Theory of odd-frequency pairings on a quasi-one-dimensional lattice in the Hubbard model

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In order to clarify whether the odd-frequency superconductivity can be realized or not, we study a quasione-dimensional triangular lattice in the Hubbard model using the random-phase approximation and the fluctuation exchange approximation. We find that odd-frequency spin-singlet *p*-wave pairing can be stabilized on a quasi-one-dimensional isosceles triangular lattice.

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I. INTRODUCTION

It is known that two electrons form Cooper pairs with gap function $\Delta_{\sigma,\sigma_n}(i\varepsilon_n, k)$ in superconductors. In general, the gap function depends on the Matsubara frequency ε_n , the combination of spins σ_1 and σ_2 , and the momentum k. In accordance with the Fermi-Dirac statistics, the sign of the gap function is reversed by the exchange of two electrons: $\Delta_{\sigma_1\sigma_2}(i\varepsilon_n, \mathbf{k}) = -\Delta_{\sigma_2\sigma_1}(-i\varepsilon_n, -\mathbf{k})$. Based on the symmetrical properties combinations of three dependences, symmetries of the gap functions can be classified into four groups; (i) even parity in Matsubara frequency space (even frequency), spin singlet, and even parity in momentum space (even parity) labeled as ESE pairing state, (ii) even-frequency spin-triplet odd-parity (ETO) pairing state, (iii) odd-frequency spinsinglet odd-parity (OSO) pairing state, and (iv) oddfrequency spin-triplet even-parity (OTE) pairing state. Almost all of the superconductors including high- T_C cuprates belong to ESE pairing state. ETO pairing state is realized in some special superconductors such as Sr₂RuO₄ or UPt₃. In contrast to these even-frequency pairings, odd-frequency pairings are not familiar.

In 1974, the possibility of realizing the odd-frequency pairing state was first proposed by Berezinskii¹ in the context of ³He, where the odd-frequency spin-triplet hypothetical pairing was discussed. After that, Vojta and Dagotto² pointed the possible realization of odd-frequency spin-triplet *s* wave (OTE pairing state) on a triangular lattice in the Hubbard model. Recent detailed calculation by Yada³ has supported this result. Balatsky and Abrahams^{4,5} proposed an odd-frequency spin-singlet *p*-wave pairing (OSO pairing state). Odd-frequency pairing has been studied on the Kondo lattice model.^{6–8} There are some experimental reports,^{9,10} which are consistent with the realization of the odd-frequency spin-singlet *p*-wave superconducting state (OSO pairing state) in Ce compounds.^{9–11} These studies have addressed the realization of odd-frequency energy-gap function in bulk.

It has been clarified recently that odd-frequency pairing correlation, i.e., pair amplitude is generated in inhomogeneous system like superconducting junctions^{12–17} or vortex core.^{18,19} It has been pointed out that OTE pair amplitude is induced in ferromagnet/superconductor junctions^{20–26} and diffusive normal metal/spin-triplet odd-parity superconductor junctions.^{15,16}

Stimulated by these pre-existing works, it is very timely to study realization of odd-frequency energy-gap function in bulk system. In this paper, we focus on the superconductivity on a quasi-one-dimensional triangular lattice. In order to clarify the dominant pairing state there, we solve the linearized Eliashberg's equation in the Hubbard model using the random-phase approximation (RPA) and the fluctuation exchange (FLEX) approximation.^{27–29}

We clarify that odd-frequency spin-singlet p wave becomes dominant pairing on a quasi-one-dimensional triangular lattice. In particular, this pairing becomes prominent on an isosceles triangular lattice due to geometrical frustration where spin-singlet *d*-wave pairing is seriously suppressed.

II. MODEL AND FORMULATION

We start with a single-band Hubbard model on an anisotropic triangular lattice as shown in Fig. 1, where t_x , t_y , and t_2 are transfer integrals along x, y, and diagonal directions, respectively.

The Hamiltonian is given by

$$H = \sum_{\langle i,j \rangle,\sigma} (t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) + \sum_{i} U n_{i\uparrow} n_{i\downarrow}, \qquad (1)$$

where t_{ij} denotes the transfer integral between two sites *i* and *j*. $\langle i,j \rangle$ is the combination of nearest and second-nearest neighbors. $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) and $n_{i\sigma}=c_{i}^{\dagger}c_{i}$ are creation (annihilation) and number operators, respectively. *U* is the on-site Coulomb repulsion. The band dispersion is given by

$$\varepsilon_k = -2t_x \cos k_x - 2t_y \cos k_y - 2t_2 \cos(k_x + k_y).$$
(2)

In this study, the number of electrons per site is fixed to unity (half filling).



FIG. 1. A two-dimensional triangular lattice with transfer integrals t_x , t_y , and t_2 .

In this paper, we calculate the Green's function $G(i\varepsilon_n, k)$ in two different ways; using (i) the RPA and (ii) the FLEX approximation.

(i) In the RPA, the Green's function is given by $G(i\varepsilon_n, k) = (i\varepsilon_n - \varepsilon_k + \mu)^{-1}$, where ε_n is the Matsubara frequency of fermion given by $\varepsilon_n = (2n-1)\pi T$ with an integer *n* and μ is the chemical potential. Using the Green's function, the irreducible susceptibility is obtained as

$$\chi_0(i\omega_m, \boldsymbol{q}) = -\frac{T}{N} \sum_{n, \boldsymbol{k}} G(i\varepsilon_n, \boldsymbol{k}) G(i\varepsilon_n + i\omega_m, \boldsymbol{k} + \boldsymbol{q}), \quad (3)$$

where ω_m is the Matsubara frequency of boson given by $\omega_m = 2m\pi T$ with an integer *m* and *N* is the number of sites. The spin susceptibility is given by

$$\chi_s(i\omega_m, \boldsymbol{q}) = \frac{\chi_0(i\omega_m, \boldsymbol{q})}{1 - U\chi_0(i\omega_m, \boldsymbol{q})} \tag{4}$$

and the charge susceptibility is given by

$$\chi_c(i\omega_m, q) = \frac{\chi_0(i\omega_m, q)}{1 + U\chi_0(i\omega_m, q)}.$$
(5)

(ii) In the FLEX approximation, first the bare Green's function $G_0(i\varepsilon_n, \mathbf{k}) = (i\varepsilon_n - \varepsilon_k + \mu)^{-1}$ is calculated. By substituting it into the Green's function in Eq. (3), we obtain the irreducible susceptibility. The spin and charge susceptibilities are given by Eqs. (4) and (5), respectively. Using the susceptibilities, the effective interaction is given by

$$V_n(i\omega_m, \boldsymbol{q}) = \frac{3}{2} U^2 \chi_s(i\omega_m, \boldsymbol{q}) + \frac{1}{2} U^2 \chi_c(i\omega_m, \boldsymbol{q}) - U^2 \chi_0(i\omega_m, \boldsymbol{q}).$$
(6)

Then, we calculate the self-energy

$$\Sigma(i\varepsilon_n, \boldsymbol{k}) = \frac{T}{N} \sum_{m, \boldsymbol{q}} V_n(i\omega_m, \boldsymbol{q}) G(i\varepsilon_n - i\omega_m, \boldsymbol{k} - \boldsymbol{q}).$$
(7)

After using the Dyson equation

$$G^{-1}(i\varepsilon_n, \mathbf{k}) = G_0^{-1}(i\varepsilon_n, \mathbf{k}) - \Sigma(i\varepsilon_n, \mathbf{k})$$
(8)

we obtain the new Green's function. The self-consistent iterations are repeated until the sufficient convergence is attained. Thus, we obtain the Green's function in which the self-energy is taken into account.

Using the Green's function, the spin susceptibility, and the charge susceptibility obtained in the RPA or the FLEX approximation, we solve the linearized Eliashberg's equation. The effective pairing interactions for spin-singlet and spintriplet channel are given by

$$V_a^s(i\omega_m, \boldsymbol{q}) = U + \frac{3}{2}U^2\chi_s(i\omega_m, \boldsymbol{q}) - \frac{1}{2}U^2\chi_c(i\omega_m, \boldsymbol{q}), \quad (9)$$

$$V_a^t(i\omega_m, \boldsymbol{q}) = -\frac{1}{2}U^2\chi_s(i\omega_m, \boldsymbol{q}) - \frac{1}{2}U^2\chi_c(i\omega_m, \boldsymbol{q}), \quad (10)$$

respectively. By substituting them into the linearized Eliashberg's equation for spin-singlet (spin-triplet) channel



FIG. 2. (Color online) t_y dependence of λ for each pairing state, fixing $t_y = t_2$, obtained by the RPA with $S_t = 0.97$ and $T/t_x = 0.04$.

$$\lambda \Delta(i\varepsilon_n, \mathbf{k}) = -\frac{T}{N} \sum_{m, \mathbf{k}'} V_a^{s(t)}(i\varepsilon_n - i\varepsilon_m, \mathbf{k} - \mathbf{k}') G(i\varepsilon_m, \mathbf{k}') G(-i\varepsilon_m, -\mathbf{k}') \Delta(i\varepsilon_m, \mathbf{k}').$$
(11)

the gap function $\Delta(i\varepsilon_n, k)$ and eigenvalue λ are obtained. This gap function $\Delta(i\varepsilon_n, k)$ is an eigenfunction of linearized Eliashberg's equation. In other words, the magnitude of it is meaningless. Hereafter, a norm of the gap function $\Delta(i\varepsilon_n, k)$ is normalized $[\sum_{n,k} |\Delta(i\varepsilon_n, k)|^2 = 1]$. Superconducting transition temperature T_C corresponds to the temperature where λ reaches unity. Thus, we consider that the larger the value of λ becomes, the more stable the superconductivity becomes. In this paper, we take $N=N_x \times N_y=128 \times 64$ k-point meshes. The Matsubara frequencies ε_n and ω_m have values from $-(2N_c-1)\pi T$ to $(2N_c-1)\pi T$ and from $-2N_c\pi T$ to $2N_c\pi T$, respectively, with $N_c=2048$.

III. RESULT

First, we study superconducting state on a quasi-onedimensional triangular lattice based on the RPA. In our model, a quasi-one-dimensional triangular lattice is represented by choosing the values of t_y and t_2 much smaller than that of t_x . The quasi-one-dimensional direction is parallel to x axis.



FIG. 3. (Color online) Temperature dependence of λ for each pairing state by the RPA with $t_y/t_x=t_2/t_x=0.1$ and $U/t_x=1.6$.



FIG. 4. (Color online) Momentum dependences of the gap functions for (a) ESE and (b) OSO pairing state by the RPA with t_y/t_x = t_2/t_x =0.1, U/t_x =1.6 and T/t_x =0.06, where the dashed and solid lines and the arrows represent the nodes of the gaps, the Fermi surfaces, and nesting vectors $Q = (\pi, \pi/2)$, respectively.

In order to clarify how symmetry of gap function depends on the dimension of the lattice, we gradually change the lattice structure varying t_y and t_2 from a two-dimensional regular triangular one $(t_x = t_y)$ to a quasi-one-dimensional triangular one $(t_x > t_y)$. Here, we choose $t_y = t_2$ for simplicity. In this case, the lattice structure is an isosceles triangular one, in which spin frustration in the directions of t_y and t_2 exists. λ of each pairing state changes as shown in Fig. 2, where Stoner factor $(S_t = U\chi_0^{max})$ is fixed to 0.97 by tuning the value of U. Here, χ_0^{max} denotes the maximum value of χ_0 . We see that OSO pairing state is dominant on a quasi-onedimensional triangular lattice $(t_y/t_x \sim 0.1)$, while ESE pairing state is dominant in almost all of the region. Hereafter, we focus on OSO pairing state.

In order to study details of the OSO pairing state on a quasi-one-dimensional triangular lattice, we calculate the temperature dependence of λ for $t_y/t_x = t_2/t_x = 0.1$ and $U/t_x = 1.6$ with the value of T/t_x running from 0.05 to 0.20. As shown in Fig. 3, λ of OSO pairing state increases much above unity at low temperatures for $U/t_x = 1.6$, where the Stoner factor S_t becomes almost unity. The value of S_t reaches unity at $T/t_x \sim 0.05$. This means that the OSO pairing state can be realized near the spin-density wave (SDW) phase. As in the case of ESE pairing, OSO pairing is mediated by antiferromagnetic spin fluctuation²⁹ since the superconductivity appears near the SDW phase.

The momentum dependences of the gap functions for the ESE and the OSO pairing states on a quasi-one-dimensional





FIG. 6. (Color online) t_2 dependence of λ for each pairing state by the RPA with $t_y/t_x=0.3$, $S_t=0.995$ and $T/t_x=0.05$.

triangular lattice with fixed Matsubara frequency $i\varepsilon_n = i\pi T$ are shown in Figs. 4(a) and 4(b), respectively, where the dashed and solid lines and the arrows represent the nodes of the gaps, the Fermi surfaces, and nesting vectors Q $=(\pi, \pi/2)$, respectively. We find that the momentum dependences of the ESE and the OSO gap functions can be approximated by $\cos k_x$ (d wave) and $\sin k_x$ (p wave), respectively. Here, we denote d(p) wave since this gap function changes sign four (two) times on the Fermi surface.^{30,31} It is noted that this p wave has no nodes on the Fermi surface in the case of quasi-one-dimensional lattice $(t_v \leq 0.6)$. The shape of the Fermi surface becomes two lines with k_x $=\pm \pi/2$ in the absence of t_{y} and t_{z} . These two lines are bent into an S shape by introducing t_v and t_2 . It is noteworthy that these two "Fermi lines" are perfectly nested with a vector $Q = (\pi, \pi/2)$ at half filling with $t_y = t_2$. Because of this, the spin susceptibility $\chi_s(i\omega_m, q)$ at $q = (\pi, \pi/2)$ becomes strong as shown in Fig. 5.

It is known that on a two-dimensional triangular lattice, the antiferromagnetic fluctuation works equally in the directions of x and y axes. Therefore, in real space, neighboring two electrons in these directions with antiparallel spins make a Cooper pair. As a result, spin-singlet $d_{x^2-y^2}$ -wave (ESE) becomes dominant. On the other hand, the antiferromagnetic fluctuation along x axis becomes dominant on a quasi-one-



FIG. 7. (Color online) Matsubara frequency dependences of the gap function $\Delta_{OSO}(i\varepsilon_n, \mathbf{k})$ at $\mathbf{k} = (\pi/2, 0)$ and the effective pairing interaction $V_a^s(i\omega_m, \mathbf{Q})$ at $\mathbf{Q} = (\pi, \pi/2)$ for spin-singlet channel by the RPA with $t_y/t_x = t_2/t_x = 0.1$, $S_t = 0.95$, and $T/t_x = 0.05$.

dimensional triangular lattice. Then neighboring two electrons along x axis with antiparallel spins make a Cooper pair. As a result, spin-singlet d wave (ESE) and p_x wave (OSO) make pairs in x direction.

The gap function for ESE pairing state has nodes on the Fermi surfaces, while that for OSO pairing state has no nodes on the Fermi surfaces, which can be called full gap, in momentum space. This point is relevant to following fact that OSO pairing state dominates over ESE pairing state for sufficiently small magnitude of t_y and t_2 .

We also explore the lattice with $t_y \neq t_2$ to clarify that $t_y = t_2$ is an indispensable condition for the realization of OSO pairing state. We gradually change the value of t_2 , fixing $t_y/t_x=0.3$. The resulting λ of each pairing state changes as shown in Fig. 6. We see that OSO pairing state is relatively

enhanced compared to ESE pairing state especially in the case of $t_y = t_2$. This result is robust against changing value of t_y . The condition with $t_y = t_2$ corresponds to geometrical frustration, which suppresses the antiferromagnetic fluctuation in these directions.

In the following, we study OSO pairing state focusing on Matsubara frequency dependence. Matsubara frequency dependences of the gap function $\Delta_{OSO}(i\varepsilon_n, k)$ for OSO pairing state at $k = (\pi/2, 0)$ and the effective pairing interaction $V_a^s(i\omega_m, Q)$ with $Q = (\pi, \pi/2)$ for spin-singlet channel on a quasi-one-dimensional triangular lattice are shown in Fig. 7. Near the SDW phase, $V_a^s(i\omega_m, Q)$ has a sharp peak at ω_m =0 in Matsubara frequency space. After a simple transformation of the linearized Eliashberg's Eq. (11), we obtain following relation:

$$\lambda = -\frac{T}{N} \frac{\sum_{n,m,k,k'} V_a^{s(t)}(i\varepsilon_n - i\varepsilon_m, k - k') G(i\varepsilon_m, k') G(-i\varepsilon_m, -k') \Delta(i\varepsilon_m, k') \Delta(i\varepsilon_n, k)}{\sum_{n,k} |\Delta(i\varepsilon_n, k)|^2}.$$
(12)

In Eq. (12), $\sum_{n,k} |\Delta(i\varepsilon_n, k)|^2$, $G(i\varepsilon_m, k')G(-i\varepsilon_m, -k')$, and $V_a^s(i\varepsilon_n - i\varepsilon_m, k - k')$ are always positive. Then negative (positive) sign of $\Delta_{OSO}(i\varepsilon_m, k')\Delta_{OSO}(i\varepsilon_n, k)$ makes positive (negative) contribution to λ . Due to the sharp peak of $V_a^s(i\omega_m, Q)$ at $\omega_m = 0$, pair scattering from ε_m to ε_n with $\varepsilon_m = \varepsilon_n$ makes main contribution to λ . The gap function $\Delta_{OSO}(i\varepsilon_n, k)$ changes sign in the process of scattering from k' to k through the nesting vector $Q = (\pi, \pi/2)$, which makes the main contribution to λ , in the momentum summation of the numerator. However, scattering process for $\omega_m \neq 0$ suppresses the value of λ since gap functions with positive and negative sign of ε_n have opposite signs each other in OSO pairing.

Next we calculate the value of λ with the FLEX approximation in order to reveal how the above results is changed by the self-energy. As in the case of the RPA, to clarify how the superconducting state depends on the dimensionality of the

lattice, we gradually change the lattice structure from a twodimensional regular triangular one $(t_x = t_y)$ into a quasi-onedimensional triangular one $(t_x > t_y)$, fixing $t_y = t_2$. λ of each pairing state changes as shown in Fig. 8. Compared to the result of the RPA in Fig. 2, the values of λ are reduced. However, similar to the case of the RPA for $t_y/t_x \leq 0.1$, the OSO pairing state still remains dominant.

We calculate the temperature dependence of λ for $t_y/t_x = t_2/t_x = 0.01$ with the value of T/t_x running from 0.001 to 0.20. As shown in Fig. 9, the value of λ for OSO pairing reaches up to 0.8. The present value of λ is considerably high as compared to the corresponding values studied by the FLEX approximation in other strongly correlated systems.^{32–36} Up to now, only the values of λ obtained for high- T_C cuprates and exotic systems with disconnected Fermi surface exceed over the present value.^{37–43} Momentum



FIG. 8. (Color online) t_y dependence of λ for each pairing state fixing $t_y = t_2$ by the FLEX approximation with $S_t = 0.97$ and $T/t_x = 0.02$.



FIG. 9. (Color online) Temperature dependence of λ for each pairing state by the FLEX approximation with $t_y/t_x=t_2/t_x=0.01$ and $U/t_x=2.5$.



FIG. 10. (Color online) Matsubara frequency dependences of $G(i\varepsilon_n, k)G(-i\varepsilon_n, -k)$ at $k = (\pi/2, 0)$ by the RPA and the FLEX approximation with $t_y/t_x = t_2/t_x = 0.1$, $S_t = 0.95$, and $T/t_x = 0.05$.

and Matsubara frequency dependences of gap function are qualitatively similar to the one obtained by the RPA. As regards the Matsubara frequency dependence, there is only quantitative difference.

Matsubara frequency dependences of value of $G(i\varepsilon_n, k)G(-i\varepsilon_n, -k)$ at $k = (\pi/2, 0)$ obtained by the RPA and the FLEX approximation, which directly affect the value of λ as noted in Eq. (12), are shown in Fig. 10. $G(i\varepsilon_n, k)G(-i\varepsilon_n, -k)$ for the FLEX approximation is smaller than that for the RPA since imaginary part of self-energy corresponds to damping of quasiparticles. Thus, the presence of self-energy decreases the value of λ in the FLEX approximation.

Matsubara frequency dependences of the normalized effective pairing interactions $V_a^s(i\omega_m, Q)/V_a^s(0, Q)$ at Q $=(\pi, \pi/2)$ for spin-singlet channel in the RPA and the FLEX approximation are shown in Fig. 11. A peak width of $V_a^{s}(i\omega_m, Q)$ for the FLEX approximation is broader than that for the RPA in Matsubara frequency space due to the presence of the self-energy. This broadness of the peak width of the effective pairing interaction $V_a^s(i\omega_m, Q)$ relatively enhances the value of $V_a^s(i\omega_m, \mathbf{Q})$ with $\omega_m \neq 0$. Subsequently, the scattering processes from positive ε_n to negative ε_n relatively increase the summation of Matsubara frequency in the numerator of Eq. (12). Thus, the OSO pairing state is suppressed. On the other hand, for the ESE pairing state, the above scattering processes do not suppress the value of λ since the gap function has always same sign in Matsubara frequency space. As a result, the OSO pairing is suppressed more significantly by the self-energy as compared to the ESE pairing. This is consistent with the fact that the critical value of t_v/t_x where OSO pairing dominates over ESE pairing in the RPA $(t_v/t_x \sim 0.2)$ is reduced to ~0.1 by using the FLEX approximation as shown in Figs. 2 and 8.

As shown above, the resulting value of λ does not reach unity due to the self-energy effect based on the FLEX approximation. However, in the FLEX approximation, vertex corrections are not taken into account. The roles of vertex corrections have been studied in the context of high- T_C cuprates, where ESE (*d*-wave) pairing is realized. It has been shown that the value of λ in the presence of vertex corrections is larger than that within the FLEX approximation.^{44,45} This is because the effective pairing interaction is enhanced



FIG. 11. (Color online) Matsubara frequency dependences of the normalized effective pairing interactions $V_a^s(i\omega_m, Q)/V_a^s(0, Q)$ at $Q = (\pi, \pi/2)$ for spin-singlet channel by the RPA and the FLEX approximation with $t_y/t_x = t_2/t_x = 0.1$, $S_t = 0.95$, and $T/t_x = 0.05$.

by the vertex corrections. We can expect that the value of λ reaches unity if we consider the vertex corrections in the present calculation.

IV. CONCLUSION

We have studied symmetry of gap functions on a quasione-dimensional triangular lattice in the Hubbard model by solving the linearized Eliashberg's equation based on the RPA and the FLEX approximation. Surprisingly, oddfrequency spin-singlet p_x wave (OSO pairing state), which is not familiar, is the most dominant near the SDW phase. The OSO pairing state becomes prominent on an isosceles triangular lattice ($t_y=t_2$), where the geometrical frustration is the most significant. Even if the self-energy is introduced by the FLEX approximation, above conclusions are not changed.

The OSO pairing state is induced in the following way. In real space, neighboring two electrons with antiparallel spins make a Cooper pair mediated by the antiferromagnetic spin fluctuation near the SDW phase. The value of the effective pairing interaction $V_a^s(i\omega_m, Q)$ for spin-singlet channel at the nesting vector $Q = (\pi, \pi/2)$ has a sharp positive peak at ω_m =0 in the Matsubara frequency space. In this case, pair scattering with conserving Matsubara frequency makes major contribution to the value of λ . Therefore, sign inversion of gap function through the nesting vector $Q = (\pi, \pi/2)$ in the momentum space enhances the value of λ in Eq. (12) because the effective pairing interaction for spin-singlet channel has a positive value. This favors p_x wave, which is full gap on the Fermi surface. In accordance with Fermi-Dirac statistics, spin-singlet p_x wave can be interpreted as oddfrequency pairing. These results in this paper suggest possibility of odd-frequency superconductivity realizing in bulk system.

In the present paper, only on-site Coulomb interaction is considered. In the presence of off-site Coulomb interaction, it is known that SDW and CDW can compete with each other in quasi-one-dimensional superconductor. In that case, competition between even-frequency spin-triplet *f*-wave pair and even-frequency spin-singlet *d*-wave pair has been pointed by several theories.^{30,31,46–48} It is a challenging issue to consider

the possible realization of odd-frequency pairing in the presence of off-site Coulomb interaction.

Besides this problem, to clarify the superconducting properties of odd-frequency superconductor is an important problem. Since phase-sensitive probes, e.g., tunneling and Josephson effects, are crucial to identify the pairing symmetry in unconventional superconductors,^{49–51} similar studies on odd-frequency superconductors become important.^{12,52–54} It is necessary to calculate temperature dependence of energygap function to reveal the superconducting properties.

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