(\beta r)} - \frac{1}{2} \left( \frac{I_1(\beta r)}{I_0(\beta r)} \right)^2 \right] + \beta^{-1} [s_{\mathbb{Z}_2}(m) - \ln(I_0(\beta M))]$$

(10)

with $M = 1 + K_1 m^2$, $m = \frac{1}{2}(m_\lambda + m_\beta)$ when the $\mathbb{Z}_2$ sector will order “ferromagnetically”, and $M = \sqrt{(1 - K_1 m^2)^2 + 4K_2^2 m^2}$, $m = \frac{1}{2}(m_\lambda - m_\beta)$, when the ordering is “antiferromagnetic”. Antiferromagnetic $\mathbb{Z}_2$ ordering can take place when $K_1 < K_2^2$, i.e. for large enough $K_2$. This situation is unphysical when viewing the reduced model as a limiting case of the multiband London model [15], i.e. when $K_1$ and $K_2$ are determined by Eqs. (6) and (7), but is included here for the sake of completeness. $m_\lambda$ and $m_\beta$ are the Ising-type magnetizations on sublattices A and B of the bipartite lattice, while $r$ is the condensate density (U(1) order parameter). Furthermore, the $I_l$’s are modified Bessel functions of order $l$ and $s_{\mathbb{Z}_2}(m) = (1+m) \ln \left( \frac{1+m}{2} \right) + (1-m) \ln \left( \frac{1-m}{2} \right)$. An immediate consequence of this mean-field form is that when $r = 0$, we have $f = \beta^{-1} s_{\mathbb{Z}_2}(m)$, which has a global minimum at $m = 0$. Thus, at the mean-field level, there can be no broken $\mathbb{Z}_2$ symmetry in a U(1)-symmetric (metallic) state. As we shall see, strong fluctuation effects alter this picture quite drastically, even in three dimensions.

With $m = 0$, $M = 1$ and the free energy Eq. (10) reduces (up to a constant term) to that of the XY model,

$$f_{\text{XY}} = r I_1(\beta r) - \frac{1}{2} \left( \frac{I_1(\beta r)}{I_0(\beta r)} \right)^2 - \beta^{-1} \ln (I_0(\beta r))$$

(11)

which displays a second order phase transition at $\beta = 2$.

In Fig. 2b, we show an improved cluster-mean field phase diagram (see supplementary material) based on a $2 \times 2 \times 2$ cluster where fluctuations are allowed. This represents a first step towards including fluctuation corrections to the mean-field phase-diagram of Fig. 2a, which is essentially based on a $1 \times 1 \times 1$ cluster. We see that the tricritical boundary line separating (II, II′) from (III, III′) is pushed considerably further away from the origin of the $K_1, K_2$ plane, due to fluctuation effects even at this level. This result in itself indicates that fluctuation effects are strong in these systems.

Figure 2c shows the phase diagram for the case with no fluctuating gauge field, obtained by Monte Carlo simulations (see supplementary material). The tricritical boundary line is altered considerably compared to what is found in Fig. 2a and Fig. 2b. Furthermore, for $K_2 = 0$ and sufficiently large $K_1$ values, the transitions in the $\mathbb{Z}_2$ and U(1) sector merge into a single joint first order transition not seen in the mean field case.

Adding a fluctuating gauge field, the discrepancy between the true (Monte Carlo) and the mean-field picture is even more striking. Figure 2d gives the phase diagram when $q = 0.1$. The $\mathbb{Z}_2$ transition now remains second order in the entire phase diagram. A new, U(1)-symmetric (metallic), but $\mathbb{Z}_2$ broken (chiral) state emerges. Typically, one expects mean-field calculations in a three-dimensional system to at least yield a correct phase diagram. Here, we see that strong intrinsic fluctuation effects in multiband superconductors with more than two bands alter this basic picture.

The nontrivial interplay between the U(1) vortices and the $\mathbb{Z}_2$ topological defects, with the ensuing large corrections to the mean-field phase-diagram, is due to the interband Josephson couplings. This coupling essentially represents a frustration of the system [13–15]. While strong fluctuation effects are well known in superconductors and superfluids in two dimensions [1–3], it is much
FIG. 2. (a) The mean field phase diagram of the $K_1K_2$ model, based on minimizing the free energy, Eq. (10). (b) The cluster mean field phase diagram of the $K_1K_2$ model based on a $2 \times 2 \times 2$ cluster. (c) The phase diagram of the $K_1K_2$ model without a fluctuating gauge field, Eq. (5). The plot is based on Monte Carlo simulations with $L = 40$, except for $K_2 = 0$, where $L = 50$ was used. (d) The phase diagram of the $K_1K_2$ model with a fluctuating gauge field, $q = 0.1$. The plot is based on Monte Carlo simulations with $L = 40$. Unprimed labels denote a state where the ordering in the $Z_2$-sector is “ferromagnetic”, while primed labels indicate that this ordering is “antiferromagnetic”. I: The borderline between the ferromagnetic and antiferromagnetic regions. On this borderline, there is only U(1) ordering, no $Z_2$ ordering. II, II’: The $Z_2$ transition is second order and happens when the U(1) sector has already ordered. III, III’: The $Z_2$ transition is first order and happens when the U(1) sector has already ordered. The solid line separating the regions (II, II’) from the regions (III, III’) indicates the boundary where the phase transition in the $Z_2$ sector changes from second order to first order. For I-III the U(1) transition is second order. IV: The $Z_2$ and U(1) sectors order at the same time through a first order transition. V: The $Z_2$ sector orders before the U(1) sector, i.e. the system displays a region of an anomalous, $Z_2$ broken metallic state. Both sectors order through second order transitions. See text for details.

more uncommon to see such strong fluctuation effects in higher-dimensional systems.

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