Diversified Ruderman-Kittel-Kasuya-Yosida Interactions in a Nonsymmorphic Crystal

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We show that there are diversified Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions between magnetic impurities, mediated by itinerant electrons, in a centrosymmetric crystal respecting a nonsymmorphic space group. We take the $P4/nmm$ space group as an example. We demonstrate that the different type of interactions, including the Heisenberg-type, the Dzyaloshinskii-Moriya (DM)-type, the Ising-type and the anisotropic interactions, can appear in accordance with the positions of the impurities in the real space. Their strengths strongly depend on the location of the itinerant electrons in the reciprocal space. The diversity stems from the position-dependent site groups and the momentum-dependent electronic structures guaranteed by the nonsymmorphic symmetries. Our study unveils the role of the nonsymmorphic symmetries in affecting magnetism, and suggests that the nonsymmorphic crystals can be promising platforms to design magnetic interactions.

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Introduction. In noncentrosymmetric systems, the Rashba spin-orbit coupling (SOC) arises due to the absence of the inversion symmetry [1]. The Rashba SOC leads to the spin-momentum lock, which plays an important role in lots of exotic quantum phenomena [2–4], such as the spin-orbit torques [5, 6], the singlet-triplet mixing superconductivity [7, 8], the various topological phases of matter [9–16], etc. Especially, when the Rashba SOC is encoded with magnetism, the DM magnetic interactions can be induced [17–21]. The DM interaction has been extensively studied in recent years, because of its essential role in inducing the magnetic skyrmion [22–30], the topological magnon [31–34] and the spin helix [35, 36]. These interesting properties make the materials with large DM interaction be promising candidates for next-generation spintronics [37, 38].

Recently, a class of centrosymmetric systems, which have the so-called local inversion-symmetry-breaking effect [39–45], have attracted great research interest. In such systems, the inversion center is off the lattice sites, making the Rashba SOC allowed even though the system being globally inversion symmetric. Interestingly, in such systems there exists the net spin-momentum lock for electrons from certain subsystems, but the effect compensates for electrons from different subsystems. Correspondingly, the DM magnetic interaction can be expected in such systems. Moreover, besides magnetism it has been demonstrated that the local inversion-symmetry-breaking effect may be essential in the odd-parity superconductivity [46–48] and the topological superconductivity [41, 49].

The RKKY interaction, which plays a central role in the diluted magnetic semiconductors, is an indirect exchange interaction between magnetic impurities mediated by itinerant electrons. It provides an another scheme for the DM magnetic interaction [50–54]. In this work, we present a detailed theoretical investigation on the RKKY interaction mediated by itinerant electrons in a centrosymmetric crystal respecting the nonsymmorphic space group $P4/nmm$. We demonstrate that though the itinerant electrons respect the inversion symmetry in the system, RKKY interactions including the Heisenberg, the DM, the Ising and the anisotropic terms, can be induced. Moreover, the specific forms of the RKKY interaction varies in accordance with the positions of the impurities in the real space, and the strength of the interaction varies according to the positions of the itinerant electrons in the reciprocal space. We discuss the rich and electronically controllable spin configurations in such systems.

Space group $P4/nmm$. We first briefly review the nonsymmorphic space group $G = P4/nmm$. The group $G$ has 16 symmetry operations in its quotient group $G/T$, satisfying a special structure [55]

$$G/T \cong D_{2d} \otimes Z_2 \cong C_{4v} \otimes Z_2,$$

where $D_{2d}$, $C_{4v}$ and $Z_2$ are three point groups defined at different positions. To have a more intuitive impression, we consider a quasi-2D lattice shown in Fig. 1(a). In the lattice, the Wyckoff positions $2a$ and $2c$ are the fixed points preserving the point group $D_{2d}$ and $C_{4v}$, respectively. The $Z_2$ group in Eq. (1) is a two-element group including the inversion symmetry which switches the two $2a$ ($2c$) Wyckoff positions in Fig. 1(a). According to Eq. (1), it is obvious that group $G/T$ can be generated by the generators of $D_{2d}$ ($C_{4v}$) and $Z_2$, which can be chosen as $\{M_y|0\}$, $\{S_{2z}|0\}$, $\{M_{xy}|\tau_0\}$, $\{C_{4z}|\tau_0\}$, and $\{I|\tau_0\}$ respectively [56].

Itinerant electrons in group $P4/nmm$. For a nonsymmorphic crystal, its group structure, i.e. the commutation relations between the symmetry operations, varies with the momentum.
in the reciprocal space [57–59]. Actually, at the BZ center, i.e. the Γ point (0, 0), the system in Fig. 1(a) respects the D_{4h} point group [60]; while it respects a little group which is not isomorphic to any point group at the BZ corner, i.e. the M point (π, π) [61]. The momentum-dependent group structures indicate the momentum-dependent properties of the itinerant electrons in a nonsymmetric group.

To describe the itinerant electrons in group P4/nmm specifically, we derive the low-energy effective theory. We start with the BZ corner. A standard group theory analysis shows that, the group P4/nmm merely has one single 4D irreducible spinful representation at the M point, meaning that all the energy bands in the system are fourfold degenerate and respect the same effective theory at M in the spinful condition [8, 62]. Considering the constraints of the crystalline symmetries and the time-reversal symmetry, we obtain the effective theory as follows [8, 48, 62]

\[
\mathcal{H}_{\text{M,2a}}(\mathbf{k}) = m(\mathbf{k}) s_0 \sigma_0 + \lambda k_x s_2 \sigma_3 + \lambda k_y s_1 \sigma_3 + t' k_z k_y s_0 \sigma_1, \tag{2}
\]

where \(m(\mathbf{k}) = t'(k_x^2 + k_y^2)\), and \(t', \lambda\) are all constants. In Eq. (2), \(s_i\) and \(\sigma_i\) (\(i = 0, 1, 2, 3\)) are Pauli matrices in the spin and sublattice spaces respectively. To have an intuitive impression on the effective theory, one can assume a single \(s\) orbital at each 2a Wyckoff position in Fig. 1(a), \(t'\) \((t')\) can be understood as the hopping between intrasublattice (intersublattice) nearest-neighbour sites, and \(\lambda\) represents the Rashba SOC stemming from the mismatch between the lattice sites and the inversion center. According to Eq. (1), one can also set the orbital at the 2c Wyckoff positions in Fig. 1(a), in which condition the effective theory at M reads as (details in SM [63])

\[
\mathcal{H}_{\text{M,2c}}(\mathbf{k}) = m(\mathbf{k}) s_0 \sigma_0 + \lambda k_x s_2 \sigma_3 - \lambda k_y s_1 \sigma_3 + t' k_z k_y s_0 \sigma_1, \tag{3}
\]

where the coefficients can be understood in a similar way with these in \(\mathcal{H}_{\text{M,2a}}\). Notice that \(\mathcal{H}_{\text{M,2a}}\) and \(\mathcal{H}_{\text{M,2c}}\) describes the same fourfold band degeneracy at M. However, corresponding to the different positions where the orbitals locate, the physical observables are different. For example, we calculate the spin textures on the Fermi surfaces for the effective theories in Eq. (2) and Eq. (3) and show the results in Fig. 1(b) and Fig. 1(c) respectively. As shown, the spin texture in Fig. 1(b) (Fig. 1(c)) is \(D_{2d}(C_{4v})\) symmetric, in accordance with the site group at the 2a (2c) Wyckoff positions chosen for \(\mathcal{H}_{\text{M,2a}}\) (\(\mathcal{H}_{\text{M,2c}}\)). The different theories in Eqs. (2)(3) demonstrate the profound roles of the real-space positions on the RKKY interactions.

At the Γ point, the system respects the point group \(D_{4h}\) and the corresponding effective theory takes the form (details in SM [63])

\[
\mathcal{H}_{\Gamma,2a}(\mathbf{k}) = m(\mathbf{k}) s_0 \sigma_0 + \lambda k_x s_2 \sigma_3 + \lambda k_y s_1 \sigma_3 + t' s_0 \sigma_1, \tag{4}
\]

where the basis is the same with that for the effective theory \(\mathcal{H}_{\text{M,2a}}\) in Eq. (2). For the basis in Eq. (3), the effective theory at Γ becomes

\[
\mathcal{H}_{\Gamma,2c}(\mathbf{k}) = m(\mathbf{k}) s_0 \sigma_0 + \lambda k_x s_2 \sigma_3 - \lambda k_y s_1 \sigma_3 + t' s_0 \sigma_1. \tag{5}
\]

Apparently, \(\mathcal{H}_{\Gamma,2a(2c)}\) describes two Kramers’ doublets which is different from the condition at M.

Comparing the effective theories near Γ and M, it can be found that, near Γ the effective SOC on the energy bands is vanishing small because of the finite \(t' s_0 \sigma_1\) term, while the system is nearly a direct product of two Rashba electron gas systems due to the dominating SOC term near M. Such difference implies the different RKKY interactions corresponding to itinerant electrons at the BZ center and corner.

**RKKY interaction in P4/nmm.** We consider two magnetic impurities \(S_i\) (\(i = 1, 2\)) located at \(R_i\), in the system in Fig. 1(a). The magnetic impurities interact with the itinerant electrons through the \(s - d\) interaction [64]

\[
\mathcal{H}_{sd} = -J \langle [S_1 \cdot s] \sigma_\alpha \delta(\mathbf{r} - R_1) + \langle S_2 \cdot s \rangle \sigma_\beta \delta(\mathbf{r} - R_2) \rangle, \tag{6}
\]

where \(J\) is the strength of the exchange coupling. In Eq. (6), \(\sigma_{\alpha/\beta}\) denotes the sublattice locked to the position \(R_i\), which takes the form \((\sigma_1 + \sigma_3)/2\) or \((\sigma_1 - \sigma_3)/2\). The RKKY interaction between the impurities can be obtained by integrating out the itinerant electrons

\[
\mathcal{H}_{\text{RKKY}} = -\frac{J^2}{2} \int \frac{d\omega}{\pi} \text{Im} \int_{\omega < \mu} \text{d}\omega \text{Tr} \langle [S_1 \cdot s] \sigma_\alpha G(R_2, R_1, \omega) \rangle \times \langle S_1 \cdot s \rangle \sigma_\beta \langle G(R_1, R_2, \omega) \rangle, \tag{7}
\]

where \(\mu\) is the Fermi energy, Tr represents the trace over the degrees of the itinerant electrons, and \(G(R_i, R_j, \omega)\) is the real-space Green function for the itinerant electrons with \(\omega\)
the frequency. After some algebra, we find the RKKY interaction in Eq. (7) takes the form

\[ H_{\text{RKKY}}(\mathbf{R}, \mu) = \Lambda \mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{D} \cdot (\mathbf{S}_1 \times \mathbf{S}_2) + \sum_{i,j} T_{ij} S_{1i} S_{2j}, \]

with \( \mathbf{R} = \mathbf{R}_1 - \mathbf{R}_2, \mathbf{D} = (D_1, D_2) \) and \( i, j = x, y, z. \) In Eq. (8), the first term is the Heisenberg-type, the second term is the DM-type, the last term includes the Ising-type terms \( (i = j) \) and the anisotropic terms \( (i \neq j). \) Its specific form and strength depend on the location of the impurities in the real space and the location of the itinerant electrons in the reciprocal space.

**Symmetry constraints.** Before going to the details, we first consider the symmetry constraints on the RKKY interaction. As we shall show, the Heisenberg and DM terms in Eq. (8) dominate other terms. Therefore, we focus on these two terms in the analysis. The Heisenberg-type magnetic interaction, \( \mathbf{S}_1 \cdot \mathbf{S}_2, \) is always invariant under the crystalline symmetries. The DM-type interaction, \( \mathbf{D} \cdot (\mathbf{S}_1 \times \mathbf{S}_2), \) is characterized by the so-called DM vector, \( \mathbf{D}. \) Moreover, to guarantee the term a scalar, \( \mathbf{D} \) must be a pseudovector. A pseudovector behaves like a vector under the proper spatial symmetry whereas remain unchanged under inversion symmetry. This imposes strict constraints on the DM interaction [21] and makes it strongly depend on the positions of the impurities in Fig. 1(a).

**Numerical results.** We simulate the range functions in Eq. (8) numerically. Here, we only show the results corresponding to the condition where the impurities locate at the \( 2a \) Wyckoff positions in Fig. 1(a). The results correspondingly to the \( 2c \) Wyckoff positions are similar and more details are presented in the SM [63]. Specifically, for impurities in the same sublattice, the range functions for the RKKY interactions in Eq. (8) mediated by the itinerant electrons near the M and \( \Gamma \) points take the form

\[ \Lambda(\mathbf{R}, \mu) = -\frac{J^2}{\pi} \text{Im} \int_{\omega < \mu} d\omega \left( g_0^2 + g_1^2 + g_2^2 \right), \]

\[ D_{1(2)}(\mathbf{R}, \mu) = -\frac{2J^2}{\pi} \text{Re} \int_{\omega < \mu} d\omega \ g_0 g_{2(1)}, \]

\[ T_{ij}(\mathbf{R}, \mu) = -\frac{J^2}{\pi} \text{Im} \int_{\omega < \mu} d\omega \ g_i g_j, \]

where

\[ g_0 = \sum_{\alpha = \pm} \int \frac{d^2k}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \frac{1}{2\Xi_{\alpha}(\mathbf{k})} \omega - E^\alpha_{\mu}(\mathbf{k}) + i0^+, \]

\[ g_i = \sum_{\alpha = \pm} \int \frac{d^2k}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \frac{1}{2\Xi_{\alpha}(\mathbf{k})} \omega - E^\alpha_{\mu}(\mathbf{k}) + i0^+, \]

with \( i, j = 1, 2, k_{1(2)} = k_x(y), \) and \( 0^+ \) being a positive infinitesimal. In Eq. (10), \( E^\alpha_{\mu}(\mathbf{k}) = m(\mathbf{k}) \pm \Xi_{\alpha}(\mathbf{k}) \) are the eigenenergies of the itinerant electrons near the \( \theta = M, \Gamma \) points, where \( \Xi_{\alpha}(\mathbf{k}) = \sqrt{\lambda^2(k_x^2 + k_y^2) + f_{\theta}^2} \) with \( f_M = t'k_xk_y \) and \( f_{\Gamma} = t'. \) If the two impurities are in the different sublattices, in Eq. (8) only the Heisenberg term survives with the range function

\[ \Lambda(\mathbf{R}, \mu) = -\frac{J^2}{\pi} \text{Im} \int_{\omega < \mu} d\omega g^2, \quad D_{1}(\mathbf{R}, \mu) = T_{ij}(\mathbf{R}, \mu) = 0, \]

for the condition where the two impurities locate in the A sublattice at the \( 2a \) Wyckoff positions, and the DM vectors in the B sublattice is shown in Fig. 2(b) as the two sublattices are related by the inversion symmetry. If the two impurities locate in the same sublattice at the \( 2c \) Wyckoff positions, i.e. the \( A' (B') \) sublattice in Fig. 1(a), the DM vectors must be compatible with the \( C_{4v} \) group and we sketch the results in Figs. 2(d)(e).

It is worth pointing out that, in the above conditions the DM interactions are allowed because the inversion symmetry is absent within the same sublattice at \( 2a (2c) \) Wyckoff positions. When the two impurities locate in the different sublattices at the \( 2a (2c) \) Wyckoff positions, the inversion symmetry always exists and the DM interaction must vanish. The symmetry constraints on the DM interaction corresponding to other impurity configurations can be analyzed similarly. We note that, the above symmetry analysis does not depend on the location of the itinerant electrons in the BZ.

**FIG. 2:** (color online) (a)(b) and (d)(e) sketch the directions of the DM vectors \( \mathbf{D} \) in Eq. (8), corresponding to the condition that the two impurities locate in the same sublattice at the \( 2a \) and \( 2c \) Wyckoff positions in Fig. 1(a) respectively. (a) (d) and (b) (e) represent the \( A (A') \) and \( B (B') \) sublattices related by the inversion symmetry in Fig. 1(a). The DM interactions in (a)(b) and (d)(e) support the antiskyrmion-type and Néel-type spin textures shown in (c) and (f) respectively.
where

\[ y' = \sum_{\alpha = \pm} \int \frac{d^2k}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2 + \pi_0)} \frac{1}{2\Xi_0(k)} \omega - E''_\alpha(k) + i0^+ \]

(12)

Based on Eqs. (9)–(12), we plot the RKKY interactions in different cases in Fig. 3 and Fig. 4. Accordingly, one can find the following features of the RKKY interactions in the system.

The DM interaction can exist only when the two impurities are in the same sublattice, which is consistent with the symmetry analysis in the above. Moreover, the itinerant electrons near M are more in favor of the DM interaction which is comparable to the Heisenberg term, as indicated in Figs. 3(a)–(c); and a larger \( \lambda \) leads to the stronger DM term in comparison with the Heisenberg term, as shown in Figs. 3(a)(b). The latter reflects the fact that, the local inversion symmetry breaking effect in the system is characterized by \( \lambda \), i.e. the strength of the inversion symmetric Rashba SOC; and the former arises from the fact that, near \( \Gamma \) the system is more like a conventional centrosymmetric system with vanishing samll effective Rashba SOC on the energy bands, while near M the system is nearly a direct product of two Rashba electron gas systems, as indicated in the effective theories in Eqs. (2)(4). Moreover, according to the effective Rashba SOC which can be featured by the spin polarizations on the energy bands shown in Fig. 1(b), one can conclude that the smaller Fermi energy for itinerant electrons near M, i.e. the smaller \( k \) near M, is better for the DM interaction.

In the condition where the two impurities locate in the same sublattice at the 2\( \alpha \) Wyckoff positions in Fig. 1(a), \( (a) \) corresponds to the condition \( \mathbf{R} \parallel [11] \), where it satisfies \( T_{xx} = T_{yy} = T_{zy} \). (b) shows \( T_{xy} \) with respect to \( g = 0.2, \theta = \pi/4 \lambda = 0.15, \mu = 0.2, | \mathbf{R} | = 27 \).

The Ising and anisotropic terms are much weaker than the Heisenberg and DM terms. In Fig. 4(a), we show the \( T_{ij} \) corresponding to the condition where the two impurities are arranged along the [11] direction in the same sublattice, i.e. \( \mathbf{R} \parallel [11] \). Along the [11] direction, it satisfies \( g_1 = g_2 \) in Eq. (10), leading to that the Ising terms equals the anisotropic terms, i.e. \( T_{xx} = T_{yy} = T_{zy} \). In addition, these terms oscillate with two different periods \( P_1 \) and \( P_2 \) as indicated in Fig. 4(a), which origin from the interference of two distinct Fermi surface as shown in Fig. 1(b). These two periods can be estimated with \( 2\pi|k_{F1} + k_{F2}|^{-1} = 6.6 \) and \( 2\pi|k_{F1} - k_{F2}|^{-1} = 26 \), with \( k_{Fi} \) the i-th Fermi wave vectors along the [11] direction [65]. In Fig. 4(b), we show the anisotropic term \( T_{xy} \) with respect to \( \mathbf{R} \) in different directions. As shown, \( T_{xy} \) is prohibited along the \( x \) \( (y) \) axis by the mirror symmetry \( \{ M_y | 0 \} \) \( \{ M_x | 0 \} \).

Discussion and conclusion. In the above, based on the symmetry and numerical analysis, we show the rich and controllable RKKY interactions among impurities in the nonsymmetric crystal respecting the \( P4/\text{mmm} \) space group. The substantial DM interaction mediated by itinerant electrons near the BZ corner, whose form varies in accordance with the positions of the magnetic impurities, can lead to rich magnetic spin textures in the system. For instance, for impurities in the same sublattice at the 2\( \alpha \) Wyckoff positions, the \( D_{2d} \) symme-
ic DM interaction in Figs. 2(a)(b) supports the anti-skyrmion
type spin texture presented in Fig. 2(c); while for impurities
in the same sublattice at the $2c$ Wyckoff positions, the $C_{4v}$
symmetric DM interaction in Figs. 2(d)(e) favors the Néel-
type skyrmion spin texture shown in Fig. 2(f) [43, 44, 66]. In
both cases, the skyrmion in the different sublattices carry op-
posite helicities [67–70]. Moreover, the relative position of
skyrmion centers in the two sublattices can be adjusted by the
intersublattice Heisenberg interaction, which is weak medi-
ated by itinerant electrons near the BZ corner as indicated in
Fig. 3(d). If the intersublattice interaction is strong, which can
be true if there are additional itinerant electrons near the BZ
center, the skyrmion spin textures in the two sublattices hy-
bridize, and a spiral magnetic order may be supported instead
[43, 44].

In summary, we theoretically investigate the RKKY in-
teraction between magnetic impurities in a nonsymmorphic
crystal respecting the space group $P4/nmm$. We show that
though the system is globally centrosymmetric, various types
of magnetic interactions, including the Heisenberg-type, the
DM-type, the Ising-type and the anisotropic RKKY interac-
tions, can appear according to the configurations of the im-
purities in the real space, and their strength can be controlled
by adjusting the locations of the itinerant electrons in the re-
ciprocal space. Our study reveals the role that the nonsym-
morphic symmetries play in affecting magnetism, and sug-
gests that the nonsymmorphic crystals are potential platforms
to support rich types of magnetic orders.

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Here, we specify the point group part of those symmetries as $m_y : (x, y, z) \mapsto (x, -y, z)$, $s_{4z} : (x, y, z) \mapsto (y, -x, -z)$, $m_{xy} : (x, y, z) \mapsto (-y, -x, z)$, $c_{4z} : (x, y, z) \mapsto (-y, x, z)$, $i : (x, y, z) \mapsto (-x, -y, -z)$. The origin of the coordinate system is defined on the site in fig. 1.

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APPENDIX A: THE CONSTRUCTION OF EFFECTIVE MODEL FROM 2c WYCKOFF POSITION

In this section, we present the detailed construction of the low-energy effective model \( \mathcal{H}_{M,2c} \) near the boundary of the BZ, i.e., M point. The bases in the reciprocal space and in the real space are related by the Fourier transform

\[
|\phi_{2c,1}(k)| = \sum_j e^{i k^j R_{2c,1}^j} |\phi_{2c,1}(R_{2c,1}^j)|, \quad |\phi_{2c,2}(k)| = \sum_j e^{i k^j R_{2c,2}^j} |\phi_{2c,2}(R_{2c,2}^j)|,
\]

where \( R_{2c,i}^j \) is the position of orbital located at the \( i \)-th 2c Wyckoff in the \( j \)-th unit cell satisfying \( R_{2c,1}^j - R_{2c,2}^j = \tau_0 \), and \( |\phi_{2c,1/2}(r - R_{2c,1/2})| \) are the localized atomic-like orbitals located in the position of \( R_{2c,1/2} \).

Firstly, we need to figure out how the symmetry operations act on the basis \( \{ |\phi_{2c,1}(r)|, |\phi_{2c,2}(r)| \} \equiv (c_{2c,1}, c_{2c,2})|0\rangle \), where \( |0\rangle \) is the vacuum state, \( c_{2c,i} \) is the creation operator of the orbitals located at \( i \)-th 2c Wyckoff position, and the spin index has been omitted for convenience. When a spatial symmetry \( \{ \hat{g} a_i \} \) acts on the basis function, we have

\[
\{ \hat{g} |0\rangle |\phi_{2c,1}^k(r)\rangle = |\phi_{2c,1}^k(g^{-1}r)\rangle = \eta_{2c,1} |\phi_{2c,1}^k(r)\rangle,
\]

\[
\{ \hat{g} |0\rangle |\phi_{2c,2}^k(r)\rangle = |\phi_{2c,2}^k(g^{-1}r)\rangle = \sum_j e^{i k^j R^j} \eta_{2c,2} |\phi_{2c,2}(g^{-1}[R - R^j - \tau_0])\rangle
\]

\[
= \eta_{2c,2} \sum_j e^{i k^j (R^j + \tau_0)} |\phi_{2c,2}(R - g^{-1} R^j - g^{-1} \tau_0)\rangle
\]

\[
= \eta_{2c,2} \sum_j e^{i (g(k) - k) \cdot R^j} t e^{i (g(k) - k) \cdot \tau_0} |\phi_{2c,2}(R - g^{-1} R^j - g^{-1} \tau_0)\rangle
\]

\[
= \eta_{2c,2} \sum_j e^{-i (g(k) - k) \cdot \tau_0} e^{i (g(k) - g) \cdot \tau_0} |\phi_{2c,2}(R - g^{-1} R^j - g^{-1} \tau_0)\rangle
\]

\[
= \eta_{2c,2} e^{-i (g(k) - k) \cdot \tau_0} \sum_j e^{i (g(k) - g) \cdot \tau_0} |\phi_{2c,2}(R - g^{-1} R^j - g^{-1} \tau_0)\rangle
\]

\[
\{ E a_i^\dagger |\phi_{2c,1}^k(r)\rangle \} = e^{-i k^j a_i^\dagger} |\phi_{2c,1}^k(r)\rangle,
\]

\[
\{ E a_i |\phi_{2c,2}^k(r)\rangle \} = e^{-i k^j a_i} |\phi_{2c,2}^k(r)\rangle,
\]

\[
\{ E |\phi_{2c,1}(r)\rangle \} = \sum_j e^{i k^j (R^j + \tau_0 - \tau_0)} |\phi_{2c,2}(R - R^j - \tau_0)\rangle = e^{-i k^j \tau_0} |\phi_{2c,2}^k(r)\rangle
\]

\[
\{ E |\phi_{2c,2}(r)\rangle \} = \sum_j e^{i k^j (R^j + \tau_0 - \tau_0)} |\phi_{2c,1}(R - R^j - \tau_0 - \tau_0)\rangle = e^{-i k^j \tau_0} |\phi_{2c,1}^k(r)\rangle
\]

where \( \eta_{2c,i} \) is the \( \hat{g} \)'s eigenvalue of the orbital located at \( i \)-th 2c Wyckoff position. Thus, the matrices of the generator of the little group \( G_k \) at the \( \Gamma \) and M points are summarized in Table A1.

---

**TABLE A1:** Matrix form for the symmetry operations, \( \{ I |\tau_0 \}, \{ M_i |0 \}, \{ C_{4z} |0 \} \) and \( T \) at \( \Gamma \) and M point.

| \( I |\tau_0 \) | \( M_i |0 \) | \( C_{4z} |0 \) | \( T \) |
|---|---|---|---|
| \( \Gamma \) | \( -s_0 \sigma_1 \) | \( -i s_2 \sigma_0 \) | \( e^{-i \pi/3} s_0 \) | \( i s_2 \sigma_0 K \) |
| \( M \) | \( -s_0 \sigma_1 \) | \( -i s_2 \sigma_3 \) | \( e^{-i \pi/3} s_0 \) | \( i s_2 \sigma_0 K \) |

---

Due to the fact that the single-particle Hamiltonian \( H(k) = f_{ij}(k)s_i \sigma_j \) is a bilinear map on the single-particle Hilbert space, the matrix form and \( f(k) \) can furnish a representation of \( D_{4h} \). We first consider the time reversal symmetry and the inversion symmetry, which constrain the system as

\[
T \mathcal{H}_{M,2c} \mathcal{T}^{-1} = \mathcal{H}_{M,2c}(-k), \quad \mathcal{H}_{M,2c} \mathcal{T}^{-1} = \mathcal{H}_{M,2c}(-k).
\]

(A3)

The four-band model \( \mathcal{H}_{M,2c}(k) \) can be generally expressed in the form of the sixteen \( \Gamma = s_i \sigma_j \) matrices. The constraints in Eq. (A3) merely allow six \( \Gamma \) matrices, i.e., \( s_0 \sigma_0, s_0 \sigma_1, s_0 \sigma_2, s_1 \sigma_3, s_2 \sigma_3 \) and \( s_3 \sigma_3 \), to appear in \( \mathcal{H}_{M,2c}(k) \). Then, we consider the constraints of the crystalline symmetries. At the \( \Gamma \) point of BZ, one can classify the above six matrices as shown in Table A2.

Therefore, \( \mathcal{H}_{M,2c}(k) \) must take the following form
The corresponding energy dispersions and the spin-polarization in the $A$-sublattice space are shown in Fig. A1(a). It can be clearly seen that the spin polarization near the $\Gamma$ point is almost 0. Note that the length of arrow representing the strength of spin-polarization in Fig. A1(a) is magnified by a factor of 20.

Similarly, at the $M$ point of BZ, one can classify the above six matrices as shown in Table A3. Therefore, $\mathcal{H}_{M,2c}(\mathbf{k})$ must take the following form

$$
\mathcal{H}_{M,2c}(\mathbf{k}) = (t(k_x^2 + k_y^2) - \mu)s_0\sigma_0 + \lambda(k_x s_2\sigma_3 - k_y s_1\sigma_3) + t' s_0\sigma_1.
$$

The corresponding energy dispersions and the spin-polarization in the $A$-sublattice space are shown in Fig. A1(b).

**APPENDIX B: THE GREEN’S FUNCTION IN THE MOMENTUM-ENERGY SPACE**

In this section, we give a detailed derivation of the Green’s function in the momentum-energy space. The low-energy effective model $H_{2a,M}$ is

$$
\mathcal{H}_{M,2a}(\mathbf{k}) = m(\mathbf{k})s_0\sigma_0 + \lambda k_x s_2\sigma_3 + \lambda k_y s_1\sigma_3 + t'k_xk_ys_0\sigma_1.
$$

where $m(\mathbf{k}) = t(k_x^2 + k_y^2)$ with $t$, $t'$, $\lambda$ all constants. The bases in the reciprocal space and in the real space are related by the Fourier transform

$$
|\phi_{2a,1}(\mathbf{k})\rangle = \sum_j e^{i\mathbf{k} \cdot \mathbf{R}_{2a,1}^j} |\phi_{2a,1}(\mathbf{R}_{2a,1}^j)\rangle, \quad|\phi_{2a,2}(\mathbf{k})\rangle = \sum_j e^{i\mathbf{k} \cdot \mathbf{R}_{2a,2}^j} |\phi_{2a,2}(\mathbf{R}_{2a,2}^j)\rangle,
$$
where \( \mathbf{R}_{2a,i}^j \) is the position of orbital located at the \( i \)-th 2c Wyckoff in the \( j \)-th unit cell satisfying \( \mathbf{R}_{2a,1}^j - \mathbf{R}_{2a,2}^j = \tau_0 \), and \( |\phi_{2a,1/2}(\mathbf{r} - \mathbf{R}_{2a,1}^j)\rangle \) are the localized atomic-like orbitals located in the position of \( \mathbf{R}_{2a,1}^j/\mathbf{R}_{2a,2}^j \). The energy dispersions are

\[
E_\pm(k_x, k_y) = t(k_x^2 + k_y^2) \pm \sqrt{\lambda^2(k_x^2 + k_y^2) + t^2k_x^2k_y^2} \equiv m(k) \pm \Xi(k),
\]

(B3)

which are two-fold degenerate. The corresponding degenerate eigenstates \( |\Psi_{\pm}(k)\rangle \) are

\[
|\Psi_{+(1)}(k)\rangle = \frac{1}{\sqrt{2}} \left[ \lambda(-ik_x + k_y)\Xi(k), -1, 0, t'k_xk_y|^{T}, |\Psi_{+(2)}(k)\rangle = \frac{1}{\sqrt{2}} \left[ -t'k_xk_y, 0, 1, \lambda(ik_x + k_y)|^{T},
\right.
\]

\[
|\Psi_{-(3)}(k)\rangle = \frac{1}{\sqrt{2}} \left[ \lambda(-ik_x + k_y)\Xi(k), 1, 0, t'k_xk_y|^{T}, |\Psi_{-(4)}(k)\rangle = \frac{1}{\sqrt{2}} \left[ t'k_xk_y, 0, 1, -\lambda(ik_x + k_y)|^{T}.
\right.
\]

(B4)

In order to obtain the retarded Green’s function in real space, we first calculate the corresponding Green’s function in momentum space:

\[
[G_{0}^R(R_i, R_j, \epsilon)]_{\mu\mu'} = \sum_{n=1}^{4} \frac{|\Psi_n(k)\rangle_{\mu} \langle\Psi_n(k)|_{\mu'}}{\epsilon - E_n(k) + i\eta},
\]

where \( k = (k_x, k_y) \). After some straightforward calculation, we have

\[
G_{M,2a}^R(k, \epsilon) = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+}, \quad g_1 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+},
\]

\[
G_{M,2c}^R(k, \epsilon) = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+}, \quad g_1 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+},
\]

(B5)

\[
G_{M,2c}^R(k, \epsilon) = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+}, \quad g_1 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+},
\]

where \( \Xi(k) = \sqrt{\lambda^2(k_x^2 + k_y^2) + t^2k_x^2k_y^2} \), \( E_{\pm}(k_x, k_y) = m(k) \pm \Xi(k) \). The real-space Green’s function can be obtained as

\[
G_{M,2a}(R_1, R_2, \epsilon) = g_0s_0s_0 + g_1s_2s_3 + g_2s_1s_3 + g' s_0s_1,
\]

(B8)

where \( g_0, g_1, g_2, g' \) are the \((R_1 - R_2)\)- and \( \omega \)- dependent functions:

\[
g_0 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+}, \quad g_1 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+},
\]

\[
g_2 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+}, \quad g' = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+}.
\]

(B9)

Similarly, for the effective model \( \mathcal{H}_{M,2c} \), the corresponding Green’s function is

\[
G_{M,2c}^R(k, \epsilon) = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+}, \quad g_1 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+},
\]

\[
g_2 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{-\alpha \lambda k_y}{\omega - E_a(k) + i0^+}, \quad g' = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2 + \tau_0)} \frac{1}{\Xi(k)} \frac{\alpha \lambda k_x}{\omega - E_a(k) + i0^+}.
\]

(B10)

(B11)

where \( g_0, g_1, g_2, g' \) are the \((R_1 - R_2)\)- and \( \omega \)- dependent functions:

\[
g_0 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+}, \quad g_1 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{1}{\omega - E_a(k) + i0^+},
\]

\[
g_2 = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2)} \frac{1}{\Xi(k)} \frac{-\alpha \lambda k_y}{\omega - E_a(k) + i0^+}, \quad g' = \frac{1}{2} \sum_{\alpha=\pm} \int \frac{d^2k}{(2\pi)^2} e^{ik(R_1 - R_2 + \tau_0)} \frac{1}{\Xi(k)} \frac{\alpha \lambda k_x}{\omega - E_a(k) + i0^+}.
\]

(B12)
For the effective model $\mathcal{H}_{\Gamma,2a}$, the corresponding Green’s function is
\begin{equation}
G_{\Gamma,2a}^R(\mathbf{k}, \epsilon) = \frac{1}{2} \frac{1}{\epsilon - E_0^R(\mathbf{k}) + i\eta^+} \left[ s_0 \sigma_0 - \frac{t'}{2} \xi(\mathbf{k}) s_0 \sigma_1 + \frac{\lambda k_y}{\xi(\mathbf{k})} s_0 \sigma_3 - \frac{\lambda k_x}{\xi(\mathbf{k})} s_2 \sigma_3 \right]
+ \frac{1}{2} \frac{1}{\epsilon - E_0^A(\mathbf{k}) + i\eta^+} \left[ s_0 \sigma_0 + \frac{t'}{2} \xi(\mathbf{k}) s_0 \sigma_1 + \frac{\lambda k_y}{\xi(\mathbf{k})} s_1 \sigma_3 + \frac{\lambda k_x}{\xi(\mathbf{k})} s_3 \sigma_3 \right],
\end{equation}
where $\xi(\mathbf{k}) = \sqrt{\lambda^2 (k_x^2 + k_y^2)} + t^2 E_{\pm}(k_x, k_y) = m(k) \pm \Xi(k)$. The real-space Green’s function can be obtained as
\begin{equation}
G_{\Gamma,2a}(\mathbf{R}_1, \mathbf{R}_2, \epsilon) = g_0 s_0 \sigma_0 + g_1 s_2 \sigma_3 + g_2 s_1 \sigma_3 + g' s_0 \sigma_1,
\end{equation}
where $g_0, g_1, g_2, g'$ are the $(\mathbf{R}_1 - \mathbf{R}_2)$- and $\omega$- dependent functions:
\begin{equation}
g_0 = \frac{1}{2} \sum_{\alpha = \pm} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \frac{1}{\Xi(\mathbf{k})} \left( \epsilon - E_0(\mathbf{k}) + i\eta^+ \right), \quad g_1 = \frac{1}{2} \sum_{\alpha = \pm} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \frac{\alpha \lambda k_x}{\Xi(\mathbf{k})} \left( \epsilon - E_0(\mathbf{k}) + i\eta^+ \right),
\end{equation}
\begin{equation}
g_2 = \frac{1}{2} \sum_{\alpha = \pm} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \frac{\alpha \lambda k_y}{\Xi(\mathbf{k})} \left( \epsilon - E_0(\mathbf{k}) + i\eta^+ \right), \quad g' = \frac{1}{2} \sum_{\alpha = \pm} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2 + \tau_0)} \frac{\alpha \lambda k_x}{\Xi(\mathbf{k})} \left( \epsilon - E_0(\mathbf{k}) + i\eta^+ \right).
\end{equation}

For the effective model $\mathcal{H}_{\Gamma,2c}$, the corresponding Green’s function is
\begin{equation}
G_{\Gamma,2c}^R(\mathbf{k}, \epsilon) = \frac{1}{2} \frac{1}{\epsilon - E_0^R(\mathbf{k}) + i\eta^+} \left[ s_0 \sigma_0 - \frac{t'}{2} \xi(\mathbf{k}) s_0 \sigma_1 + \frac{\lambda k_y}{\xi(\mathbf{k})} s_0 \sigma_3 - \frac{\lambda k_x}{\xi(\mathbf{k})} s_2 \sigma_3 \right]
+ \frac{1}{2} \frac{1}{\epsilon - E_0^A(\mathbf{k}) + i\eta^+} \left[ s_0 \sigma_0 + \frac{t'}{2} \xi(\mathbf{k}) s_0 \sigma_1 - \frac{\lambda k_y}{\xi(\mathbf{k})} s_1 \sigma_3 + \frac{\lambda k_x}{\xi(\mathbf{k})} s_3 \sigma_3 \right],
\end{equation}
where $\Xi(\mathbf{k}) = \sqrt{\lambda^2 (k_x^2 + k_y^2)} + t^2 E_{\pm}(k_x, k_y) = m(k) \pm \Xi(k)$. The real-space Green’s function can be obtained as
\begin{equation}
G_{\Gamma,2c}(\mathbf{R}_1, \mathbf{R}_2, \epsilon) = g_0 s_0 \sigma_0 + g_1 s_2 \sigma_3 + g_2 s_1 \sigma_3 + g' s_0 \sigma_1,
\end{equation}
where $g_0, g_1, g_2, g'$ are the $(\mathbf{R}_1 - \mathbf{R}_2)$- and $\omega$- dependent functions:
\begin{equation}
g_0 = \frac{1}{2} \sum_{\alpha = \pm} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \frac{1}{\Xi(\mathbf{k})} \left( \epsilon - E_0(\mathbf{k}) + i\eta^+ \right), \quad g_1 = \frac{1}{2} \sum_{\alpha = \pm} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \frac{\alpha \lambda k_x}{\Xi(\mathbf{k})} \left( \epsilon - E_0(\mathbf{k}) + i\eta^+ \right),
\end{equation}
\begin{equation}
g_2 = \frac{1}{2} \sum_{\alpha = \pm} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \frac{\alpha \lambda k_y}{\Xi(\mathbf{k})} \left( \epsilon - E_0(\mathbf{k}) + i\eta^+ \right), \quad g' = \frac{1}{2} \sum_{\alpha = \pm} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2 + \tau_0)} \frac{\alpha \lambda k_x}{\Xi(\mathbf{k})} \left( \epsilon - E_0(\mathbf{k}) + i\eta^+ \right).
\end{equation}

**APPENDIX C: THE DERIVATION OF THE RKKY INTERACTION FROM THE GREEN’S FUNCTION**

In this section, we give the detailed derivation of the RKKY interaction from the real-space Green’s function. In the above section, we show that the real-space Green’s function has the form:
\begin{equation}
G_0(\mathbf{R}_1, \mathbf{R}_2, \epsilon) = g_0 s_0 \sigma_0 + g_1 s_2 \sigma_3 + g_2 s_1 \sigma_3 + g' s_0 \sigma_1,
\end{equation}
where $g_i$ depends on the locations of the Fermi surface and the orbitals.

Firstly, we consider the RKKY interaction between the same sublattice $A$, which is given by
\begin{equation}
H_{\text{RKKY}} = -\frac{J^2}{\pi} \text{Im} \int_{\epsilon < \mu} d\epsilon \text{Tr} \left[ S_2 \cdot \frac{\sigma_0 + \sigma_z}{2} \otimes s G_0^R(\mathbf{R}_2, \mathbf{R}_1, \epsilon) S_1 \cdot \frac{\sigma_0 + \sigma_z}{2} \otimes s G_0^R(\mathbf{R}_1, \mathbf{R}_2, \epsilon) \right]
\end{equation}
\begin{equation}
= -\frac{J^2}{\pi} \text{Im} \int_{\epsilon < \mu} d\epsilon \text{Tr} \left[ S_2 \cdot s G_{0,A}^R(\mathbf{R}_2, \mathbf{R}_1, \epsilon) S_1 \cdot s G_{0,A}^R(\mathbf{R}_1, \mathbf{R}_2, \epsilon) \right]
\end{equation}
where $G_{0,A}^R(\mathbf{R}_2, \mathbf{R}_1, \epsilon)$ is defined as
\begin{equation}
G_{0,A}^R(\mathbf{R}_1, \mathbf{R}_2, \epsilon) = \langle \sigma_z = +1 | G_0(\mathbf{R}_1, \mathbf{R}_2, \epsilon) | \sigma_z = +1 \rangle = g_0 s_0 + g_1 s_2 + g_2 s_1.
\end{equation}
The integrand of Eq. (C2) can be expanded as
\[
\sum_{\alpha, \beta=1}^{3} S_{\alpha^2} S_{\beta^2} \text{Tr}[s_{\alpha}(g_0 s_0 - g_2 s_1 - g_1 s_2)s_{\beta}(g_0 s_0 + g_2 s_1 + g_1 s_2)],
\]  \hspace{1cm} (C4)
where we use the fact that \(g_0(\mathbf{R}_1, \mathbf{R}_2) = g_0(\mathbf{R}_2, \mathbf{R}_1), \ g_1(\mathbf{R}_1, \mathbf{R}_2) = -g_1(\mathbf{R}_2, \mathbf{R}_1), \) and \(g_2(\mathbf{R}_1, \mathbf{R}_2) = -g_2(\mathbf{R}_2, \mathbf{R}_1). \) The Eq. (C4) contains five terms:
\[
(g_1^2 + g_2^2 + g_0^2)S_1 \cdot S_2, \ 2ig_2g_0(S_1 \times S_2)_x, \ 2ig_1g_0(S_1 \times S_2)_y, \ -2g_2^2 S_1z S_2x, \ -2g_1^2 S_1y S_2y, \ -2g_1g_2(S_1z S_2y + S_1y S_2x). \]  \hspace{1cm} (C5)
Finally, the RKKY interaction \(H_{\text{RKKY}}^A \) between the same sublattice \(A\) can be divided into four type: the Heisenberg-type \(\Lambda(\mathbf{R}, \mu)\) \(S_1 \cdot S_2\), the DM-type \(D_i(S_1 \times S_2)_i\), the Ising-type \((T_{ij} S_1 S_2)_i\) and the anisotropic terms \((T_{ij} S_1 S_2)_i\), of which strength can be calculated by
\[
\Lambda(\mathbf{R}, \mu) = -\frac{J^2}{\pi} \text{Im} \int_{\omega<\mu} d\omega \ (g_0^2 + g_1^2 + g_2^2), \quad D_i(\mathbf{R}, \mu) = -\frac{2J^2}{\pi} \text{Re} \int_{\omega<\mu} d\omega \ g_0 g_2, \quad T_{ij}(\mathbf{R}, \mu) = -\frac{J^2}{\pi} \text{Im} \int_{\omega<\mu} d\omega \ g_i g_j, \]  \hspace{1cm} (C6)
Similarly, the RKKY interaction between the same sublattice \(B\), which is given by
\[
H_{\text{RKKY}}^B = -\frac{J^2}{\pi} \text{Im} \int_{\omega<\mu} d\omega \ Tr[S_2 \cdot [\frac{\sigma_0 - \sigma_z}{2} \otimes s]G^R_0(\mathbf{R}_2, \mathbf{R}_1, \epsilon)S_1 \cdot [\frac{\sigma_0 - \sigma_z}{2} \otimes s]G^R_0(\mathbf{R}_1, \mathbf{R}_2, \epsilon)] \]  \hspace{1cm} (C7)
where \(G^R_{0,B}(\mathbf{R}_1, \mathbf{R}_2, \epsilon)\) is defined as \(G^R_{0,B}(\mathbf{R}_1, \mathbf{R}_2, \epsilon) \equiv \langle \sigma_z = -1|G_0(\mathbf{R}_1, \mathbf{R}_2, \epsilon)|\sigma_z = -1 \rangle = g_0 s_0 - g_1 s_2 - g_2 s_1. \) \hspace{1cm} (C8)
The RKKY interaction \(H_{\text{RKKY}}^{AB} \) between the distinct sublattice \(A\) and \(B\), which is given by
\[
H_{\text{RKKY}}^{AB} = -\frac{J^2}{\pi} \text{Im} \int_{\omega<\mu} d\omega \ Tr[S_2 \cdot [\frac{\sigma_0 + \sigma_z}{2} \otimes s]G^R_0(\mathbf{R}_2, \mathbf{R}_1, \epsilon)S_1 \cdot [\frac{\sigma_0 - \sigma_z}{2} \otimes s]G^R_0(\mathbf{R}_1, \mathbf{R}_2, \epsilon)] \]  \hspace{1cm} (C10)
where \(G^R_{0,AB}(\mathbf{R}_2, \mathbf{R}_1, \epsilon)\) is defined as \(G^R_{0,AB}(\mathbf{R}_1, \mathbf{R}_2, \epsilon) \equiv \langle \sigma_z = +1|G_0(\mathbf{R}_1, \mathbf{R}_2, \epsilon)|\sigma_z = -1 \rangle = g' s_0. \) \hspace{1cm} (C11)
The RKKY interaction \(H_{\text{RKKY}}^{AB} \) between the distinct sublattice only contains the Heisenberg-type term, of which strength can be calculated by
\[
\Lambda(\mathbf{R}, \mu) = -\frac{J^2}{\pi} \text{Im} \int_{\omega<\mu} d\omega \ g'^2, \]  \hspace{1cm} (C12)