Effect of \(d-f\) hybridization on the Josephson current through Eu-chalcogenides

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Abstract

A superconducting ring with a \(\pi\) junction made from superconductor/ferromagnetic-metal/superconductor (S-FM-S) exhibits a spontaneous current without an external magnetic field in the ground state. Such \(\pi\) ring provides so-called quiet qubit that can be efficiently decoupled from the fluctuation of the external field. However, the usage of the FM gives rise to strong Ohmic dissipation. Therefore, the realization of \(\pi\) junctions without FM is expected for qubit applications. We theoretically consider the possibility of the \(\pi\) coupling for S/Eu-chalcogenides/S junctions based on the \(d-f\) Hamiltonian. By use of the Green’s function method we found that \(\pi\) junction can be formed in the case of the finite \(d-f\) hybridization between the conduction \(d\) and the localized \(f\) electrons.

Key words: Josephson junction, Spin filter effects, Spintronics, Quantum computer, Green’s function method

PACS: 74.50.+r, 03.65.Yz, 05.30.-d

1. Introduction

The interplay between superconductivity and ferromagnetism has been the subject of study for many decades [1]. Recently theoretical and experimental investigations into the properties of superconductor/ferromagnetic-metal/superconductor (S-FM-S) heterostructures [1,2] have seen an upsurge in interest after the experimental observation of 0-\(\pi\) transitions in the Josephson current through S-FM-S junction by Ryananov et al. [3] and by Kontos et al. [4]. In terms of the Josephson relationship \(I_J = I_C \sin \phi\), where \(\phi\) is the phase difference between the two superconductor layers, a transition from the 0 to \(\pi\) states implies a change in sign of \(I_C\) from positive to negative. Physically, such a change in sign of \(I_C\) is a consequence of a phase change in the pairing wave-function induced in the FM layer due to the proximity effect. Josephson junctions presenting a negative \(I_C\) are usually called \(\pi\) junctions and such behavior has been observed experimentally.

Recently, quiet qubits consisting of a superconducting loop with a S-FM-S \(\pi\) junction have been theoretically proposed [5,6]. In the quiet qubits, a quantum two level system (qubits) is spontaneously generated and therefore it is expected to be robust to the decoherence by the fluctuation of the external magnetic field. From the viewpoint of the quantum dissipation, however, the structure of S-FM-S junctions is inherently identical with S-N-S junctions (N is a normal nonmagnetic metal). Therefore a gapless quasiparticle excitation in the FM layer is

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Preprint submitted to Elsevier Science
inevitable. This feature gives a strong Ohmic dissipation [7] and the coherence time of S-FM-S quiet qubits is bound to be very short.

On the other hand, as was predicted by Tanaka and Kashiwaya [8], the π junction can be formed in Josephson junctions with ferromagnetic insulators (FI). By following their theory, we have theoretically proposed a superconductor phase- [9] and flux-type qubits [10–12] based on S-FI-S π junctions. Moreover, we have showed that the effect of the dissipation due to the quasi-particle excitation on macroscopic quantum tunneling is negligibly small [11]. However, in above studies, we have used a very simple δ-function model as the FI barrier. Therefore, the correspondence between this toy mode and the actual band structure of FI is still unclear. In this paper, we will formulate a numerical calculation method for the Josephson current through FI by taking into account the band structure of FI. Then we will discuss the possibility of the formation of the π-coupling for the Josephson junction through the Eu chalcogenides.

2. Spin-filter effect in Eu-chalcogenides

Recently spin filtering effect are intensively studied by use of the the Eu chalcogenides [13–15]. The Eu chalcogenides stand out among the FIs as ideal Heisenberg ferromagnets, with a high magnetic moment and a large exchange splitting of the conduction band for Eu d-electrons. Utilizing the exchange splitting ($V_{ex}^d$) to filter spins, these materials produce a near-fully spin-polarized current when used as a tunnel barrier. Of the Eu chalcogenides, EuO has the largest $V_{ex}^d$ and the highest Curie temperature ($T_{Curie} \sim 69$ K for bulk).

In EuO, the large saturation magnetic moment $\mu g J = 7 \mu_B$ per Eu$^{2+}$ originates from the seven unpaired electrons localized at the 4f levels in the energy gap between the valence band and the conduction band, shown schematically in Fig. 1. Ferromagnetic order of the 4f spins causes exchange splitting of the conduction band, lowering (raising) the spin-up (down) band symmetrically by $V_{ex}^d/2$. Thus, free carriers in the conduction d band are spin-polarized. A large exchange splitting of 0.54 eV was first determined by measuring the redshift of the absorption edge in single crystals of EuO cooled below $T_{Curie}$ [16].

When an ultrathin film of EuO is used as the tunnel barrier between two metallic electrodes, the exchange splitting of the conduction band gives rise to a lower barrier height for spin-up electrons and a higher barrier height for spin-down electrons. Because of the tunnel current depends exponentially on the barrier height [13,14], the tunneling probability for spin-up electrons is much greater than for spin-down electrons, leading to a highly spin-polarized current. This phenomenon is called the spin-filter effect.

3. Numerical calculation of Josephson current

In this section, we develop a numerical calculation method of the Josephson current for S-FI-S junctions [17,18]. Let us consider the two-dimensional two-band tight-binding model for a S-FI-S junction as shown in Fig. 1. The vector $r = jx + my$ points to a lattice site, where $x$ and $y$ are unit vectors in the $x$ and $y$ directions, respectively. In the $y$ direction, we apply the periodic boundary condition for the number of lattice sites being $W$.

Electronic states in superconductor are described by the mean-field Hamiltonian

$$H_{BCS} = \frac{1}{2} \sum_{r,r'} \left[ \hat{c}^\dagger_r \hat{h}_{r,r'} \hat{c}_{r'} - \hat{c}^\dagger_r \hat{h}^*_{r,r'} \hat{c}_{r'} \right] + \frac{1}{2} \sum_{r \in S} \left[ \hat{c}^\dagger_r \hat{\Delta} \hat{c}_{r} - \hat{c}^\dagger_r \hat{\Delta}^* \hat{c}_{r} \right],$$

$$\hat{h}_{r,r'} = [-t \delta_{|r-r'|,1} + (-\mu + 4t) \delta_{r,r'}] \hat{\sigma}_0,$$
magnetic properties of the Eu chalcogenides. So we
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splitting of
with $\tilde{c}_r = (c_{r,\uparrow}, c_{r,\downarrow})$, where $c_{r,\sigma}^\dagger$ is the
creation (annihilation) operator of an electron at $r$ with
spin $\sigma = (\uparrow \text{ or } \downarrow)$, $\tilde{c}$ means the transpose of $\tilde{c}$, and
$\delta_0$ is $2 \times 2$ unit matrix. In superconductors, the
hopping integral $t$ is considered among nearest neighbor
sites and we choose $\Delta = i\Delta \delta_2$, where $\Delta$ is the
amplitude of the pair potential in the $s$-wave symmetry
channel, and $\delta_2$ is a Pauli matrix.

In a ferromagnetic insulator, we have used a following
two-band Hamiltonian:

$$H_{\text{FI}} = H_d + H_f + H_{df},$$

$$H_d = -t_d \sum_{r,r',\sigma} d_{r,\sigma}^\dagger d_{r',\sigma} - \sum_{r} (4t_d - \mu_d)d_{r,\uparrow}^\dagger d_{r,\uparrow}$$

$$- \sum_{r} (4t_d - \mu_d + V_{\text{ex}}^d)d_{r,\uparrow}^\dagger d_{r,\downarrow},$$

$$H_f = -t_f \sum_{r,r',\sigma} f_{r,\sigma}^\dagger f_{r',\sigma} - \sum_{r} (4t_f - \mu_f)f_{r,\uparrow}^\dagger f_{r,\uparrow}$$

$$- \sum_{r} (4t_f - \mu_f + V_{\text{ex}}^f)f_{r,\uparrow}^\dagger f_{r,\downarrow},$$

$$H_{df} = V_{df} \sum_{r,\sigma} (d_{r,\sigma}^\dagger f_{r,\sigma} + f_{r,\sigma}^\dagger d_{r,\sigma}),$$

where $d_{r,\sigma}^\dagger$ ($f_{r,\sigma}^\dagger$) is the creation operator, $t_d$ ($t_f$) is the
hopping integral and $V_{\text{ex}}^d$ ($V_{\text{ex}}^f$) is the exchange
splitting of $d$ ($f$) electrons. The Fermi energy of $d$
and $f$ bands are, respectively, given by $\mu_d = -g_d$
and $\mu_f = 8t_f + g_f$, where $g_d$ ($g_f$) is the energy gap
of the $d$ ($f$) band (see Fig.1). The third term $H_{df}$
of the Hamiltonian describes the mixing between
$d$ and $f$ bands. It was recognized for a long
time that the $d$-$f$ mixing is very important to understand
magnetic properties of the Eu chalcogenides. So we
have taken into account the $d$-$f$ mixing term in the
Hamiltonian.

The Hamiltonian is diagonalized by the Bogoliubov
transformation and the Bogoliubov-de Gennes
(BdG) equation is numerically solved by the recursive
Green function method [19]. We calculate the
Matsubara Green function,

$$\tilde{G}_{\omega_n}(r, r') = \left( \begin{array}{cc} \hat{g}_{\omega_n}(r, r') & \hat{f}_{\omega_n}(r, r') \\ -\hat{f}_{\omega_n}(r, r') & -\hat{g}_{\omega_n}(r, r') \end{array} \right),$$

where $\omega_n = (2n + 1)\pi T$ is the Matsubara frequency,
$n$ is an integer number, and $T$ is a temperature. The
Josephson current is given by

$$I_J(\phi) = -ie\ell T \sum_{\omega_n} \sum_{m=1}^W \text{Tr} \left[ \tilde{G}_{\omega_n}(r, r) - \tilde{G}_{\omega_n}(r, r') \right]$$

with $r' = r + \mathbf{z}$. Throughout this paper we fix the
following parameters: $W = 25$, $\mu = 2t$, $\Delta_0 = 0.01t$,
and $T = 0.01T_c$ ($T_c$ is the superconductor transition
temperature).

4. Josephson current through Eu-chalcogenides

Below, we consider the Josephson transport
through the Eu-chalcogenides. In calculation, we
use the following parameters in consideration of
EuO [20,21]: $t_d = 1.25eV$, $g = g_d + g_f = 1.12eV$,
$t_f = 0.125eV$, and $V_{\text{ex}}^d = 0.528eV$.

We first discuss the Josephson current through the
spin-filtering barrier only [Fig. 3(a)], i.e., the $d$-
band. The phase diagram depending on the strength
of $V_{\text{ex}}^d$ ($0 \leq V_{\text{ex}}^d/t_d \leq 6$) and the thickness of FL $L_F$
is plotted in Fig. 3(b). In this case, the $\pi$ junction is not
formed irrespective of $L_F$, and $V_{\text{ex}}$. Therefore, only
the spin-filter effect dose not lead to the $\pi$-junction
behaviors.

Next we consider the Josephson transport
through the Eu-chalcogenides with both $d$ and
$f$-bands. In calculation we set $L_F = 5$ and systematically change the values of the exchange splitting
of $f$ electron $V_{\text{ex}}^f$ ($= 0.0 \sim 10.0eV$) and the $d$-$f$
hybridization $V_{df}$ ($= -1.25 \sim 1.25 eV$). Fig. 4 shows
the numerically obtained $0 - \pi$ phase diagram. The
$\pi$ junction can be realized at the certain values of
$V_{df}$ and $V_{\text{ex}}^f$. We found that the $\pi$ junction can be
formed if (1) $d$ and $f$ bands are overlapped each other
and (2) the $d$-$f$ hybridization $V_{df}$ is strong enough.
More detailed discussion for above results
will be given in elsewhere [17].
Fig. 3. (a) The density of states for each spin direction for the spin-filtering barrier (5d band of Eu). (b) The phase diagram depending on the strength of $V_{\text{ex}}$ and $L_F$ for the spin-filtering barrier. In this case, no $\pi$ junction is formed.

Fig. 4. The phase diagram depending on the $d-f$ hybridization $V_{df}$ and the exchange splitting of the $f$ band $V_{\text{ex}}^{\text{f}}$ for the S/Eu-chalcogenides/S Josephson junctions. The black and white regime correspond to the $\pi$ and 0 junction, respectively.

5. Summary

To summarize, we have studied the Josephson effect in S/Eu-chalcogenides/S junction by use of the recursive Green's function method. The $\pi$ junction behavior is realized if the $d$ and $f$ bands are overlapped and the $d-f$ hybridization is strong. Such Eu-chalcogenides based $\pi$ junctions may becomes a element in the architecture of "quiet qubit".

Acknowledgements

This work was supported by CREST-JST and a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture of Japan (Grant No. 19710085).

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