Realization of Berezinskii’s superconductivity in quasi-one-dimensional systems

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We revisit the pairing symmetry competition in quasi-one-dimensional systems. We show that spin-triplet \(s\)-wave pairing, where the pair is formed by electrons with different times and has an odd-frequency symmetry, can be realized in systems with strong one-dimensionality when the strength of charge fluctuation dominates over spin fluctuation. The present study provides a novel microscopic mechanism for this exotic pairing originally proposed by Berezinskii in 1974.

Superconductivity in strongly correlated systems has been a long standing issue in condensed matter physics. To avoid the strong on-site Coulomb repulsion, a Cooper pair tends to be formed by two electrons located in separate places with the non-zero angular momentum \(L\). Spin-singlet \(d\)-wave (\(L = 2\)) \textsuperscript{1} and spin-triplet \(p\)-wave (\(L = 1\)) \textsuperscript{2} pairings belong to this class. On the other hand, two electrons located in separate times are also able to avoid the Coulomb repulsion in forming a Cooper pair. There is a possibility that a sign of the pairing function changes in exchanging times of two electrons. Then the Fourier transformed pairing function is an odd function of frequency. This type of pairing is called odd-frequency (odd-\(\omega\)) one originally proposed by Berezinski\textsuperscript{8}.

Berezinski\textsuperscript{8} proposed odd-\(\omega\) spin-triplet \(s\)-wave pairing (Berezinski\textsuperscript{8}’s pairing) in a bulk system. However, realization of such a pairing has been believed to be difficult in bulk systems due to the presence of gapless excitation. Bergeret \textit{et al.} revived this exotic pairing in the context of ferromagnet / superconductor (F/S) issues \textsuperscript{4}. They have proposed that Berezinskii’s pairing can be induced locally in ferromagnet although the bulk pairing symmetry in superconductor is spin-singlet \(s\)-wave. Stimulated by this proposal there have been several works about this pairing in F/S junctions \textsuperscript{5,6}. Besides ferromagnet junctions, Berezinski\textsuperscript{8}’s pairing has been predicted in diffusive normal metal attached to spin-triplet \(p\)-wave superconductor \textsuperscript{7}. It is a really interesting issue to resolve whether Berezinskii’s pairing is possible in bulk superconductor or not.

Strictly speaking, there are two classes of odd-\(\omega\) superconductors, \textit{i.e.}, spin-singlet and spin-triplet ones. Odd-\(\omega\) spin-singlet superconductor \textsuperscript{8} has an odd-parity in accordance with Fermi-Dirac statistics. Thus the resulting superconducting state is fragile against impurity scattering similar to spin-singlet \(d\)-wave and spin-triplet \(p\)-wave pairing ones. Furthermore, temperature dependence of Knight shift below transition temperature \(T_{C}\) becomes similar to that of spin-singlet \(d\)-wave superconductor. On the other hand, odd-\(\omega\) spin-triplet \(s\)-wave superconductor, the original proposal by Berezinskii, can have a clear difference from preexisting pairings, since it has an unchanged Knight shift below \(T_{C}\) even in the presence of impurity scattering. Thus, in order to discover odd-\(\omega\) superconductors experimentally, study on the mechanism of Berezinski\textsuperscript{8}’s pairing is highly desired. Although there have been several studies on the generation of odd-\(\omega\) pairing up to now \textsuperscript{8,10}, there has not been clear microscopic mechanism which supports the realization of Berezinski\textsuperscript{8} pairing. The aim of the present paper is to present a clear microscopic mechanism for realizing this exotic pairing.

To resolve this issue, we focus on quasi-one-dimensional (Q1D) systems. Up to now, superconductivity in Q1D systems has been studied in the context of, \textit{e.g.}, an organic superconductor (TMTSF)\textsubscript{2}X. It has been shown that spin-triplet \(f\)-wave pairing (\(L = 3\)) can dominate over spin-singlet \(d\)-wave (\(L = 2\)) one \textsuperscript{11} when charge fluctuation dominates over spin fluctuation \textsuperscript{12-14} as we shall discuss below. In real space, these correspond to Cooper pairs formed between separate places. However, when the system becomes strongly Q1D, it is difficult to form Cooper pairs with separate places due to the geometrical constraint, so actually there is a chance that even- and odd-\(\omega\) pairings compete. In the present paper, combining this “odd-\(\omega\) > even-\(\omega\)” situation with the “triplet > singlet” effect, we show that spin-triplet \(s\)-wave (\(L = 0\)) pairing, namely, the original Berezinski\textsuperscript{8}’s pairing, can be realized in a strongly Q1D system with strong charge fluctuation. This is actually exemplified by solving the linearized Eliashberg’s equation in the Q1D extended Hubbard model. The present study provides a novel and realistic mechanism for realizing this exotic pairing proposed more than thirty years ago.

Before going into the actual model and the calculation results, we make a general argument for the pairing symmetry in a Q1D system. We assume a many body system on a Q1D lattice, where the hopping integral in the \(y\) direction \(t_{y}\) is smaller than that in the \(x\) direction \(t_{x}\). The on-site Coulomb repulsion enhances spin fluctuation at the nesting vector \(Q\). In addition, we assume a situation where the off-site Coulomb repulsion enhances charge fluctuation at \(Q\). When the pairing interaction is mainly mediated by spin and charge fluctuations at
the effective pairing interactions for spin-singlet and spin-triplet channels can be given by

\[ V_{\text{eff}}^s(i\nu_m, Q) = \frac{3}{2} V_{sp}(i\nu_m, Q) - \frac{1}{2} V_{ch}(i\nu_m, Q) \]
\[ V_{\text{eff}}^t(i\nu_m, Q) = -\frac{1}{2} V_{sp}(i\nu_m, Q) - \frac{1}{2} V_{ch}(i\nu_m, Q), \]

respectively, where \( V_{sp} \) and \( V_{ch} \) are contributions from spin and charge fluctuations, respectively. \( \nu_m = 2m\pi T \) is the bosonic Matsubara frequency with an integer \( m \) at the temperature \( T \). In strongly correlated systems, the effective pairing interaction at \( \nu_m = 0 \) tends to give a large contribution to pairing. When the off-site Coulomb repulsion is absent or small, spin-singlet pairing is favored (\( |V_{\text{eff}}^s| > |V_{\text{eff}}^t| \)) due to the prominence of spin fluctuation. We call this “SF > CF case”. On the other hand, when the off-site Coulomb repulsion is so remarkable as to make charge fluctuation exceed spin fluctuation, spin-triplet pairing is favored (\( |V_{\text{eff}}^t| > |V_{\text{eff}}^s| \)). We call this “CF > SF case”. It is also noted that the effective pairing interaction for spin-singlet (spin-triplet) channel has a positive (negative) sign as far as the contribution by charge fluctuation does not become too large. Since the superconducting gap function \( \Delta \) has to satisfy a condition \( V_{\text{eff}}^s(Q)\Delta(k_F)\Delta(k_F + Q) < 0 \) on the Fermi surface, it is required for spin-singlet (spin-triplet) pairing to satisfy a condition \( \Delta(k_F)\Delta(k_F + Q) < 0 (\Delta(k_F)\Delta(k_F + Q) > 0) \) with \( k_F = (i\omega_n, k_F) \) and \( Q = (0, Q) \) consisting of the momentum on the Fermi surface \( k_F \) and the fermionic Matsubara frequency \( \omega_n = (2n - 1)\pi T \). In the following, we discuss all four classes of pairings in accordance with the Fermi-Dirac statistics. They are (i) even-\( \omega \) spin-singlet even-parity (ESE), (ii) even-\( \omega \) spin-triplet odd-parity (ETO), (iii) odd-\( \omega \) spin-singlet odd-parity (OSO), and (iv) odd-\( \omega \) spin-triplet even-parity (OTE) pairings. Berezinskii’s pairing belongs to class (iv). We consider four cases by combining strongly (weakly) Q1D lattice and SF > CF (CF > SF) case.

First, we discuss a weakly Q1D lattice. In this case, electrons avoid the strong Coulomb repulsion in real space. Anisotropic pairing with the non-zero angular momentum is induced and it has even-\( \omega \) symmetry. It is difficult for odd-\( \omega \) pairing to be stabilized due to the nature of pairing with separate times. In the SF > CF case, which favors spin-singlet pairing, ESE one has an advantage. This pairing has \( d \)-wave symmetry, where two nodes of \( \Delta \) run close to the Fermi surface as shown in Fig. 1(A). Reversely in the CF > SF case, which favors spin-triplet pairing, ETO one dominates. This pairing has \( f \)-wave symmetry, where two nodes of \( \Delta \) also run close to the Fermi surface as shown in Fig. 1(B) [15].

Next, we consider a strongly Q1D lattice. In this case, avoidance of electrons is limited in real space. This can induce pairing with separate times and make odd-\( \omega \) pairing comparable to even-\( \omega \) one. If we focus on the above leading pairings \( d \)- and \( f \)-wave, the gap nodes will run almost on the entire Fermi surface (see Fig. 1(A),(B)), which destabilizes those pairings. Odd-\( \omega \) symmetry allows pairing with lower angular momentum than that of even-\( \omega \) one, namely, the number of gap nodes in momentum space is smaller. As a result of the competition between gap nodes in momentum and frequency spaces (see the insets of Fig. 2), odd-\( \omega \) pairing can replace even-\( \omega \) one as leading one. In the SF > CF case, OSO pairing has an advantage. This pairing has \( p \)-wave symmetry, which has no nodes of \( \Delta \) on the Fermi surface in momentum space as shown in Fig. 1(C). Finally in the CF > SF case, spin-triplet pairing dominates over spin-singlet one, and the OTE pairing can take place. This is indeed the spin-triplet \( s \)-wave pairing originally proposed by Berezinskii. Here, note that the mechanism is entirely novel in that the odd-\( \omega \) pairing can replace even-\( \omega \) one as leading one. In the SF > CF case, OSO pairing has an advantage. This pairing has \( p \)-wave symmetry, which has no nodes of \( \Delta \) on the Fermi surface in momentum space as shown in Fig. 1(C). Finally in the CF > SF case, spin-triplet pairing dominates over spin-singlet one, and the OTE pairing can take place. This is indeed the spin-triplet \( s \)-wave pairing originally proposed by Berezinskii. Here, note that the mechanism is entirely novel in that the odd-\( \omega \) pairing can replace even-\( \omega \) one as leading one. In the SF > CF case, OSO pairing has an advantage. This pairing has \( p \)-wave symmetry, which has no nodes of \( \Delta \) on the Fermi surface in momentum space as shown in Fig. 1(C). Finally in the CF > SF case, spin-triplet pairing dominates over spin-singlet one, and the OTE pairing can take place.
for spin-singlet (spin-triplet) channel within the RPA this model, we solve the linearized Eliashberg’s equation respectively. We choose \( \sigma \) and \( t \) are the on-site and off-site Coulomb repulsions, respectively. \( V \) acts between electrons neighboring in the \( x \) direction. The momentum dependence is given by \( V(q) = 2V \cos q_x \) with the momentum \( q = (q_x, q_y) \). In this model, we solve the linearized Eliashberg’s equation for spin-singlet (spin-triplet) channel within the RPA

\[
\lambda \Delta(k) = -\frac{T}{N} \sum_{k'} V_{\text{eff}}(k - k')|G_0(k')|^2 \Delta(k'),
\]

where \( N \) is the number of sites and \( k \equiv (\omega_n, \mathbf{k}) \). \( G_0(k) = (\omega_n - \varepsilon_k + \mu)^{-1} \) is the bare Green’s function with the chemical potential \( \mu \). \( \lambda \) is the eigenvalue for \( \Delta \). \( \lambda \) becomes unity just at \( T_C \). The more stable the superconducting state is, the larger \( \lambda \) tends to be. We calculate \( \lambda \) and \( \Delta \) for ESE, ETO, OSO, and OTE symmetries. The effective pairing interactions for spin-singlet and spin-triplet channels within the RPA are given by

\[
V_{\text{eff}}(q) = U + V(q) + \frac{3}{2} U^2 \chi_{\text{sp}}(q)
- \frac{1}{2} \{U + 2V(q)\}^2 \chi_{\text{ch}}(q),
\]

\[
V_{\text{eff}}(q) = V(q) - \frac{1}{2} U^2 \chi_{\text{sp}}(q)
- \frac{1}{2} \{U + 2V(q)\}^2 \chi_{\text{ch}}(q),
\]

respectively, with \( q \equiv (iv_n, q) \). The spin and charge susceptibilities are given by

\[
\chi_{\text{sp}}(q) = \frac{\chi_0(q)}{1 - U \chi_0(q)}
\]

\[
\chi_{\text{ch}}(q) = \frac{\chi_0(q)}{1 + \{U + 2V(q)\} \chi_0(q)},
\]

respectively, with the irreducible susceptibility

\[
\chi_0(q) = -\frac{T}{N} \sum_k G_0(q + k) G_0(k).
\]

In the present paper, we normalize the gap function \( \sum_k |\Delta(k)|/N = 1 \). We take the number of sites \( N = N_x \times N_y = 256 \times 64 \). The number of electrons is unity per site (half-filled), which gives the nesting vector \( \mathbf{Q} = (\pi, \pi/2) \) both on weakly and strongly Q1D lattices. The fermionic and bosonic Matsubara frequency have values from \(-2N_\uparrow \pi T\) to \(2N_\uparrow \pi T\) and from \(-2N_\uparrow \pi T\) to \(2N_\uparrow \pi T\), respectively, with \( N_\uparrow = 2048 \).
In Fig. 3, $\Delta$ for four kinds of pairings are plotted against $T$ in the four cases. There are two insets in panels Fig. 3(A)-(D), where (k) $k_x$ and ($\omega$) $\omega_n$ dependences of $\Delta$ are plotted at $T = 0.05t_x$. In the inset (k), we choose $k_y = 0$ and $\omega_n = \pi T$. $k_F$ in the inset denotes the location of the Fermi surface at $k_y = 0$. In order to give clear comparison with inset ($\omega$), we plot only the $k_x \geq 0$ portion, while the $k_x < 0$ portion is given by $\Delta(k) = +(-)\Delta(-k)$ for even- (odd-) parity pairings. In the inset ($\omega$), we choose $k$ where $\Delta$ gets the largest value on $k_y = 0$.

First, we focus on a weakly Q1D lattice ($t_y = t_d = 0.35t_x$). In the SF > CF case ($U = 2t_x, V = 0$), ESE pairing is the most stable as shown in Fig. 3(A). This pairing has d-wave gap, whose $k_x \geq 0$ portion is shown in the inset (k) of Fig. 3(A). There is a node of $\Delta$ near $k_x = k_F$ in momentum space, while there are no nodes in Matsubara frequency space as shown in the inset ($\omega$) of Fig. 3(A). In the CF > SF case ($U = 1.995t_x, V = t_x$), ETO pairing is the most stable as shown in Fig. 3(B). This pairing has f-wave gap, whose $k_x \geq 0$ portion is shown in the inset (k) of Fig. 3(B) [10]. There is also a node of $\Delta$ near $k_x = k_F$ in momentum space, while there are no nodes in Matsubara frequency space as shown in the inset ($\omega$) of Fig. 3(B).

Next, we focus on a strongly Q1D lattice ($t_y = t_d = 0.1t_x$). In the SF > CF case ($U = 1.6t_x, V = 0$), OSO pairing is the most stable as shown in Fig. 3(C). This pairing has p-wave gap, whose $k_x \geq 0$ portion is shown in the inset (k) of Fig. 3(C) [10]. There are no nodes of $\Delta$ near $k_x = k_F$ in momentum space, and instead there is a node in Matsubara frequency space as shown in the inset ($\omega$) of Fig. 3(C). And finally for the CF > SF case ($U = 1.595t_x, V = 0.8t_x$), OTE pairing is indeed the most stable as shown in Fig. 3(D). This pairing has s-wave gap, whose $k_x \geq 0$ portion is shown in the inset (k) of Fig. 3(D). There are also no nodes of $\Delta$ near $k_x = k_F$ in momentum space, and instead there is a node in Matsubara frequency space as shown in the inset ($\omega$) of Fig. 3(D). It is remarkable that the realization of Berezinskii’s pairing has been verified based on a microscopic calculation. These four cases are summarized in Fig. 4.

To summarize, we have shown that odd-$\omega$ spin-triplet $s$-wave pairing originally proposed by Berezinskii can be realized in systems with strong one-dimensionality when the strength of charge fluctuation exceeds over that of spin fluctuation. Experimentally, it is interesting to look for this exotic pairing in Q1D materials where spin and charge fluctuations coexist. Moreover, we may expect applying magnetic field to enhance spin-triplet pairing (even when charge fluctuation is not so strong) [14], so combining this effect with the strong one-dimensionality may increase chances for realizing Berezinskii’s pairing in actual materials. Also, we hope anomalous properties specific to this pairing will be observed in Q1D systems [8, 10].

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