Broken Time-reversal Symmetry in Josephson Junction with an Anderson impurity and multi band superconductors

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A Josephson junction consisting of an Anderson impurity weakly coupled with two-band and single-band superconductors exposes a time reversal breaking ground state when the coupling between the two bands exceeds a certain threshold. The critical regime occurs around local moment formation. This indicates a fundamental and distinct role of strong correlations: Driving a system into a time reversal breaking ground state. One of the observable consequences is that the impurity magnetization in this phase is reduced.

Motivation: Recently, there is a renewed interest in the physics of multi-band superconductors which are believed to encode the physics behind the new Iron based superconductors\(^1\)\(^2\)\(^3\). Historically, interest in two-band superconductors is related to experiments suggesting that in some transition metals, there should be a second mechanism responsible for pairing beyond that of electron-phonon interaction\(^4\)\(^5\)\(^6\)\(^7\). For example, in Nb\(_3\)Sn the isotopic effect is found to be very weak\(^8\). Inter-band coupling also provides a natural mechanism for augmenting \(T_c\)\(^7\)\(^9\).

The physics associated with a two-band superconductor can be examined in a Josephson junction involving two-band superconductors on one of its sides and a third superconductor on the other side\(^10\). Within a Ginzburg-Landau formalism the order parameters \(\psi_1, \psi_2\) of the two bands are coupled among themselves by a term \(-J\text{Re}[\psi_1^*\psi_2]\), and to the single-band superconductor (on the opposite side of the junction) with tunneling strengths \(\Gamma_1\) and \(\Gamma_2\). A time-reversal violating ground state (TRVGS) was found for \(\Gamma_1 \approx \Gamma_2\), due to frustration between the three order parameters, while otherwise, a time reversal conserving ground state (TRCGS) prevails. A natural question which motivates the present research is what would happen if the Josephson junction contains an Anderson impurity. Indeed, strong correlations are expected to affect these findings and alter the pertinent physics in a profound way.

In this work we study a system consisting of an Anderson impurity (level energy \(\epsilon\) and correlation strength \(U\)) weakly coupled on the left with a two-band superconductor (order parameters \(\psi_n = \Delta_n e^{i\theta_n}, n = 1, 2\) and inter-band Josephson coupling \(J\)) and on the right to a single-band superconductor (order parameter \(\psi_3 = \Delta_3 e^{i\theta_3}\)). This is briefly denoted as \(2B - U - 1B\) Josephson junction (see Fig. 1). A TVRGS occurs if the free energy \(\mathcal{F}[\theta] \equiv \langle \theta_1, \theta_2, \theta_3 \rangle\) has a minimum at some point \(\theta\) for which there is a non-zero Josephson current loop \(\mathcal{J}\) even in the absence of magnetic field (see Ref.\(^{10}\) for the case of \(2B - 1B\) Josephson junction without Anderson impurity). On the technical part, the mean-field (Hartree-Fock) approach to the \(1B - U - 1B\) problem\(^{12,13}\) can be used to treat the \(2B - U - 1B\) system.
as well. It enables the elucidation of the ground-state configuration $\bar{\theta}(J, U)$ together with the free energy $F(\bar{\theta})$, the Josephson current $J_c(\bar{\theta})$ the impurity occupation $n_{imp}(\bar{\theta})$ and magnetization $m_{imp}(\bar{\theta})$. As it turn out, however, the physics is distinct since there are now three order parameters and two of them are coupled.

**Our main result** pertains to the nature of the ground state TR symmetry in the $U - J$ plane, for high asymmetry parameter, $\delta \equiv \frac{U}{J} \gg 1$, where no TRGS exists\(^\text{10}\) on the line $U = 0$. Two phases are identified, one for which there is TRCGS and one for which there is TRGS, separated by a sharp border line. The TRGS occurs for $U_1(\delta) < U < U_2(\delta)$ and for $J > J_c(U, \delta) > 0$. Here $U_1 < U_0$ and $U_2 > U_0$ where $U_0$ defined by $\varepsilon + \frac{U_0}{2} = 0$ is the particle hole symmetric point and $J_c(U, \delta)$ is some critical threshold.

**Formalism:** The mean-field Hamiltonian is written as,

$$H = H_L + H_R + H_I + H_{imp}. \quad (1)$$

The first two terms $H_L, H_R$ describe (within the BCS formalism) the two band superconductor on the left ($H_L$) and the single band superconductor on the right ($H_R$). Explicitly, in terms of quasi-particle field operators, $H_L = \sum_{n=1}^{2} H_n$ and $H_R = H_3$ are written as,

$$H_n = \int \Psi_n^\dagger(r) \mathcal{H}_n \Psi_n(r) dr, \quad \mathcal{H}_n(r) = \begin{bmatrix} \psi_{n1}^\dagger(r) \\ \psi_{n1}(r) \end{bmatrix}, \quad (2)$$

The two-band Hamiltonian densities $\mathcal{H}_{n=1,2}$ are derived rom the two-band model Hamiltonian of Ref.\(^\text{3}\). In this Hamiltonian (equation (1) therein), there is only intraband pairing (and no interband pairing) and the electrons in the two bands are coupled only through an interband Josephson effect (see below). The single band Hamiltonian density $\mathcal{H}_3$ has the standard Bogoliubov-De Gennes structure. Thus,

$$\mathcal{H}_n = \begin{pmatrix} \varepsilon_n(-i\nabla) - \mu & \Delta_n e^{i\theta_n} + J_m e^{i\theta_m} \\ \Delta_n e^{-i\theta_n} + J_m e^{-i\theta_m} & -\varepsilon_n(-i\nabla) + \mu \end{pmatrix}, \quad \mathcal{H}_3 = \begin{pmatrix} \varepsilon_3(-i\nabla) - \mu & \Delta_3 e^{i\theta_3} \\ \Delta_3 e^{-i\theta_3} & -\varepsilon_3(-i\nabla) + \mu \end{pmatrix}. \quad (3)$$

In Eqs.\(^\text{3}\) $m \neq n = 1, 2$ and the various quantities are defined as follows: $\varepsilon(-i\nabla)$ is the kinetic energy operator derived from the corresponding energy dispersion functions $\varepsilon_n(k)$, and $\mu$ is the chemical potential. Moreover, $\Delta_n e^{i\theta_n} \equiv V_n \psi_n$ where $\psi_n \equiv \int dr \psi_{n1}(r) \psi_{n1}(r)$ is the order parameter of superconductor $n = 1, 2, 3$ and $V_n$ is the corresponding strength of the pairing potential. Similarly, $J_m e^{i\theta_m} \equiv I \psi_m$ encodes the pairing field in band $n \neq m$ due to electrons pairing in band $m$ (interband Josephson effect) and $I$ is the strength of the coupling between the two bands.

The tunneling part $H_I$ contains hopping between the impurity to each one of the three superconductors (with different strengths $t_{n=1,2,3}$), which occurs at a single point. Finally, the strong correlation part has the usual structure of an Anderson impurity Hamiltonian. Explicitly,

$$H_I = -\sum_{n=1}^{3} t_n [\Psi_n^\dagger(0) \tau_3 C + C^\dagger \tau_3 \Psi_n^\dagger(0)] + h.c., \quad C = \begin{bmatrix} c_1 \\ c_3 \end{bmatrix}, \quad H_{imp} = \bar{\varepsilon} C^\dagger \tau_3 C + \frac{1}{2} U |C^\dagger C|^2, \quad \bar{\varepsilon} = \varepsilon + \frac{U}{2}. \quad (4)$$

The procedure for calculating the free energy $F(\theta_1, \theta_2, \theta_3)$ is a modified version of the algorithm used in Refs.\(^\text{12,13}\). It involves an Euclidean path integral for the partition function $Z = e^{-\beta F}$ in terms of Grassman fields and employing Hubbard-Stratonovich transformation for treating the quartic term in $H_{imp}$ at the expense of an additional integration on a new field $\gamma$. The latter is carried out within the saddle point approximation leading to a self consistent equation (Hartree-Fock approximation). Notice that unlike Ref.\(^\text{10}\) where the pairing field away from the impurity is also solved
self-consistently within a Ginzburg-Landau approximation, the pairing fields $\Delta_n$’s are assumed to take a constant value in the superconductors.

Beside the density of states at the Fermi energy $N(\mu)$ (assumed constant) and the impurity level (partial) widths $\Gamma_n = \pi n^2 N(\mu)$ for the superconductor $n = 1, 2, 3$, the basic input quantities are defined below, [with $\omega = \omega_k = (2k + 1)\pi T$ ($k = 0, 1, 2, \ldots$) a Matsubara frequency at temperature $T = 1/\beta$ and $\sum_\omega f(\omega) = \sum_k f(\omega_k)$]:

$$\alpha_{n=1,2}(\omega) = \Gamma_n[\Delta_n^2 + J_n^2 + 2\Delta_n J_n \cos(\theta_1 - \theta_2) + \omega^2]^{-\frac{1}{2}}, \quad \alpha_3 = \Gamma_3[\Delta_3^2 + \omega^2]^{-\frac{1}{2}}, \quad \eta(\omega) = \omega[1 + \sum_n \alpha_n(\omega)].$$

$$q_1(\omega) = \alpha_1(\omega)\Delta_1 + \alpha_2(\omega)J_1, \quad q_2(\omega) = \alpha_2(\omega)\Delta_2 + \alpha_1(\omega)J_2, \quad q_3(\omega) = \alpha_3(\omega)\Delta_3.$$

$$F(\omega; \theta) \equiv \sum_{n=1}^3 q_n^2 + 2 \sum_{n \neq n'} q_n q_{n'} \cos(\theta_n - \theta_n').$$

The self consistent equation for the field $\gamma$ (analogous to Eq. 7 in Ref.12 or Eq. 12 in Ref.13) reads,

$$\frac{1}{2U} - T \sum_\omega \frac{[\gamma^2 + \eta(\omega)^2 - \tilde{\varepsilon}^2 - F(\omega; \theta)]}{[\gamma^2 - \eta(\omega)^2 - \varepsilon^2 - F(\omega; \theta)]^2 + 4\gamma^2 \eta(\omega)^2} = 0,$$

whose solution $\bar{\gamma}(\theta)$ is used below.

**Analysis of the results:** The free energy associated with the impurity is the coefficient of $-\beta$ in the exponent of the partition function $Z = e^{-\beta F}$, and the formalism described above yields for it the following expression,

$$F(\theta) = \frac{\bar{\gamma}^2}{2U} + \tilde{\varepsilon} - \frac{1}{2T} \sum_\omega \ln \beta^4 \{[\bar{\varepsilon}^2 - \eta(\omega)^2 - \varepsilon^2 - F(\omega; \theta)]^2 + 4\bar{\varepsilon}^2 \eta(\omega)^2 \}.$$

It will be examined as function of $J$ and $U$ fixing other parameters as,

$$\Delta_{1,3} = 1.0, \quad \Delta_2 = 0.8, \quad \Gamma_1 = 0.5, \quad \Gamma_2 = \Gamma_3 = 0.2, \quad \varepsilon = -2, \quad T = 0.0005,$$

(energies are expressed in unit of $\Delta_1 = 1$). Note the ratio $\delta \equiv \frac{\Gamma_2}{\Gamma_1} = 2.5$ and recall that for noticeable different Josephson tunneling strengths $\Gamma_1 \neq \Gamma_2$, there is no TRVGs in a $2B - 1B$ junction10.

Employing gauge invariance and setting $\theta_3 = 0$, the minimum $\tilde{\theta} = (\tilde{\theta}_1, \tilde{\theta}_2, 0)$ of $F(\theta)$ is located. If $\sin \tilde{\theta}_1 = \sin \tilde{\theta}_2 = 0$ one evidently has a TRCGS where the Josephson current vanishes. On the other hand, when the above condition is not satisfied, one has a TRVS. In the absence of Anderson impurity and close to perfect symmetry $\delta \approx 1$ it occurs for $J > 0$ at $\tilde{\theta}_1 \approx -\tilde{\theta}_2 \approx \frac{\pi}{2}$. For $U \neq 0$ the property $\tilde{\theta}_1 \approx -\tilde{\theta}_2 \approx \frac{\pi}{2}$ is expected to be somewhat modified, and regions with $\sin \tilde{\theta}_1, \sin \tilde{\theta}_2 \neq 0$ are those where TRVGs is realized.

The phase diagram displaying these two domains is shown in Fig. 2. The order parameter phases of the TRVGs just above the border line $J_c(U, \delta)$ are displayed in Fig. 2, and indeed, they are neither 0 nor $\pi$ so that $\sin \tilde{\theta}_1, \sin \tilde{\theta}_2 \neq 0$. The scenario emerging from Fig. 2 is as follows: For a given asymmetry parameter $\delta \gg 1$ there is a domain in the $U - J$ plane for which TRVGs is realized. It is bounded on the left and right by vertical lines $U = U_1(\delta)$ and $U = U_2(\delta)$ and below by a border line $J_c(U, \delta) > 0$. It is checked that $U_1(\delta) < U_0 = 2|\varepsilon|$ is a slowly increasing function of $\delta$ starting at $U_1(1) = 0$ while $U_2(\delta) > U_0$ is very weakly dependent on $\delta$. Moreover, $J_c(U, \delta)$ is an increasing function of $U$ and $\delta$ (actually it saturates around $U_0$).

To understand the mechanism which drives the formation of the TRVGs state, we first consider the case of single-band superconductor Josephson junction12. It was found that the effective Josephson coupling between the two superconductors mediated through the Anderson Impurity changes sign when $U$ goes through a critical value $U_c$. The two superconductors are in phase ($\delta = 0$) at $U < U_c$, and are out of phase ($\delta = \pi$) at $U > U_c$. Associated with this
FIG. 2: (a) Phase diagram showing the line $J_c(U, \delta)$ separating TRCGS from TRVGS in the $U - J$ plane. All parameters (except $U$ which varies) are defined in Eq. (5). Note the sharp cutoff points at $U_1(\delta) \approx 3.5$ (below the point $B$), and $U_2(\delta) \approx 6.1$ (below the point $C$). (b) The phases $\bar{\theta}_1, \bar{\theta}_2$ of the order parameters at the ground state configuration (minimum point of the free energy, Eq. (7)), are displayed along the line $ABCD$ of Fig. 2a. Along the border line $J_c(U, \delta)$ we have $\sin \bar{\theta}_1, \sin \bar{\theta}_2 \neq 0$.

transition is the formation of a large magnetic moment at the Anderson impurity at $U > U_c$. We now replace one of the superconductor by a two-band superconductor. In this case the effective Josephson coupling $F_{jos}$ between the different $\theta_n$'s generated by the impurity has the form

$$F_{jos} \sim T_{13}(U) \cos(\theta_1 - \theta_3) + T_{23}(U) \cos(\theta_2 - \theta_3) + T_{12}(U) \cos(\theta_1 - \theta_2) + O(\cos(\theta_n) \cos(\theta_m)) + \ldots,$$

where $T_{13}(U)$ and $T_{23}(U)$ become small around $U \sim U_c$ and higher order terms in $F_{jos}$ becomes important in determining the phase structure. The higher order Josephson terms arises from $\alpha_n(\omega)$'s and $F(\omega; \theta)$ in Eq. (5) which has much more complicated structure than the case of one-band superconductor considered in Ref. 12. Apparently, the coupling between the superconductors and the formation of $\pi$ junction for large $U$ introduces additional frustration among the phases $\theta_n$ which gives rise to TRVGS when the first order coupling terms $T_{13}, T_{23}$ become small, i.e. around the critical regime $U \sim U_0$.

The question now is whether this phase where TRVGS occurs can be traced experimentally. A promising direction is to inspect the impurity magnetization $m$ and its behavior as the phase boundary is crossed. Specifically, we fix the repulsive potential $U$ and inspect the magnetization as $J$ is varied, thereby crossing the phase boundary at $J_c(U, \delta)$.

In Ref. 12 it was found that for a 1B-U-1B junction, the ground state energy and the magnetization develop kinks near the critical point (when studied as function of the phase difference between left and right superconductors). Here, on the other hand, the behavior of the ground state energy (as function of $J$) appears to be very smooth and rather slowly varying. It should be stressed that here we do not vary the phases of the order parameters, as they are fixed at the ground state position ($\bar{\theta}_1, \bar{\theta}_2$). The mean field magnetization $m = \frac{2\gamma}{U}$ and the ground state order-parameter phases ($\bar{\theta}_1, \bar{\theta}_2$) are displayed as function of $J$ for $U = 4$ in Fig. 3. The magnetization in the TRVGS phase is smaller than in the TRCGS phase because according to the spin analog developed in Ref. 10, the former phase is characterized by frustration. The fact that $\bar{\theta}_1, \bar{\theta}_2$ also shows step behavior as $J$, and that these steps are commensurate with those of the magnetization lead us to conjecture that the system has many frustrated states close in energy.

**Conclusions:** The study of $2B - U - 1B$ carried out here is motivated by the renewed interest in multi-band superconductors (stemming from the analysis of the Iron based superconductors). The pertinent physics is fundamentally
FIG. 3: Impurity magnetization $m$ (upper line) at the ground state is displayed as function of $J$ for $U = 4$ with other parameters defined in Eq. (3). Also displayed are the phases $\theta_1, \theta_2$ (divided by $2\pi$) of the order parameters indicating the ground state configuration. Both the magnetization and the phases undergo a remarkable change of behavior at the border line where $J = J_c(U, \delta)$ (according to Fig. 2b, $J_c(U = 4, \delta) \approx 0.1$). The magnetization becomes smaller due to frustration in the TR VGS phase and the commensurability of steps indicates that the system passes through higher and higher frustrated ground-states. At the same time, it is verified that the ground state energy is a very smooth function of both $J$ and $U$.

distinct from that of a $1B - U - 1B$ system$^{12,13}$ and the $2B - 1B$ junction discussed in Ref.$^{10}$ since the roles of strong correlations $U$ and the coupling $J$ between the two order parameters in the two-band superconductor interface. It has been shown that for $J > J_c(U, \delta) > 0$ and for $U_1 < U < U_2$ a TRVGS emerges which supports a non-zero Josephson current even without a magnetic field. The role of strong correlations as controlling the TR symmetry of the ground-state is evidently remarkable. As far as an experimental detection is concerned, beside the experiments proposed in Ref.$^{10}$, our preliminary results indicate that some quantities (such as impurity magnetization) undergo a dramatic change as $J$ pass through the phase boundary $J_c(U, \delta)$, hence a Josephson junction with Anderson impurity can serve as a potential tool for probing the relative phase of the two order parameters in a two-band superconductor (which is a very elusive quantity).

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1. S. Raghu, Xiao-Liang Qi, Chau-Xing Liu, D. J. Scalapino and S. C. Zhang, Phys. Rev. B 77, 220503 (2008).
2. P. A. Lee and Xiao-Gang Wen, arXiv:0804.1739.
3. Xiao-Yong Feng and Tai-Kai Ng, arXiv:0812.1068.
4. H. Suhl, B. T. Matthias and R. Walker, Phys. Rev. Lett. 3, 552 (1959).
5. V. A. Moskalenko, FMM 8, 503 (1959).
6. W. S. Chaw, Phys. Rev. 176, 525 (1968).
7. J. Kondo, Prog. Theor. Phys. 23, 1 (1963).
8. G. E. Devlin and E. Corenzwit, Phys. Rev. 120, 1964 (1960).
9. O. Entin-Wohlman and Y. Imry, Phys. Rev. B 40, 6731 (1989).
10 T. K. Ng and N. Nagaossa, arXiv:cond-mat/08.
11 S. Mukhopadhyay et. al., arXiv:0903.0674 (2009).
12 A. V. Rozhkov and D. P. Arovas, Phys. Rev. Lett. 82, 2788 (1999).
13 Y. Avishai and A. Golub, Phys. Rev. B61 11293 (2000).