Random phase approximation for superconducting states in multi-orbital Hubbard models with spin-orbit coupling

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Abstract. To better understand electronic and magnetic properties of superconducting (SC) states in 5d transition metal oxides, we derive an analytical formula of the dynamical correlation function for multi-orbital systems with the spin-orbit coupling (SOC), which is accessible to the experimental responses. Starting with a multi-orbital BCS Hamiltonian including the SC gap function, we introduce the dynamical correlation function in the non-interacting case. Based on the diagrammatic techniques, we derive the dynamical correlation function for the interacting case within the random phase approximation. With the help of a numerical calculation, we also show the temperature dependence of the magnetic susceptibility for two different SC states in the presence of the SOC.

1. Introduction
5d transition metal oxide Sr₂IrO₄ has been focused both experimentally [1, 2, 3, 4, 5, 6, 7, 8] and theoretically [9, 10, 11, 12, 13, 14, 15, 16, 17, 18] because of the unexpected quantum phenomena arising from not only its electron correlation but also highly entangled spin and orbital degrees of freedom due to the large spin-orbit coupling (SOC). Sr₂IrO₄ has a layered perovskite structure where the two-dimensional square lattice is formed by Ir atoms [1], and its electronic properties are attributed to the five 5d electrons of Ir occupying the t₂g orbitals. In addition, the large SOC splits the sixfold degenerate t₂g orbitals into the effective total angular momentum jₑff = |−l+s| states: the fourfold degenerate jₑff = 3/2
states and the doubly degenerate \( j_{\text{eff}} = 1/2 \) states. Thus the four electrons fill the \( j_{\text{eff}} = 3/2 \) states and the remaining electron occupies one of the \( j_{\text{eff}} = 1/2 \) states, contributing mostly to determine the electronic properties.

Several experiments have revealed that an antiferromagnetic insulating state appears at low temperatures [3], and very recently, a pseudogap-like structure (Fermi arc) has been observed in the electron-doped \( \text{Sr}_2\text{IrO}_4 \) [6, 7, 8], analogous to high-\( T_c \) cuprate superconductors [19, 20, 21]. These similarities naturally expect superconductivity in \( \text{Sr}_2\text{IrO}_4 \) once mobile carriers are introduced. However, this has not been reported experimentally up to date. On the other hand, theoretical studies have proposed that pseudospin \( j_{\text{eff}} = |l - s| \) singlet pairing superconductivity is favored due to the large SOC. For example, variational Monte Carlo method, functional renormalization group method, and dynamical mean field theory with continuous time quantum Monte Carlo method are employed to show that a \( d_{x^2-y^2} \)-wave pairing is favored in the electron-doped region [14, 15, 18] and a \( s_{+} \)-wave [15, 18] or \( p \)-wave [17] pairing in the hole-doped region. To detect the unconventional superconductivities experimentally, it is highly desirable to theoretically derive the experimental responses of the pseudospin singlet pairing.

For this end, it is important to evaluate the dynamical correlation function for superconducting (SC) states in the presence of the SOC because experimental responses are obtained from its linear combinations. To achieve this, we derive the random phase approximation (RPA) for multi-orbital systems with the SOC, where the electron correlation can be incorporated by an infinite summation over all bubble and ladder diagrams connected to the Coulomb interactions. In this paper, we evaluate the magnetic susceptibility in the pseudospin singlet SC states, which can be obtained from the linear formulation of the dynamical correlation function. Here we adopt an effective model for the iridium oxide \( \text{Sr}_2\text{IrO}_4 \). However, the formalism derived here is general and is applicable to other systems where the spin and orbital degrees of freedom is entangled due to the SOC.

2. Formulation

Our goal in this paper is to calculate the following dynamical correlation function in SC states:

\[
\langle \hat{\mathcal{X}}(q) \rangle_{q \neq 0} = \frac{1}{\mathcal{N}} \int_0^\beta d\tau \ e^{i\alpha\tau} \sum_{kk'} \langle T e^{-i\tau} (c_{k\sigma}(\tau)c_{k+q\alpha}(\tau)c_{k'\sigma}^\dagger(0)c_{k'-q\alpha}(0)) \rangle_c,
\]

where \( q = (q_x, q_y) \) and \( \epsilon_m = 2mk_BT \) is Matsubara frequency for bosons (at temperature \( T \) and \( m \in \mathbb{N} \)), and \( c_{k\sigma} (c_{k\sigma}^\dagger) \) with \( \alpha = (\sigma, \sigma') \) represents the field operator for an electron annihilation (creation) with wave number \( k \), spin \( \sigma \) (\( \uparrow, \downarrow \)), and orbital \( \alpha \) (\( xy, yz, zx \)). The subscript “c” denotes the inclusion of only connected diagrams.

2.1. Tight-Binding Model

Let us start with an effective model for \( \text{Sr}_2\text{IrO}_4 \). We consider its effective \( t_{2g} \) three-orbital tight-binding model on the square lattice with a SOC,

\[
H_0 = \sum_{kk'} \epsilon_k^{\alpha\gamma} \hat{\xi}_k^\alpha \hat{\xi}_k^\gamma,
\]

where

\[
\hat{\xi}_k = \begin{pmatrix}
\xi_{kx}^x & i\lambda/2 & 0 & 0 & 0 & -\lambda/2 \\
-i\lambda/2 & \xi_{kx}^x & 0 & 0 & 0 & i\lambda/2 \\
0 & 0 & \xi_{ky}^y & \lambda/2 & -i\lambda/2 & 0 \\
0 & 0 & \lambda/2 & \xi_{ky}^y & -i\lambda/2 & 0 \\
0 & i\lambda/2 & i\lambda/2 & \xi_{kxy}^x & 0 \\
-\lambda/2 & -i\lambda/2 & 0 & 0 & 0 & \xi_{kxy}^x
\end{pmatrix},
\]

and

\[
\epsilon_k^{\alpha\gamma} = \begin{pmatrix}
\xi_{kx}^x & 0 & 0 & 0 & 0 \\
0 & \xi_{kx}^x & 0 & 0 & 0 \\
0 & 0 & \xi_{ky}^y & 0 & 0 \\
0 & 0 & 0 & \xi_{ky}^y & 0 \\
0 & 0 & 0 & 0 & \xi_{kxy}^x \\
0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]
\( \epsilon_k^\Delta = \epsilon_k^\mu - \mu \) represents the energy dispersion \( \epsilon_k^\mu \) measured from the chemical potential \( \mu \) and \( \lambda \) is the strength of the SOC. According to the previous studies [11, 14], the band structure of Sr\(_2\)IrO\(_4\) obtained from the first-principles calculation [2] can be well reproduced using the following tight-binding energy dispersion for the three \( t_{2g} \) orbitals:

\[
\begin{align*}
\epsilon_k^{\Delta x} &= -2t_5 \cos k_x - 2t_4 \cos k_y, \\
\epsilon_k^{\Delta y} &= -2t_4 \cos k_x - 2t_5 \cos k_y, \\
\epsilon_k^{\Delta z} &= -2t_1 (\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y \\
&\quad - 2t_3 (\cos 2k_x + \cos 2k_y) + \mu_{xy},
\end{align*}
\]

(5)

with \((t_1, t_2, t_3, t_4, t_5, \mu_{xy}, \lambda) = (0.36, 0.18, 0.09, 0.37, 0.06, -0.36, 0.37)\) eV. Notice that the SOC \( \lambda \) is as large as the hopping parameters.

\( H_0 \) can be diagonalized by a unitary matrix \( \hat{U}_k \) as

\[
H_0 = \sum_k \epsilon_k^\Delta \hat{U}_k \left( \hat{U}_k^\dagger \epsilon_k \hat{U}_k \right) \hat{U}_k^\dagger \hat{c}_k = \sum_k \hat{a}_k^\dagger \hat{h}_k \hat{a}_k,
\]

(6)

where

\[
\hat{a}_k^\dagger = \left( a_{k1\uparrow}^\dagger a_{k1\downarrow}^\dagger a_{k2\uparrow}^\dagger a_{k2\downarrow}^\dagger a_{k3\uparrow}^\dagger a_{k3\downarrow}^\dagger \right)
\]

(7)

and

\[
\hat{h}_k = \text{diag} \left( E_1^1, E_1^2, E_2^1, E_2^2, E_3^1, E_3^2 \right).
\]

(8)

Here, \( E_k^l \) represents the \( l \)-th energy eigenvalue in descending order, i.e., \( E_1^1 \geq E_2^2 \geq E_3^3 \), and \( a_{klj} \) is its annihilation operator for the Kramers doublet \( j(=\uparrow, \downarrow) \). The previous studies have revealed that the quasiparticle \( a_{klj} \) for the highest band \( E_1^1 \) is mostly composed of the effective total angular momentum \( j_{\text{eff}} \) = 1/2 doublet, where \( j_{\text{eff}} = -l + s \) is ”pseudospin” operator, and \( s \) and \( l \) are the spin and orbital angular momentum, respectively. Therefore, \( E_1^1 \) is referred to as the \( j_{\text{eff}} \) = 1/2 band in the following.

As is obvious in the above, the intrinsic spin \( \sigma \) is no longer a good quantum number, but instead the pseudospin \( j_{\text{eff}} \) becomes a good quantum number. Thus, when the possible superconductivity is considered in carrier doped Sr\(_2\)IrO\(_4\), it is expected that a pseudospin SC pairing is favored to form Cooper pairs with opposite wave number \( \pm \kappa \) and opposite (singlet) or parallel (triplet) pseudospins. The pseudospin superconductivity depends on the carrier doping: in the electron-doped regions only the single \( j_{\text{eff}} \) = 1/2 (\( l = 1 \)) band becomes dominant because the other bands are far below the Fermi level [14, 15, 18], while in the hole-doped regions several \( j_{\text{eff}} \) bands (especially, the two highest bands with \( l = 1 \) and 2) contribute to form Cooper pairs [15, 17, 18].

We also consider the Coulomb interaction term including the intra- and inter-orbital on-site Hubbard interactions \((U \text{ and } U', \text{ respectively})\), the Hund’s coupling \((J)\), and the pair hopping \((J')\), described by the following Hamiltonian:

\[
H_{\text{int}} = U \sum_i \sum_a n_i^a n_i^a + U' \sum_i \sum_{a < b} n_i^a n_i^b \\
- J \sum_i \sum_{a < b} \left( 2S_i^a \cdot S_i^b + \frac{1}{2} n_i^a n_i^b \right) + J' \sum_i \sum_{a < b} c_{i\alpha}^\dagger a_{i\alpha}^\dagger c_{i\beta} a_{i\beta} + \text{h.c.},
\]

(9)

where \( n_i^\alpha = c_{i\alpha}^\dagger c_{i\alpha} \), \( n_i^\alpha = n_i^\alpha + n_i^\alpha \), and \( S_i^\alpha = \sum_{\sigma \sigma'} c_{i\alpha}^\dagger \tau_{\sigma \sigma'} c_{i\alpha} \) (\( \tau_{\sigma \sigma'} \) is the elements of the Pauli matrix \( \tau \)). We impose that \( U = U' + 2J \) and \( J = J' \) for simplicity [22].
2.2. BCS Hamiltonian

Next, we consider a multi-orbital BCS Hamiltonian $H_{BCS}$ in the presence of the SOC by introducing a SC gap function $\Delta_k$ into $H_0$ (apart from a constant term),

$$
H_{BCS} = \frac{1}{2} \sum_k C_k^\dagger \hat{H}_{BCS}^{\text{spec}} C_k = \frac{1}{2} \sum_k \hat{\mathcal{H}}_{k} \left| \hat{\Delta}_k \right| \hat{c}_k + \hat{\Delta}^\dagger \hat{c}^\dagger_k ,
$$

where $C_k$ is a matrix representation of the field operators,

$$
C_k = (c_k^\dagger, e_k^\dagger, \cdots, c_k^\dagger, e_k^\dagger, \cdots, c_k^\dagger) .
$$

The capital subscript $A$ ($B$) is used to represent the $A$-th element of $\hat{C}_k$, and $\hat{\Delta}$ indicates the summation over $A = 1, 2, \cdots, 12$. Here the dimension of $\hat{C}_k$ is specified as $12 = 3(\text{orbital}) \times 2(\text{spin}) \times 2(\text{Nambu})$ since the effective model for Sr$_2$IrO$_4$ is considered. The $H_{BCS}$ can be diagonalized by the unitary matrix $\hat{U}_k$ as

$$
H_{BCS} = \frac{1}{2} \sum_k C_k^\dagger \hat{U}_k (\hat{U}_k^\dagger \hat{H}_{BCS}^{\text{spec}} \hat{U}_k) \hat{U}_k^\dagger C_k
$$

$$
= \frac{1}{2} \sum_k \hat{B}_k^\dagger \hat{E}_k \hat{B}_k = \frac{1}{2} \sum_k \hat{B}_k^\dagger \hat{E}_k \hat{B}_k ,
$$

where $\hat{B}_k$ represents the field operator of the Bogoliubov quasiparticles (in the vector form) in the Nambu representation, and $\hat{E}_k$ is its quasiparticle energy. The unitary transformation from the $\hat{B}_k$ to $\hat{C}_k$ is given as

$$
\hat{C}_k = \hat{U}_k \hat{B}_k \quad \hat{C}_k = \hat{B}_k \hat{U}_k^\dagger
$$

$$
\Rightarrow
$$

In Eq. (10), the SC gap function $\hat{\Delta}_k$ is introduced as an input parameter. When we consider the pseudospin SC pairing for Sr$_2$IrO$_4$, $\hat{\Delta}_k$ can be obtained from the unitary transformation of the pseudospin SC gap function $D_k$ via $\hat{c}_k^\dagger \hat{\Delta}_k \hat{c}_k^\dagger = \hat{D}_k \hat{c}_k^\dagger$. For instance, the specific form of the $d_{12\rightarrow y^2}$-wave pseudospin $\hat{j}_{12\rightarrow y^2}$ is given by $\hat{[D_k]}_{12} = - \hat{[D_k]}_{21} = D_d (\cos k_x - \cos k_y) / 2$ and the other elements are zero, while that of the $s_\alpha$-wave pseudospin singlet pairing is given by $\hat{[D_k]}_{12} = - \hat{[D_k]}_{21} = + D_s$, $\hat{[D_k]}_{34} = - \hat{[D_k]}_{43} = - D_s$, and the other elements are zero. Here, $D_d$ and $D_s$ denote the amplitudes of the $d_{12\rightarrow y^2}$- and $s_\alpha$-wave pseudospin singlet pairing, respectively.

2.3. Green’s Functions

To formulate the RPA scheme for SC states, we here introduce a Green’s function defined as

$$
\hat{G}(k) = - \int^\beta_0 d\tau e^{i\omega_n \tau} \langle T_\tau \hat{C}_k^\dagger(\tau) \hat{C}_k(0) \rangle
$$

$$
= \begin{pmatrix} \hat{G}(k) & \hat{F}(k) \\ \hat{F}(k) & \hat{G}(k) \end{pmatrix},
$$

where $\beta = 1 / k_B T$, $k = (k, i\omega_n)$, and $\omega_n = (2n + 1) k_B T$ is a Matsubara frequency for fermions with $n \in \mathbb{N}$. The elements of the $6 \times 6$ matrix $G$ ($G$) and $F$ ($F$) are the normal and anomalous Green’s functions,
respectively. In the non-interacting case, the Green’s function \( \hat{G}_0(k) \) can be obtained immediately from the BCS Hamiltonian matrix, i.e.,

\[
\hat{G}_0(k) = \left( i\omega_n - \hat{H}_k^{\text{BCS}} \right)^{-1} = \hat{U}_k \left( i\omega_n - \hat{\epsilon}_k \right)^{-1} \hat{U}_k^\dagger
\]

(15)

\[
\frac{\hat{G}_0(k)}{\hat{F}_0(k)} = \frac{\hat{G}_0(k)}{\hat{F}_0(k)}\begin{pmatrix} \hat{G}_0(k) \\ \hat{F}_0(k) \end{pmatrix}
\]

2.4. Dynamical Correlation Function in the Non-interacting Case

Let us consider the dynamical correlation function in the non-interacting case,

\[
[\hat{\chi}_0(q)]_{\alpha\beta\gamma\delta} = \frac{1}{N\beta} \int_0^\beta d\tau e^{i\epsilon_n\tau} \sum_{kk'} \langle T_\tau \hat{c}^\dagger_{k\beta}(\tau)\hat{c}_{k'\gamma}(0)\hat{c}_{k'\delta}(0)\hat{c}_{k\gamma}(0) \rangle_{0c},
\]

(16)

where the subscript “0” denotes the statistical average over the one-body Hamiltonian \( H_{\text{BCS}} \). With Wick’s theorem, \( \hat{\chi}_0(q) \) can be represented by using both normal and anomalous Green’s functions as

\[
[\hat{\chi}_0(q)]_{\alpha\beta\gamma\delta} = \frac{1}{N\beta} \sum_k \left[ \hat{G}_0(q + k) \right]_{\alpha\beta} \left[ \hat{G}_0(-k) \right]_{\gamma\delta} - \frac{1}{N\beta} \sum_k \left[ \hat{F}_0(q + k) \right]_{\alpha\delta} \left[ \hat{F}_0(-k) \right]_{\beta\gamma}
\]

(17)

where the summation over \( k \) is the short hand notation of the summation over \( k \) and \( i\omega_n \). The diagrammatic representation of Eq. (17) is depicted in Fig. 1. In addition to the first term in Eq. (17) composed of the normal Green’s functions (\( G \) and \( \hat{G} \)), it is necessary to include the second one composed of the anomalous Green’s functions (\( F \) and \( \hat{F} \)) in SC states.

Furthermore, one can perform the summation over \( i\omega_n \) in Eq. (17) by considering the Bogoliubov quasiparticle basis. To achieve this, it is convenient to consider the dynamical correlation function in the Nambu representation

\[
[\hat{X}_0(q)]_{ABCD} = \frac{1}{N} \int_0^\beta d\tau e^{i\epsilon_m\tau} \sum_{kk'} \langle T_\tau \hat{C}_{k\beta}^\dagger(\tau)\hat{C}_{k\alpha}(0)\hat{C}_{k'\alpha}(0)\hat{C}_{k'\beta}(0) \rangle_{0c}.
\]

(18)

By using the unitary matrix \( \hat{U}_k \) and the quasiparticle dispersion \( \hat{\epsilon}_k \), we obtain the following form of \( \hat{X}_0(q) \):

\[
[\hat{X}_0(q)]_{ABCD} = \frac{1}{N} \sum_k \left[ \hat{U}_{k+q} \right]_{AA} \left[ \hat{U}_{k+q}^\dagger \right]_{AC} \left[ \hat{U}_{k+q}^\dagger \right]_{BD} \hat{U}_k \left[ \hat{U}_k \right]_{BD} \frac{f(\hat{E}_{k+q\beta}) - f(\hat{E}_{k\beta})}{i\epsilon_m - (\hat{E}_{k+q\beta} - \hat{E}_{k\beta})}
\]

\[ - \frac{1}{N} \sum_k \left[ \hat{U}_{k+q} \right]_{AA} \left[ \hat{U}_{-k} \right]_{DD} \left[ \hat{U}_k \right]_{BD} \frac{f(\hat{E}_{k+q\beta}) - f(\hat{E}_{k\beta})}{i\epsilon_m - (\hat{E}_{k+q\beta} - \hat{E}_{k\beta})}
\]

(19)

where \( f(x) = (e^{\beta x} + 1)^{-1} \) is the distribution function for fermions, and \( \hat{A}'(\hat{B}') = \text{Mod}(6 + \hat{A}(\hat{B}) - 1, 12) + 1 \). For the derivation, we have used the following identity for the summation over the Matsubara frequencies:

\[
\frac{1}{\beta} \sum_{i\omega_n} \frac{1}{i\omega_n + i\epsilon_m - \hat{E}_{k+q\beta}} \times \frac{1}{-i\omega_n + i\epsilon_{KB}} = \frac{f(\hat{E}_{k+q\beta}) - f(\hat{E}_{k\beta})}{i\epsilon_m - (\hat{E}_{k+q\beta} - \hat{E}_{k\beta})}
\]

(20)

Notice that the elements of \( \hat{X}_0(q) \) for \( A, B, C, \) and \( D = 1, 2, \cdots 6 \) correspond to those of \( \hat{\chi}_0(q) \) as \( \hat{C}^\dagger_k = (\hat{c}^\dagger_k, \hat{c}^\dagger_{-k}) \).
The explicit expression of the interaction tensor $\hat{h}$, which is schematically represented in Figure 2. Here, the product of the tensors is defined as 

$$\hat{h} = \sum \text{second one composed of the anomalous Green’s functions } (G \text{ and } \bar{G}), \text{ the second one composed of the normal Green’s functions } (F \text{ and } \bar{F}).$$

In the presence of the SOC, however, the bubble and ladder diagrams can not be separated from each other due to the entanglement of the spin and orbital degrees of freedom. Therefore, one needs to introduce a general expression for $\hat{h}$ being taken account of the spin and orbital indices, as depicted in Figure 1.

![Figure 1](image)

**Figure 1.** Schematic representation of the dynamical correlation function $\hat{\chi}_0(q)$ in the non-interacting case in SC states. In addition to the first term composed of the normal Green’s functions ($G$ and $\bar{G}$), the second one composed of the anomalous Green’s functions ($F$ and $\bar{F}$) is also taken into account because of SC states. Notice that the order of the vertex indices is different in the first and second terms.

### 2.5. Dynamical Correlation Function in the RPA

The dynamical correlation function $\hat{\chi}(q)$ in the RPA can be obtained diagrammatically with the infinite summation over all bubble and ladder diagrams of $\hat{\chi}_0(q)$ connected by the Coulomb interactions [23, 24, 25]. In a one-band Hubbard model with the on-site Hubbard interaction $U$, the bubble diagrams can be interpreted as the charge and longitudinal spin fluctuations, while the ladder ones as the transverse spin fluctuations. In the presence of the SOC, however, the bubble and ladder diagrams cannot be separated from each other due to the entanglement of the spin and orbital degrees of freedom. Therefore, one needs to introduce a general expression for $\hat{\chi}_0(q)$ being taken account of the spin and orbital indices, as depicted in Figure 1.

To obtain the analytical expression for $\hat{\chi}(q)$, let us consider the Bethe-Salpeter equation for $\hat{\chi}(q)$, i.e.,

$$\hat{\chi}(q) = \hat{\chi}_0(q) + \hat{\chi}_0(q)\hat{V}\hat{\chi}(q),$$

(21)

which is schematically represented in Figure 2. Here, the product of the tensors is defined as $[\hat{A}\hat{B}]_{\alpha\beta\gamma\delta} = \sum_{\mu\nu} A_{\alpha\beta\mu\nu}B_{\nu\gamma\delta}$. $\hat{V}$ is the Coulomb interaction in the tensor form whose elements contain the intra- and inter-orbital on-site Hubbard interactions $U$ and $U'$, respectively, the Hund’s coupling $J$, and the pair hopping $J$ in $H_{\text{int}}$ of Eq. (9). The solution for $\hat{\chi}(q)$ can be obtained immediately as

$$\hat{\chi}(q) = \left(1 - \hat{\chi}_0(q)\hat{V}\right)^{-1}\hat{\chi}_0(q).$$

(22)

The explicit expression of the interaction tensor $\hat{V}$ is given as

$$V_{a\uparrow,b\uparrow,c\downarrow,d\downarrow} =
\begin{cases}
U' - J & (a = c \neq b = d) \\
-(U' - J) & (a = b \neq c = d) \\
0 & \text{(others)}
\end{cases},$$

$$V_{a\uparrow,b\uparrow,c\downarrow,d\downarrow} =
\begin{cases}
-U & (a = b = c) \\
-J & (a = c \neq b = d) \\
-U' & (a = b \neq c = d) \\
-J & (a = d \neq b = c) \\
0 & \text{(others)}
\end{cases},$$

$$V_{a\uparrow,b\uparrow,c\downarrow,d\downarrow} =
\begin{cases}
U & (a = b = c = d) \\
U' & (a = c \neq b = d) \\
J & (a = b \neq c = d) \\
J & (a = d \neq b = c) \\
0 & \text{(others)}
\end{cases},$$

(23)
Let us first consider the theoretical expression for the magnetic susceptibility, which can be derived from the linear combination of the dynamical correlation function \( \hat{\chi}(q) \). We now show the numerical results for the magnetic susceptibility in the pseudospin singlet SC states.

3. Results

We now show the numerical results for the magnetic susceptibility in the pseudospin singlet SC states. Let us first consider the theoretical expression for the magnetic susceptibility, which can be derived from the linear combination of the dynamical correlation function \( \hat{\chi}(q) \).

The magnetic susceptibility \( \chi_M^{\mu\nu}(q) \) can be written as,

\[
\chi_M^{\mu\nu}(q) = \frac{1}{N} \int_0^\beta d\tau e^{i\tau q} \langle T_\tau M_\mu(\tau)M_\nu^*(0) \rangle_\omega, \tag{24}
\]

where the magnetic moment operator \( M_\mu^q \equiv L_\mu^q + 2S_\mu^q \) with wave number \( q \) and \( \mu = (\pm, \pm) \) is the sum of the spin and orbital angular momentum operator \( S_\mu^q \) and \( L_\mu^q \), respectively. \( M_\mu^q, L_\mu^q, \) and \( S_\mu^q \) represent the raising and lowering operators, and \( M_\mu^q, L_\mu^q, \) and \( S_\mu^q \) are the \( z \) component of the operators. Thus, \( \chi_M^{\mu\nu}(q) \) and \( \chi_M^{zz}(q) \) represent the transverse and longitudinal magnetic susceptibilities, respectively. \( M_\mu^q \) can be expressed by the field operators as

\[
M_\mu^q = \sum_{\alpha\beta} \sum_k c_\alpha^k \hat{M}_\mu^{\alpha\beta} c_{\beta+kq}, \tag{25}
\]

where \( \hat{M}_\mu^{\alpha\beta} \) denotes the matrix representation of the magnetic moment operator. From the definition of \( M_\mu^q \), \( \hat{M}_\mu^{\alpha\beta} \) can be obtained from the sum of the matrix representation for the spin and orbital angular momentum operator \( \hat{S}_\mu^{\alpha\beta} \) and \( \hat{L}_\mu^{\alpha\beta} \), respectively, as

\[
\hat{M}_\mu^{\alpha\beta} = \hat{L}_\mu^{\alpha\beta} + 2\hat{S}_\mu^{\alpha\beta}, \tag{26}
\]

where the explicit forms of \( \hat{S}_\mu^{\alpha\beta} \) and \( \hat{L}_\mu^{\alpha\beta} \) are given as

\[
\hat{S}_z^{\pm} = \frac{1}{2} \begin{pmatrix} 1 & \hat{0} \\ \hat{0} & \hat{0} \end{pmatrix}, \hat{S}_z^{\mp} = \frac{1}{2} \begin{pmatrix} 0 & \hat{0} \\ \hat{0} & 0 \end{pmatrix}, \hat{S}_z = \begin{pmatrix} 1 & \hat{0} \\ \hat{0} & 0 \end{pmatrix},
\]

and

\[
\hat{L}_z = \begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{L}_z = \begin{pmatrix} 0 & 0 & \pm1 \\ 0 & \pm1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\]

Figure 2. Schematic representation of the dynamical correlation function \( \hat{\chi}(q) \) in the RPA. This can be obtained from the Bethe-Salpeter equation, where all the diagrams connected by the interaction tensor are summed until the infinite order.
Finally, one can obtain the magnetic susceptibility $\chi_M^{uv}(q) = \chi_M^{uu}(q = 0)$ as the linear combination of the dynamical correlation function $\hat{\chi}(q)$,

$$\chi_M^{uv}(q) = \sum_{\alpha\beta\gamma\delta} [\hat{M}_\alpha^{\mu}(q) T_{\gamma\delta}]_{\beta\gamma\delta}. \quad (29)$$

Figure 3 displays the temperature dependence of the uniform magnetic susceptibility $\chi_M^{uv} = \chi_M^{uu}(q = 0)$ in the pseudospin singlet SC states. Here, the $d_{x^2-y^2}$- and $s_z$-wave pseudospin singlet pairings are assumed in the left and right panels, respectively, in Figure 3. We assume that the temperature dependence of the amplitude $D_{d(s)}(T)$ of the SC gap function is determined by the gap equation

$$D_k = -\frac{1}{N} \sum_{k'} V_{kk'} \frac{D_{k'}}{2E_{k'}} \tanh \frac{E_{k'}}{2T} \quad (30)$$

with the pairing interaction $V_{kk'} = -|V|(\cos k_x - \cos k'_x)(\cos k_y - \cos k'_y)$ for the $d_{x^2-y^2}$-wave pairing and $V_{kk'} = -|V|$ for the $s_z$-wave pairing. We set the single-particle parameters $(t_1, t_2, t_3, t_4, t_5, \mu_{sy}) = (0.36, 0.18, 0.09, 0.37, 0.06, -0.36)$ eV and the intra-orbital on-site Hubbard interaction $U = 0.75$ eV. The two-dimensional $k$-point mesh in the first Brillouin zone is chosen to be $(k_x, k_y) = (64, 64)$. The amplitude of the SC gap at $T = 0$ is also set to be $D_{d(s)}(0) = 4k_BT_c$ and the transition temperature $T_c$ to be $k_BT_c = 0.1t_1$. In addition to this, we set the SOC $\lambda = 0.5$ (0.3) eV, the Hund’s coupling $J = 0.05U$ (0.3U), and the electron density $n = 5.1$ (4.8) for the $d_{x^2-y^2}$ ($s_z$)-wave pseudospin singlet pairing superconductivity. These parameters are selected simply because the previous studies [14, 15, 18] have shown that the $d_{x^2-y^2}$ ($s_z$)-wave pseudospin singlet superconducting pairing is dominant in the electron- (hole-) doped region with large (small) SOC $\lambda$ and small (large) Hund’s coupling $J$. The effective model of the electron-doped Sr$_2$IrO$_4$ with large $\lambda$ becomes a one-band system and thus the $d_{x^2-y^2}$-wave pairing is favored by the intra-band repulsive ($k$-dependent) pairing interaction in analogy to cuprate superconductors. On the other hand, the effective model of the hole-doped Sr$_2$IrO$_4$ with small $\lambda$ becomes a two-band system and therefore the $s_z$-wave pairing is favored by the inter-band repulsive pairing interaction in analogy to iron-based superconductors.

Figure 3 shows clearly that the transverse and longitudinal magnetic susceptibilities are different from each other. This difference is originated from the SOC and Hund’s coupling $J$, which induce magnetic anisotropy. One can also notice that these magnetic susceptibilities decrease below $T_c$ with decreasing $T$ but they do not become zero at $T = 0$. This is understood because neither spin nor orbital angular momentum is good quantum number in the presence of the SOC and therefore the formation of singlet Cooper pairs does not completely freeze the magnetic fluctuations even at $T = 0$. 

![Figure 3](image-url)

Figure 3. Magnetic susceptibility $\chi_M^{uv} = \chi_M^{uu}(q = 0)$ in the pseudospin singlet SC states. The $d_{x^2-y^2}$ and $s_z$-wave pseudospin singlet pairings are assumed in the left and right panels, respectively.
4. Summary
To summarize, we have formulated the RPA for multi-orbital systems with the SOC in order to understand the electronic and magnetic properties for SC states in $5d$ transition metal oxides such as Sr$_2$IrO$_4$. Starting with the effective model for iridium oxide insulator Sr$_2$IrO$_4$, we have considered the BCS Hamiltonian by introducing the SC gap function, from which the normal and anomalous Green’s functions can be obtained. The dynamical correlation function for the non-interacting case can be obtained from the Green’s functions, and the electron correlation can be incorporated by an infinite summation over all bubble and ladder diagrams connected via the Coulomb interactions. The formalism given here is general and is applicable to other multi-orbital systems with a SOC. Finally, we have evaluated the magnetic susceptibility in the pseudospin singlet SC states with the formalism given here is general and is applicable to other multi-orbital systems with a SOC. We have also shown that these magnetic susceptibilities decrease below $T_c$ but they are finite even at $T = 0$. This is because the magnetic fluctuations are not completely frozen in the SC states with the pseudospin singlet pairing.

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