Collective Spin Modes in Superconducting Double Layers

Christian Helm, Franz Forsthofer, and Joachim Keller
Institute for Theoretical Physics, University of Regensburg,
D-93040 Regensburg, Germany

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Abstract

We investigate a double layer system with tight-binding hopping, intra-layer and inter-layer interactions, as well as a Josephson like coupling. We find that an antiferromagnetic spin polarization induces additional spin-triplet pairing (with $S_z = 0$) to the singlet order parameter. This causes an undamped collective mode in the superconducting state below the particle-hole threshold, which is interpreted as a Goldstone excitation.

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1 INTRODUCTION AND MODEL

Collective density fluctuations in superconductors due to the breakdown of the global gauge invariance are well known theoretically. However, since these modes couple to charge oscillations, the long range Coulomb force usually pushes up their energies to the plasma frequency. One possibility to avoid the Coulomb interaction completely, is to consider spin fluctuations instead of charge fluctuations between the layers. In the following we will show the existence of such a sharp, collective spin mode in the gap, which might have been observed in inelastic neutron scattering on Y-Ba-Cu-O.

We consider an electronic double-layer system described by the Hamiltonian $H = H_0 + H_S$:

$$H_0 = \sum_{k\sigma} \epsilon_k (c_{1k\sigma}^{\dagger} c_{1k\sigma} + c_{2k\sigma}^{\dagger} c_{2k\sigma}) + t_k (c_{2k\sigma}^{\dagger} c_{1k\sigma} + c_{1k\sigma}^{\dagger} c_{2k\sigma})$$

(1)
Here $t_k$ describes a tight-binding coupling between the two layers $i = (1, 2), j = 3 - i$, while $V∥ (V⊥)$ are intra-(inter)-layer pairing interactions and the Josephson-like coupling $J$ describes the coherent transfer of two particles from one layer to the other. In a previous publication [2] we treated this model using the Nambu formalism including vertex corrections to calculate charge fluctuations between the layers.

In this paper we are primarily interested in the calculation of correlation functions involving the operator

$$S = \sum_k c_{2k\uparrow}^\dagger c_{2k\downarrow} - c_{2k\downarrow}^\dagger c_{2k\uparrow} - c_{1k\uparrow}^\dagger c_{1k\downarrow} + c_{1k\downarrow}^\dagger c_{1k\uparrow}. \quad (3)$$

describing the difference of the spin polarization in the two layers and the operators coupling to it ($\Delta_{ij} := c_{ik\uparrow}^\dagger c_{j\downarrow} - c_{j\downarrow}^\dagger c_{ik\uparrow}$)

$$\Phi_T = -i \sum_k \Delta_{21}^\dagger - \Delta_{12}^\dagger - \Delta_{21} + \Delta_{12},$$

$$M = -i \sum_k c_{2k\uparrow}^\dagger c_{1k\downarrow} - c_{1k^\uparrow}^\dagger c_{2k\downarrow} - c_{2k\downarrow}^\dagger c_{1k\uparrow} + c_{1k\uparrow}^\dagger c_{2k\downarrow}. \quad (4)$$

The quantity $M$ corresponds to the spin current between the two layers. $\Phi_T$ and $A_T$ describe pairing in different layers in a spin-triplet state with total spin $S_z = 0$ and are the real and imaginary part of the inter-layer triplet-pairing amplitude $\Delta_{ij} := \Delta_{12} - \Delta_{21}$. To shorten the notation, we introduce

$$P^{ij} := \sum_k \Psi_k^\dagger D^{ij} \Psi_k, \quad D^{ij} := \sigma_i \otimes \tau_j, \quad \Psi_k := (c_{1k\uparrow}, c_{1k\downarrow}^\dagger, c_{2k\uparrow}, c_{2k\downarrow}^\dagger)^t. \quad (5)$$

$\tau_i$ ($\sigma_i$) being the Pauli matrices in the Nambu or two-layer space, respectively (examples: $S = -P^{30}, A_T = -P^{22}, \Phi_T = -P^{21}$).

2 ANALYTICAL RESULTS AND GOLDSTONE MODES

In general the correlation functions $\ll P^{ij}, P^{lm} \gg$ have to be determined numerically. However, for constant hopping $t_k = t$ with $t, \omega \ll \Delta$ ($\Delta$ is
the superconducting s-wave gap) and weak coupling the collective modes can be calculated analytically (for \( \omega_S, \omega_0 \ll \Delta \)) in the cases i (ii) of pure intra-(inter)-layer pairing.

We obtain for case (i) case (ii)

\[
\begin{align*}
\ll S, S \gg & \approx 4N_0 \frac{(2t)^2}{\omega_S^2 - \omega^2} \quad 4N_0 \frac{\omega^2_S}{\omega^2 - \omega_S^2}, \\
\ll \Phi_T, S \gg & = 0 \quad 4iN_0 \frac{\omega^2_S}{\omega^2 - \omega_S^2} \frac{\omega}{2\Delta} \frac{V_\perp - J}{2J}, \\
\ll A_T, S \gg & \approx 4N_0 \frac{\omega^2_S}{\omega^2 - \omega_S^2} \frac{t}{2t\omega} \frac{V_\perp + V_\perp + 2J}{V_\perp - J} \quad 0, \\
\ll M, S \gg & \approx -4iN_0 \frac{\omega^2_S}{\omega^2 - \omega_S^2} \frac{2t\omega}{2{t\omega}} \quad -4iN_0 \frac{2t\omega}{\omega^2 - \omega_S^2}, \\
\omega_S^2 & = (2t)^2 + \omega^2_0 \quad (2t)^2 + \omega^2_0, \\
\omega^2_0 & = \frac{-(V_\parallel - V_\perp + 2J)}{(V_\perp - J)(V_\parallel + J)} \frac{(2\Delta)^2}{N_0} \quad \frac{-2J}{(2\Delta)^2} \frac{V_\perp - J^2}{N_0}.
\end{align*}
\]

(6)

A spin polarization \( S \) with opposite sign in the two layers obviously induces inter-layer triplet-amplitudes \( A_T (\Phi_T) \).

These results are closely connected to the collective modes discovered in density-density-correlation functions like \( \ll P, P \gg \) in our previous work. For pure inter-(intra)-layer pairing one has the exact relation

\[
\ll P, P \gg_{\text{inter(intra)}} = \ll S, S \gg_{\text{inter(intra)}},
\]

(7)

which follows from a unitary change of representation \( \tilde{A} = UAU^\dagger, | \tilde{\psi} \rangle = U | \psi \rangle \) with \( U := \exp(-i\pi \sum_k (c_{1k\parallel}^\dagger c_{2k\parallel}^\dagger + c_{2k\parallel}c_{1k\parallel}^\dagger)) \).

The Goldstone theorem predicts the existence of excitations with vanishing energy, if a continuous, dynamical symmetry \( \Omega ([\Omega, H] = 0) \) is spontaneously broken, e.g. the groundstate \( | 0 \rangle \) is not an eigenstate of \( \Omega \). Thereby it can help to classify the resonances found in the correlation functions as so-called Goldstone modes connected with certain symmetries of \( H \).

Assuming pure singlet pairing in equilibrium, the superconducting ground-state is given by

\[
| \theta_\parallel, \theta_\perp \rangle = \prod_k \left( 1 + \alpha_k | e^{2\theta_\parallel} \Delta_{k,\parallel}^\dagger + \alpha_k e^{2\theta_\perp} \Delta_{k,\perp}^\dagger \Delta_{k,\parallel}^\dagger + \Delta_{k,\parallel} \right) | 0 \rangle
\]

(8)
Table 1: Broken symmetries if $\alpha_\parallel \neq 0$ or $\alpha_\perp \neq 0$.

| case | parameters | $\alpha_\parallel \neq 0$ | $\alpha_\perp \neq 0$ |
|------|-------------|---------------------------|---------------------------|
| 1    | $t, J, V_\parallel - V_\perp = 0$ | $\Omega_{03}, \Omega_{33}, \Omega_{13}, \Omega_{21}$ | $\Omega_{03}, \Omega_{13}, \Omega_{30}, \Omega_{20}$ |
| 2    | $t, J \neq 0, V_\parallel = V_\perp$ | $\Omega_{03}, \Omega_{13}$ | $\Omega_{03}, \Omega_{13}$ |
| 3    | $t, J \rightarrow 0, V_\parallel \neq V_\perp$ | $\Omega_{03}, \Omega_{33}$ | $\Omega_{03}, \Omega_{30}$ |
| 4    | $t, J, V_\parallel - V_\perp \neq 0$ | $\Omega_{03}$ | $\Omega_{03}$ |

with $\Delta_{\parallel, S} := \Delta_{11} + \Delta_{22}$ and $\Delta_{\perp, S} := \Delta_{12} + \Delta_{21}$ being the singlet-order parameters for intra- and inter-layer pairing, respectively. The analytical calculations of case i (ii) refer to pure intra-(inter-)layer pairing with $\alpha_\perp = 0$ ($\alpha_\parallel = 0$).

Table 1 shows (for different parameters $t, J, V_\parallel, V_\perp$) the symmetries $\Omega_{ij}(\phi) := \exp(i\phi P^j)$, which are broken in the presence of intra-(inter)-layer pairing $\alpha_\parallel \neq 0$ ($\alpha_\perp \neq 0$). The spontaneous breakdown $\Omega_{03} | \theta_\parallel, \theta_\perp \rangle = | \theta_\parallel + \phi, \theta_\perp + \phi \rangle$ of the global gauge symmetry, which is generated by the total particle number, in $| \theta_\parallel, \theta_\perp \rangle$ is a defining property of the superconducting phase (case 4), as it is invariably connected with non-vanishing Cooper-pair amplitudes ($\langle \Delta_{ij} \rangle \neq 0$).

In Eq. 6 Goldstone modes ($\omega_S = 0$) appear in case i (ii), if and only if $t, J, V_\parallel - V_\perp = 0$ ($t, J = 0$). We can identify these resonances in case i (ii) with the modes in table 1 in the cases 1 (3), which are connected with the symmetries $\Omega_{23}$ ($\Omega_{30}$). The transformations

$$\Omega_{23}(\phi) | \theta_\parallel, \theta_\perp \rangle = \prod_k \left(1+\alpha_\parallel e^{i2\phi} \cos(2\phi) \Delta^\dagger_{\parallel, S} + \alpha_\perp e^{i2\phi} (\Delta^\dagger_{\perp, S} - \sin(2\phi) \Delta^\dagger_{\perp, T}) \right) | 0 \rangle,$$

$$\Omega_{30}(\phi) | \theta_\parallel, \theta_\perp \rangle = \prod_k \left(1+\alpha_\parallel e^{i2\phi} \Delta^\dagger_{\parallel, S} + \alpha_\perp e^{i2\phi} (\cos(2\phi) \Delta^\dagger_{\perp, S} - i \sin(2\phi) \Delta^\dagger_{\perp, T}) \right) | 0 \rangle$$

show that in both cases the $S_z=0$-component $\Delta_{\perp, T}$ of the triplet-order parameter is excited, which for $\Omega_{23}$ ($\Omega_{30}$) also creates non-vanishing expectation values $\langle A_T \rangle$ ($\langle \Phi_T \rangle$) and finite responses $\ll A_T, S \gg$ ($\ll \Phi_T, S \gg$) to an external spin polarization $S$. Thereby $\Omega_{23}$ mixes intra-layer pairs $\langle \Delta_{\parallel, S} \rangle$ with triplet-inter-layer pairs $\langle \Delta_{\perp, T} \rangle$, which is connected with a spin transfer between the layers without breaking up Cooper pairs. On the other hand, $\Omega_{30}$ leaves the modulus of the pairing amplitudes invariant, but creates a phase difference between $\Delta_{12}$ and $\Delta_{21}$, which is the origin of a supercurrent of inter-layer pairs, the so-called spin Josephson-effect. This terminology
is motivated by the close analogy to the usual Josephson effect, where a charge rather than a spin transfer is driven by a phase difference of intra-rather than inter-layer pairs. The density-modes $\Omega_{20}$ ($\Omega_{33}$), which correspond according to the relation (7) to the spin modes $\Omega_{23}$ ($\Omega_{30}$), can be observed as poles in $\langle P, P \rangle$ calculated in our previous work [2] rather than in $\langle S, S \rangle$. According to Eq. 6 all these modes cannot be excited in the absence of particle transfer ($t, J = 0$) between the layers. Finally, $\Omega_{13}$ connects groundstates with different ratios of inter- and intra-layer-pairing, which for $t, J = 0$ in case 1 and 2 are energetically degenerate.

3 NUMERICAL RESULTS

We carried out numerical calculations for $\langle S, S \rangle$ using two slightly different effective masses $2m_1/\hbar^2 = 1$ eV$^{-1}A^{-2}$, $2m_2/\hbar^2 = 1.2$ eV$^{-1}A^{-2}$ for the two bands $\epsilon_k \pm t_k = \hbar^2k^2/2m_{2/1}$ and parameters: $\mu = 0.3$ eV, $\omega_c = 0.25$ eV (cut-off in k-space), $(V_\parallel + V_\perp + 2J)N_0 = -0.44$, $(V_\parallel - V_\perp)N_0 = \pm 0.2$ ($N_0$: averaged density of states of the two bands). Then the pairing is mixed and for $(V_\parallel - V_\perp)N_0 < 0$ ($> 0$) dominated by intra-(inter)-layer pairing.

Figure 1: $\mathrm{Im} \langle S, S \rangle$ at $T = 0$ in the case of dominant inter-layer (a) and intra-layer (b) pairing for different $J$. The spectral weight of the collective mode is given by the height of the $\delta$-peak times 10 in (a) or times 100 for peaks marked with arrows and in (b).

Fig. 1 shows the imaginary part of the spin-polarization function for different $J$ in the case a (b) of dominant inter-(intra)-layer pairing at $T = 0$. 

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The collective modes appear as \( \delta \)-peaks below the onset of particle hole excitations around 60 meV. In the appropriate parameter range the resonances in case a (b) coincide with the poles calculated analytically in Eq. [3] in case ii (i), but they exist in a much larger parameter range. For larger positive or negative \( J \)-values than given in the figures the mode frequencies pass zero indicating an instability of the system.

The spectral weight of the phase mode decreases for dominant inter-layer pairing going from negative to positive \( J \) as indicated by the spectral weight \( \omega^2_S \) in the approximation formula (6).

For positive \( J \) a further collective mode, the so-called amplitude mode, can be seen in both cases. It is inside the particle-hole spectrum for small \( J \), but undamped for large \( J \) (arrows (a) or small peaks below the particle-hole threshold (b)). Because of the mixing of intra-layer and inter-layer pairing the spin excitation couples to both the phase \( \Phi_T \) and the amplitude \( A_T \) of the triplet order-parameter. This causes two collective modes, which were already discussed in [2].

\[ \text{Figure 2: } \text{Im} \ll S, S \gg \text{ for different temperatures in the case of dominant inter-layer pairing for constant } N_0 J = 0.01 \text{ or constant } N_0 J = -0.3. \]

The temperature dependence of the spin polarization function in Fig. 2 shows the broadening of the collective mode at about 50 meV with increasing \( T \). In case b a further collective mode appears at \( T_c \).

To conclude, the anti-ferromagnetic spin polarization couples to the phase and amplitude of the triplet-order parameter with \( S_z = 0 \). This causes a collective mode where spin-up and spin-down particle tunnel in opposite direction (\textit{spin Josephson-effect}). This might be connected with a
resonance found in magnetic neutron scattering on Y-Ba-Cu-O at finite $q$, which shows the same temperature dependence as our mode[4].

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