The prolonged decay of RKKY interactions by interplay of relativistic and non-relativistic electrons in semi-Dirac semimetals

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Abstract

The Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction has been extensively explored in isotropic Dirac systems with linear dispersion, which typically follows an exponential decaying rate with the impurity distance \( R \), i.e., \( J \propto 1/R^d \) \((1/R^2−1)\) in \( d \)-dimensional systems at finite (zero) Fermi energy. This fast decay makes it rather difficult to be detected and limits its application in spintronics. Here, we theoretically investigate the influence of anisotropic dispersion on the RKKY interaction, and find that the introduction of non-relativistic dispersion in semi-Dirac semimetals (S-DSMs) can significantly prolong the decay of the RKKY interaction and can remarkably enhance the Dzyaloshinskii–Moriya interaction around the relativistic direction. The underlying physics is attributed to the highly increased density of states in the linear-momentum direction as a result of the interplay of relativistic and non-relativistic electrons. Furthermore, we propose a general formula to determine the decaying rate of the RKKY interaction, extending the typical formula for isotropic DSMs. Our results suggest that the S-DSM materials are a powerful platform to detect and control the magnetic exchange interaction, superior to extensively adopted isotropic Dirac systems.

Over the past decades, the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction has been extensively studied in a variety of materials, e.g., graphene [1–6], \( \alpha\text{-}T_5 \) model [7], Dirac/Weyl semimetals (DSMs/WSMs) [8–10], phosphorene [11], edge/surface bands of topological materials [12–17] and so on. These researches have showed a potential application for the RKKY interaction to realize magnetization in non-magnetic materials. A typical example is the realization of quantized anomalous Hall effect in topological insulators [16, 18]. Moreover, the RKKY interaction has been proven to characterize the intrinsic properties of materials, e.g., the band topology [17, 19], rich spin textures [9], and the Rashba splitting [20]. Although the RKKY interaction has wide prospect in the area of spintronics, there are still many obstacles to overcome. One is that the RKKY interaction is too weak to be detected since it usually decays fast with the increased impurity distance \( R \). For example, in materials with isotropic linear dispersion, the RKKY interaction presents a fast decaying law as \( \sin(2k_F R)/R^d \) \((1/R^2−1)\) at finite (zero) Fermi energy. To overcome this obstacle, new research perspectives are expected. In addition to some special devices (e.g., the PN junction [21]), materials with peculiar dispersions are promising candidates to realize the prolonged RKKY interaction.

Recently, semi-Dirac semimetals (S-DSMs) have attracted more and more attention in condensed matter physics due to their highly anisotropic electronic structure. Different from the isotropic linear dispersions
around the Dirac points, the low-energy model of S-DSM exhibits a linear dispersion in some directions but disperses quadratically in the others, which allows the coexistence of relativistic and non-relativistic electrons. This peculiar dispersion leads to many new physical properties, such as the anisotropic transports [22, 23], nonsaturating large magnetoresistance [24], unique optical properties [25–27], and quantum thermoelectrics [28]. Nevertheless, the magnetic property, especially the RKKY interaction between magnetic impurities, with respect to S-DSMs receives no attention. It is expected that the strong anisotropic dispersion of the S-DSMs will affect the RKKY interaction significantly.

In this letter, we theoretically investigate the influence of anisotropic dispersion on the RKKY interaction, and take S-DSMs as examples of anisotropic structure and compare them with isotropic DSMs/WSMs. We find that the decaying rate of the RKKY interaction in S-DSMs, including all types of two or three dimensions, can be highly prolonged along the relativistic axis, in contrast to the fast-decaying RKKY interaction in DSMs/WSMs. Furthermore, we propose a general formula to determine the decaying rate of the RKKY interaction for anisotropic DSMs with arbitrary dimensions.

RKKY theory—RKKY interaction describes an indirect exchange interaction, mediated by itinerant electrons, between two impurities embedded in the material. We start from the Hamiltonian

\[ H = H_0 + \lambda \sum_{i=1,2} s_i \cdot s_i, \]

where \( H_0 \) stands for the host materials and \( \lambda \) is spin exchange between the itinerant electron spin \( s_i (s_i = \sum_{\alpha, \beta} c_{i \alpha} \sigma_{\alpha \beta} c_{i \beta}^\dagger \) with \( \sigma_{\alpha \beta} \) being the matrix element of the Pauli operator) and the impurity spin \( S_i \), located at \( r_i \). For weak coupling \( \lambda \), we can use the standard perturbation theory [29–31], and up to the second order of \( \lambda \), the RKKY interaction at zero temperature can be calculated by,

\[ H_{\text{RKKY}} = -\frac{\lambda^2}{\pi} \Im \int_{-\infty}^{\infty} \text{Tr}[(s_1 \cdot \sigma) G(R, \omega) (s_2 \cdot \sigma) G(-R, \omega)] d\omega, \]

where \( G(\pm R, \omega) \) is the retarded Green’s function with respect to \( H_0 \) in real space and \( u_F \) is the Fermi energy. After tracing the spin degrees of freedom in equation (2), the RKKY interaction can be written in the form of

\[ H_{\text{RKKY}} = \sum_{\alpha, \beta = x, y, z} J^{\alpha \beta} s_1^\alpha s_2^\beta, \]

with

\[ J^{\alpha \beta} = -\frac{\lambda^2}{\pi} \Im \int_{-\infty}^{\infty} \sum_{\alpha, \beta = x, y, z} \Lambda_{ij} (R, \omega) \text{Tr}[\sigma_\alpha \sigma_\beta \sigma_\beta] d\omega, \]

where we denote matrix of Green’s function as \( G(\pm R, \omega) = \sum_{\alpha, \beta = x, y, z} \Lambda_{ij} (\pm R, \omega) \sigma_i \) and \( \Lambda_{ij} (R, \omega) = G_i (R, \omega) G_j (-R, \omega) \). In equation (4), the trace part determines the spin exchange type and \( \Lambda_{ij} (R, \omega) \) determines the decaying rate with impurity distance \( R = r_2 - r_1 \). Physically, \( \Lambda_{ij} (R, \omega) \) characterizes the spin \( \sigma_i \) disturbance [32] of site \( r_1 \) as a response to the spin \( \sigma_j \) of site \( r_2 \).

Universal RKKY decay for isotropic materials—obviously, the decay of the RKKY interaction is determined by \( \Lambda_{ij} (R, \omega) \), which is closely related to material type. Considering a \( d \)-dimensional system with linear Dirac cone, \( H_0 = v k \cdot \sigma \), where \( v \) is the Fermi velocity, we have

\[ G_i (R, \omega) = \frac{1}{R^{(d-1)/2}} \omega^{(d-1)/2} e^{i \omega R/v}, \]

with \( R = |R| \). The resulting RKKY interaction is

\[ J^{\alpha \beta} (u_F \neq 0) \propto \frac{1}{R^d} \sin \left( \frac{2u FR}{v} \right), \]

\[ J^{\alpha \beta} (u_F = 0) \propto \frac{1}{R^{d+\zeta}} = \frac{1}{R^{d-1}}, \]

where \( \zeta = d - 1 \) is the exponent of the density of states (DOS) of DSMs. The above laws have been extensively reported in isotropic systems with linear dispersion, such as graphene [1–6], and DSMs/WSMs [8–10]. If the isotropic system is usual quadratical dispersion \( H_0 = v k^2 \sigma_0 \), the RKKY interaction follows a
law \([33]\) as \(f^\text{re}(u_F = 0) = 0\) and \(f^\text{re}(u_F \neq 0) \propto \sin \left(2R\sqrt{u_F/v^2}\right)/R^d\) which shares a same decaying rate but with a different oscillation as compared to equation \((6)\).

Universal RKKY decay for S-DSM materials—the above argument is valid only for isotropic systems since \(e^{i\nu R/\nu}\) in equation \((5)\) is obtained under the \(\theta_0\)-independent condition \([\tan(\theta_0) = R_y/R_x]\). In S-DSMs with anisotropic dispersions, the corresponding Green’s function is direction-dependent.

We employ a general Hamiltonian of a minimal low-energy model of S-DSM

\[
H_{S_{\text{-DSM}}} = v_F (k_x^2 + \xi_1 k_y^2 + v_1 (\xi_2 k_x \sigma_z + k_y \sigma_\tau)),
\]

which collects all S-DSM models in 2D and 3D materials: (1) case I: for \(\xi_1 = 0\) and \(\xi_2 = 0\), it reduces to S-DSM in 2D case \([34–39]\), (2) Case II: for \(\xi_1 = 0\) and \(\xi_2 = 1\), it is linear momentum along two directions and square along the other one, called as 3D-type I. (3) Case III: for \(\xi_1 = 1\) and \(\xi_2 = 0\), it is linear momentum along one direction and square along other two directions, called as 3D-type II. Noting that the Pauli matrices \(\sigma_{x,y,z}\) in equation \((8)\) can act either in pseudo-spin basis \([34–36]\) or real-spin basis \([37–39]\), depending on specific materials. For example, the pseudo-spin 2D S-DSM can be extracted from \((\text{TiO}_2)_3/(\text{VO}_2)_3\) multilayer system \([34–36]\), and the real-spin one can be obtained from the topological surface band under the effect of a helical spin density wave \([38]\) or a spiral magnetization superlattice \([39]\). Without loss of generality, we firstly assume that the Hamiltonian of equation \((8)\) is written in real-spin basis. Later in this paper, the effect of the pseudo-spin case on the RKKY interaction would be discussed.

Different from the numerous candidates for 2D S-DSM, few literature focus on 3D S-DSMs. The two types of 3D S-DSMs used in our paper can be obtained by applying linearly polarized light in WSMs \([40]\) and nodal-line semimetals \([41]\) (NLSMs), respectively. For example, one can consider a low-energy model of WSM with broken time-reversal symmetry as \([40]\),

\[
H_{W_{\text{WSM}}} = v_F (k_x^2 - m^2) \sigma_z + v_1 (k_x \sigma_x + k_y \sigma_y),
\]

where \(\sigma_{x,y,z}\) refer to the Pauli matrices of the spin degrees of freedom, and two Weyl points are located at \((\pm m, 0, 0)\). After introducing a beam of linearly polarized light of frequency \(\omega\), a vector potential \(A = A(1, 0, 0) \cos(\omega t)\) with period \(T = 2\pi/\omega\) is generated. By applying the Peierls substitution \(h k \rightarrow h k + e A\), the system Hamiltonian becomes time-dependent. Using the Floquet theory \([42]\) with the off-resonant condition of \(A^2/\omega \gg 1\), the modified part of the Hamiltonian induced by light reads as

\[
V_0 + \frac{\hbar}{\omega} \sum_{n \geq 1} [V_{++,V_{--}}(\omega + n\omega)] = O(1/\omega^2)\]

with \(V_{++,V_{--}} = \int_0^T H(t)e^{-i\omega t} dt,\) and the effective Hamiltonian can be written as

\[
H_{W\text{WSM}} = H_{W_{\text{WSM}}} + \frac{v_F e^2 A^2}{2m^2} \sigma_z,
\]

where the term related to \(A\) refers to the photoinduced modification. By setting proper amplitude \(A\) of the vector potential with \(e^2 A^2/2 = m^2\), the Weyl partners are merged into a point, i.e., the WSM is changed to be the type I of 3D S-DSM \((\xi_1 = 0\) and \(\xi_2 = 1\) in equation \((8)\)). Similarly, the type II of 3D S-DSM can also be obtained when the nodal ring of NLSM is shrunk into a point by the linearly polarized light.

The Green’s function with respect to \(H_{S_{\text{-DSM}}}\) of equation \((8)\) reads as

\[
G(\pm R, \omega) = \frac{1}{(2\pi)^d} \int \frac{d^d k}{(\omega + i0^+)^d} \frac{\omega \sigma_0 + H_{S_{\text{-DSM}}}}{E_{S_{\text{-DSM}}} - E_{S_{\text{-DSM}}}} e^{i k R},
\]

with \(E_{S_{\text{-DSM}}}\) denoting the eigenenergy of the Hamiltonian \(H_{S_{\text{-DSM}}}\). The analytical results of \(G(\pm R, \omega)\) for different S-DSMs can be obtained after some algebraic calculations (see the appendix \(A\)).

\(A:\) along relativistic direction—firstly, we perform the calculations for impurities deposited along the relativistic axis (see the appendix \(A\)), and depict the results in table \(1\). For this case, the decaying rate of the interaction \((u_F \neq 0)\) with the distance \(R\) between impurities can be expressed as a general form

\[
f^{\text{re}}(u_F \neq 0) \propto \left(\frac{1}{R^d/s_{1/2}} + O\left(\frac{1}{R^d}\right)\right) [A \sin (2k_yR) + B \cos (2k_yR)],
\]

where \(k_e = u_F/v_F\). Similar oscillation \(2Ru_F/v_F\) is also found in DSM-type materials \([1–5, 8–10]\). The index \(s\) in the above equation labels the number of dimension of square momentum, namely, \(s = 0, 1, 2\) correspond to the DSDs, 2D DSM (or 3D-type I S-DSM), and 3D-type II S-DSM, respectively. For \(u_F \neq 0\), we focus on the slowest-decaying RKKY components \((1/R^{d−s_{1/2}})\). Obviously, the positive number \(s\) could reduce the decaying rate as compared with isotropic systems \(f^{\text{re}} \propto 1/R^d\) in equation \((6)\). Specifically, for finite Fermi energy, the RKKY component of 2D S-DSM falls off as \(R^{-3/2}\), which decays much more slowly than that of doped phosphorene \([11, 43]\) or 2D DSM where \(f^{\text{re}}_{2D} \propto R^{-3}\) (equation \((6)\)). Compared to the fast
decaying rate of $R^{-3}$ in 3D DSMs/WSMs [8–10] with $s = 0$, the interaction in S-DSM exhibits a slowest decaying rate as $R^{-2}$ for the type II of 3D S-DSMs with $s = 2$ and as $R^{-5/2}$ for the type I of 3D S-DSMs with $s = 1$. This is attributed to the non-relativistic term, which enters into the anisotropic energy $E_{\text{S-DSM}}$ of equation (9) and competes with the relativistic term to contribute a slowly-decaying rate. This law is unexpected since the slowly-decaying RKKY interaction is usually only realized by the edge/surface state [12–17], the strain [11], the PN junction [21], etc. So far, few reports have discussed the slowly-decaying (or prolonged) RKKY interaction just mediated by the bulk states, without using any other means.

For zero Fermi energy, we find

$$f_{\alpha\beta}^{0\beta}(u_F = 0) \propto \frac{1}{R^{d-1-\frac{3}{2}+\gamma}} \equiv \frac{1}{R^{2d-1-1}}. \quad (11)$$

Compared to the case of $u_F \neq 0$, there are two changes: (1) the spatial oscillation $\sin \left(2Ru_F/\nu\right)$ vanishes; (2) the decaying rate of the interaction is increased by the exponent $\zeta = d - 1 - s/2$ of the DOS $|\omega|^\zeta$. Similar effect also have been stated in DSMs/WSMs [8–10] but with $s = 0$. Thus, $f_{\alpha\beta}^{0\beta}(u_F = 0)$ always decays more slowly than that of DSM-type materials [1–5, 8–10], where $f_{\alpha\beta}^{0\beta}(u_F = 0) \propto 1/R^{2d-1}$ in equation (7). Noting that the relation between the decaying rate and the dimension $s$ of non-relativistic terms is still similar to the case of $u_F \neq 0$, i.e., S-DSMs with larger $s$ would result in a slower decaying rate, as listed in table 1.

$B$: along non-relativistic direction—compared to the case with impurities in the relativistic axis, a faster decaying-rate is exhibited for the RKKY component $f_{\rho\rho}$ when impurities are deposited in the non-relativistic axis. Performing the similar calculations, we find

$$f_{\rho\rho}^{0\rho}(u_F \neq 0) \propto \left[ \frac{1}{R} + O \left( \frac{1}{R^{d-1}} \right) \right] \left[ C \cos \left( 2k'_F R \right) + D \cos \left( 2k'_F R \right) \right] \quad (12)$$

$$f_{\rho\rho}^{0\rho}(u_F = 0) \propto \frac{1}{R^{2d-1-1}}, \quad (13)$$

where $k'_F = \sqrt{u_F}/\sqrt{\nu}$. All the results for different S-DSM models are shown in table 2. For $u_F \neq 0$, we focus on the slowest-decaying RKKY components $(1/R^d)$. It is found that the decay of the interaction $f_{\rho\rho}^{0\rho}(u_F \neq 0)$ in S-DSMs is only related to the dimensionality $d$, i.e., $R^{-2}$ ($R^{-3}$) for 2D (3D) S-DSMs, independent on the dimension $s$ of the non-relativistic terms. The reason is that, in this impurity configuration, the interplay of relativistic and non-relativistic electrons is eliminated by the finite Fermi energy. This would result in the same decaying rate and the same oscillation $\sin \left(2R/\sqrt{u_F}/\sqrt{\nu}\right)$ as that of isotropic systems [33] with quadratical dispersion. For $u_F = 0$, all RKKY components of S-DSMs decays faster as compared to the case of $u_F \neq 0$. The reasons are: (1) similar to $f_{\rho\rho}^{0\rho}$, the exponent $\zeta = d - 1 - s/2$ of the DOS $|\omega|^\zeta$ would result in a fast decaying rate for $f_{\rho\rho}^{0\rho}$; (2) compared to the phase factor $e^{iR/\nu}$ of the Green’s function $G_0$ (or $G_1$ in DSMs of equation (5)), the modified phase factor $e^{i\sqrt{u_F}/\sqrt{\nu}}$ of $G_0$ induced by the non-relativistic term would further accelerate the decaying rate of $f_{\rho\rho}^{0\rho}$. As a result, $f_{\rho\rho}^{0\rho}(u_F = 0)$ exhibits a fastest decaying rate than that of $f_{\rho\rho}^{0\rho}(u_F = 0)$ and $f_{\rho\rho}^{0\rho}(u_F = 0)$ in isotropic systems (equation (7)). Noting that the anisotropic decaying laws shown in tables 1 and 2 are peculiar as compared to the case of doped phosphorene [43], where the RKKY interaction follows a same decaying law $(R^{-2})$ whether in armchair direction or zigzag direction although the dispersion of the phosphorene is highly anisotropic.

$C$: along non-principal directions—For impurities deposited in non-principal directions, deviating from relativistic and non-relativistic axes, the decay of the RKKY interaction can be analyzed only with numerical calculations. From the above discussions, we know that the decaying rate of the interaction can be affected...
 interaction decays more fast than heavily by the interplay of relativistic and non-relativistic electrons, leading to the slower decay in the relativistic direction than that in the non-relativistic direction. Thus, when impurities are deposited in a non-principal direction, the intermediate decaying rate would arise, as shown in figure 1, where the interaction decays more fast than \( J^0_p (\theta_R = \pi/2) \) but more slowly than \( J^0_p (\theta_R = 0) \).

\[ D: \text{underlying physics—} \text{to more deeply understand the anisotropic RKKY interaction, we employ the direction-dependent DOS } \rho (\omega, \theta), \text{which is } \rho (\omega, \theta) = -(1/\pi) \text{Im} \text{ Tr } \int G (k, \omega) k dk \text{ for 2D case. The angle } \theta \text{ is defined as } \tan(\theta) = v_F k_z/e \text{ in the Hamiltonian of } \varepsilon_{k_x} + v_F k_z \sigma, \text{ where } \varepsilon_{k_x} = v_F k_x (v_F k_z) \text{ denotes 2D S-DSM (DSM). We obtain } \rho_{\text{DSM}} (\omega, \theta) = \left| \omega \right| \left( \pi^2 v_F^2 \right) \text{ for 2D DSMs and } \rho_{\text{S-DSM}} (\omega, \theta) = \sqrt{\left| \omega \right|} \left[ \pi^2 v_F \sqrt{v_F \cos(\theta)} \right] \text{ for 2D S-DSMs. Obviously, different from the isotropic DSMs, the DOS for S-DSMs is significantly anisotropic, especially along the linear-momentum direction, i.e., } \theta = \pi/2, \text{ where the DOS of S-DSMs is much larger than that of DSMs, as shown in figure 2(a). To understand this, one can review the general form of } \rho_{\text{DSM}} (\omega, \theta) \text{ for DSM, i.e., } \rho_{\text{DSM}} (\omega, \theta) \propto \int \frac{d k}{v_F} \text{ with } k_F = \omega/v_F \text{ being the Fermi wave number. Here, } \rho_{\text{DSM}} (\omega, \theta) \text{ is isotropic since the velocity } v = \sqrt{v_F} E_{\text{DSM}} = v_F \text{ is constant. To compare S-DSMs with DSMs, one can use a parameter transformation } (k^2_x, v_F k_z) = (k^2_x, v_F k'_z) \text{ to change } \rho_{\text{S-DSM}} \text{ to a similar form as that of } \rho_{\text{DSM}}, \text{i.e., } \rho_{\text{S-DSM}} (\omega, \theta) \propto \int \frac{d k}{v_F} \text{ with } k'_F = \omega/v_F. \text{ Due to the introduce of the non-relativistic term, the velocity of electrons in S-DSMs is modified to an effective one with } v_{\text{eff}} = \sqrt{v_F \cos(\theta)} \text{ [tan(}\theta\text{) = } k'_F/k'_z\text{], which is anisotropic and different from the case of DSMs. Moreover, the vanished effective velocity } v_{\text{eff}} (\theta = \pi/2) = 0 \text{ in the relativistic direction would generate a maximal DOS since } \rho_{\text{S-DSM}} (\omega, \theta) \text{ is inversely proportional to } v_{\text{eff}}. \text{ This large DOS should naturally result in a slower decaying rate in the real space. To see it, we consider an electron scattering off a magnetic impurity, whose full electronic Green’s function under Born approximation is modified to be }

\[ G (k, k', \omega) = \delta(k - k') G (k, \omega) + G (k, \omega) (\lambda S_2 \cdot \sigma) G (k', \omega). \] (14)\]
The change of real-space local DOS reads [44]

\[ \delta \rho(R, \omega) = -\frac{\lambda}{\pi} \text{Im} \int dq e^{iqR} \sum_k \text{Tr} G(k, \omega) (S_2 \cdot \sigma) G(k - q, \omega) \]

\[ = -\frac{\lambda}{\pi} \text{Im} \text{Tr} G(R, \omega) (S_2 \cdot \sigma) G(-R, \omega), \tag{15} \]

in which the decay of \( \delta \rho(R, \omega) \) is determined by \( \text{Im}[A_{ij}(R, \omega)] \). We illustrates the change of \( \text{Im}[A_{00}(R, \omega)] \) with the impurity distance \( R \) in figure 2(b), which shows that the anisotropic decaying rate in the real space is close related to the anisotropic DOS (figure 2(a)). From above expressions, one also can see that physically, the RKKY interaction characterizes the change of spin density of itinerant electrons at site \( r_1 \) caused by a magnetization at site \( r_2 \) when electrons complete a round trip from \( r_1 \) to \( r_2 \), similar to the semiclassical picture of charge density of isotropic materials [5]. For certain direction, large spin density will remain more electrons participating the exchange interaction between magnetic impurities and so prolong the RKKY decay.

**E: anisotropic spin model and DM spin exchange interaction**—the general form of RKKY interaction in equation (3) can divide into Heisenberg type \( J^\text{f} \) and Dzyaloshinskii–Moriya (DM) type \( J^\text{DM} \),

\[ H_{\text{RKKY}} = \sum_{i=x,y,z} J^f_i S_i^1 S_i^2 + J^\text{DM} e \cdot (S_i \times S_j), \tag{16} \]

where \( e = (\hat{x}, \hat{y}, \hat{z}) \) is the unit vector and the spin-frustrated terms \( \sum_{i\neq j=x,y,z} J^f_i S_i^1 S_j^2 + S_j^1 S_i^2 \) vanish if the impurities are distributed along principle axes.

The detailed spin textures for the RKKY interaction of S-DSMs, as well as DSMs, are shown in the appendix A. Compared to the case of DSMs, there exists a significant difference for the short-range (or weak \( u_0 \)) behavior of the RKKY interaction, i.e., a stronger magnetic anisotropy would arise in S-DSMs in the condition of small \( k_F R \) as impurities are deposited on the relativistic axis. Specifically speaking, the RKKY components \( J^f_i \) are anisotropic with \( J^f_x \neq J^f_y \neq J^f_z \), which would generate the XYZ spin model for all S-DSMs and distinguishes itself from the XYZ (e.g., \( J^f_x = J^f_y \neq J^f_z \)) spin model of DSMs. The underlying physics is attributed to the competition of the RKKY interactions with different decaying rates. Taking 2D S-DSM as an example, the RKKY components of finite Fermi energy in the long-range limit exhibits an anisotropy of \( J^f_x = J^f_y \neq J^f_z \) (see equation (A11) of the appendix A), where \( J^f_x \) falls off as \( R^{-3/2} \) and \( J^f_y \propto R^{-2} \). When the short-range limits (small \( R \)) is considered, the higher-order terms \( R^{-2} \) with different coefficients in \( J^f_x \) become considerable, which compete with the term of \( R^{-3/2} \) and lead to \( J^f_x \neq J^f_y \neq J^f_z \).
Next, we focus on the influence of the anisotropic dispersion on the DM term. Starting from equation (4), the DM coefficient can be obtained with

\[ J_{\text{DM}} = -\frac{4\lambda^2}{\pi} \Re \int_{-\infty}^{\infty} \omega \, d\omega \, G_0(G_x, G_y, G_z). \] (17)

Here, the appearance of DM term must satisfy two conditions: (1) finite Fermi energy. If \( u_F = 0 \), all the models show the vanished DM interaction due to the protected electron–hole symmetry, similar to the case of WSMs [8, 9]. (2) Breaking the symmetry of spatial inversion. Note that \( G(R, \omega) = \sum_{l=0,\pi,\pi} G_l(R, \omega) \) and if impurities are distributed along the square-momentum direction, only diagonal components \( G_0 \) and \( G_z \) in the spin space are nonzero, i.e., \( G(R, \omega) = G_0 \sigma_0 + G_z \sigma_z \). It is easy to confirm \( G(-R, \omega) = G(R, \omega) \) and so \( J_{\text{DM}} = 0 \). Once the impurities are deposited along the linear-momentum direction, the nondiagonal components \( G_x \) and \( G_y \) are included, which breaks the inversion symmetry, \( G(-R, \omega) \neq G(R, \omega) \), and so finite DM interaction emerges. In figure 3, we plot the dependence of DM exchange interaction for 2D on impurity direction \( \theta_R \). Compared with isotropic DM interaction for the DSMs, the DM interaction for S-DSMs exhibits strong anisotropic, which is largest for linear-momentum direction \( (\theta_R = \pi/2) \) and vanishes for \( k^2 \) direction \( (\theta_R = \pi/2) \). These results also are in agreement with derived analytical expressions for limit cases (see derivation in the appendix A). Also, the introduction of non-relativistic contribution in the S-DSMs can reduces the dependence of DM interaction on \( u_F \), in comparison with the case of DSMs.

If the Hamiltonian of equation (8) is expressed in the pseudospin space (\( \sigma_i \rightarrow \tau_i \) in equation (8)), taking orbital space as an example, the term \( \text{Tr}[\sigma_i \sigma_j \sigma \sigma \rho] \) in equation (4) have to be rewritten as \( \text{Tr}[\sigma_i \sigma_j] \text{Tr}[\tau_i \tau_j] \) according to the references [9, 12]. Thus, the DM terms would vanish and only the Heisenberg-type RKKY interaction survives with an isotropic XXX \( (J_{\text{X}}) = J_{\text{XX}} = J_{\text{YY}} = J_{\text{XY}} \) spin model, similar to the case of graphene [1–5]. But the decay of the RKKY interaction still follows the law shown in equations (10)–(13).

**Conclusions**—we have theoretically explored the RKKY interaction between magnetic impurities in S-DSMs including all 2D and 3D models. Due to the coexistence of the relativistic and non-relativistic electrons, the RKKY interaction of S-DSMs is anisotropic and violates the decaying law proposed in isotropic systems. We find that the introduction of non-relativistic electrons in the S-DSMs can significantly prolong the decay of the RKKY interaction along relativistic direction, in comparison with the case of isotropic DSMs. For example, the decaying rate \( R^{-5} \) for 3D DSMs is reduced to be \( R^{-3} \) for type-II 3D S-DSMs, which can greatly facilitate the experiment detection and magnetic doping technology. The underlying physics is ascribed to the interplay of relativistic and non-relativistic electrons. Furthermore, we give a general formula to determine the decaying rate from the system dimension and the non-relativistic dimension. In addition, we find that the anisotropy of S-DSMs can greatly affect the DM component of the RKKY interaction, which is largest for impurities in the relativistic direction but vanishes in non-relativistic direction.

All these peculiar magnetic characteristics implies that the S-DSMs are a powerful platform to detect and control the magnetic exchange interaction, superior to extensively adopted isotropic systems.

Experimentally, a variety of candidates for S-DSMs with different approaches have been proposed, such as multilayer \( (\text{TiO}_2)_n/(\text{VO}_2)_n \) nanostructures [34–36], deformed graphene [45], and silicene oxide [46]. The RKKY interactions can be probed experimentally with present techniques, e.g., spin-polarized scanning tunneling spectroscopy [47], which can measure the magnetization curves of individual atoms, or the electron-spin-resonance technique coupled with an optical detection scheme [48, 49].
Acknowledgments

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. Derivation for RKKY interaction in S-DSMs and DSMs

We employ an general Hamiltonian of a minimal low-energy model of S-DSM

\[ H_{S-DSM} = v_p (k_x^2 + 
\xi_1 k_y^2) \sigma_z + v_1 (\xi_2 k_y \sigma_x + k_z \sigma_y), \]

which collects all S-DSM models in 2D and 3D materials: (1) case I: for \( \xi_1 = 0 \) and \( \xi_2 = 0 \), it reduces to S-DSM in 2D case [34–39]. (2) Case II: for \( \xi_1 = 0 \) and \( \xi_2 = 1 \), it is linear along two directions and square momentum along the other one, called as 3D-type I. (3) Case III: for \( \xi_1 = 1 \) and \( \xi_2 = 0 \), it is linear along one direction and square momentum along other two directions, called as 3D-type II. The corresponding Green’s function reads,

\[ G(\pm \mathbf{R}, \omega) = \frac{1}{(2\pi)^d} \int d^dk [\omega_n - H_{S-DSM}(\mathbf{k})]^{-1} e^{\pm i\mathbf{kR}}, \]

\[ = \frac{1}{(2\pi)^d} \int d^dk \omega_{\alpha n} + H_{S-DSM} \omega_{\sigma n} - E_{\sigma n} \omega_{\sigma n} - E_{S-DSM} \omega_{\sigma n} \]

\[ e^{\pm i\mathbf{kR}}, \quad \text{(A2)} \]

where \( \omega_+ = \omega + i0^+ \), \( d \) is the dimensionality, and \( E_{S-DSM} \) denotes the eigenenergy of the Hamiltonian \( H_{S-DSM} \), given by,

\[ E_{S-DSM} = \pm \sqrt{v_p^2 (k_x^2 + \xi_1 k_y^2)^2 + v_1^2 (\xi_2 k_y^2 + k_z^2)}. \]

Noting that the Pauli matrices \( \sigma_{x,y,z} \) in equation (A1) can act either in pseudo-spin basis [34–36] or real-spin basis [37–39], depending on specific materials. For example, the pseudo-spin 2D S-DSM can be extracted from (TiO\(_2\))\(_3\)/(VO\(_2\))\(_3\) multilayer system [34–36], and the real-spin one can be obtained from the topological surface band under the effect of a helical spin density wave [38] or a spiral magnetization superlattice [39]. We assume that the Hamiltonian of equation (A1) is written in real-spin basis in this appendix. In the main text, the effect of the pseudo-spin case on the RKKY interaction would also be discussed.

A.1. The case of 2D S-DSMs

For the case of 2D S-DSMs (i.e., \( \xi_{1,2} = 0 \)) with real-spin basis [37–39], the Green’s function of equation (A2) can be rewritten as

\[ G_{2D}(\pm \mathbf{R}, \omega) = \frac{1}{2\pi} \int_0^\infty dk_x \int_{-\infty}^{\infty} dk_y \omega_+ \sigma_n + v_p k_x^2 \sigma_x + v_1 k_y \sigma_x + \omega_{\alpha n} - \left(\frac{v_p^2 k_x^2 + v_1^2 k_y^2}{\omega_{\sigma n}}\right) e^{\pm ik_x R_x} \cos (k_y R_y). \]

\[ \text{(A4)} \]

Using a parameter transformation \((k_x^2, v_p k_x) = (k_x', v_p k_x')\), the above Green’s function can be rewritten as

\[ G_{2D}(\pm \mathbf{R}, \omega) = \frac{v_p}{2\pi} \int_0^\infty \frac{dk_x'}{\sqrt{v_p^2 k_x'^2 + v_1^2 k_y^2}} \int_0^\infty \frac{dk_y'}{\omega_+} \cos \left( v_p k_x' R_x/v_1 \right) \sigma_n + v_p k_y' \cos \left( v_p k_x' R_x/v_1 \right) \sigma_x \pm ik_y' \sin \left( v_p k_x' R_x/v_1 \right) \sigma_x \]

\[ \times \cos \left( \sqrt{v_p^2 k_x'^2 + v_1^2 k_y^2} \right). \]

\[ \text{(A5)} \]
Note that, the above Green’s function has the following form,

\[ G_{2D}(\pm \mathbf{R}, \omega) = G_0\sigma_0 \pm G_x\sigma_x + G_z\sigma_z. \]  

(A6)

Plugging the Green’s function of equation (A6) into equation (A2) of the main text and summing over the spin degrees of freedom, the RKKY components can be written in the form of

\[ H_{\text{RKKY}}^{2D} = \sum_{i=x,y,z} J_i S_i^z S_i^z + J^{\text{OM}} e \cdot (S_1 \times S_2), \]  

(A7)

with

\[ J^x = -\frac{2\lambda^2}{\pi} \text{Im} \int_{-\infty}^{\infty} (G^0_0 + G^x_j - G^x_z) d\omega, \]

\[ J^y = -\frac{2\lambda^2}{\pi} \text{Im} \int_{-\infty}^{\infty} (G^0_0 - G^y_j - G^y_z) d\omega, \]

\[ J^z = -\frac{2\lambda^2}{\pi} \text{Im} \int_{-\infty}^{\infty} (G^0_0 + G^z_j + G^z_z) d\omega, \]

\[ J^{\text{OM}} = -\frac{4\lambda^2}{\pi} \text{Re} \int_{-\infty}^{\infty} G_0 G_j d\omega, \]

where \( e = (0, 1, 0) \).

According to equations (A5) and (A6), the matrix elements \( G_{ij}^{\text{DM}} \) of the Green’s function with impurities in the relativistic axis \( (R_x = 0, R_z \neq 0) \) can be solved after some algebraic calculations, given by

\[ G_0 = -\sqrt{\frac{1+i}{2\pi \nu_i}} \frac{R_z}{\nu_i^2 v_l} \left( \frac{\nu_i}{\nu_l} \right)^{1/4} \omega_+^{3/4} K_{1/4} \left( -\frac{iR_x \omega_+}{\nu_l} \right) \Gamma \left( \frac{5}{4} \right), \]

\[ G_y = -\sqrt{\frac{1+i}{2\pi \nu_i}} \frac{R_x}{\nu_i^2 v_l} \left( \frac{\nu_i}{\nu_l} \right)^{1/4} K_{3/4} \left( -\frac{iR_x \omega_+}{\nu_l} \right) \Gamma \left( \frac{5}{4} \right), \]

\[ G_z = -\frac{(1)^{7/8}}{\sqrt{2} \pi^{3/2} \nu_i} \frac{v_x}{v_y^2 R_z} \left( \frac{\nu_x}{\nu_y} \right)^{1/4} K_{1/4} \left( -\frac{iR_x \omega_+}{\nu_l} \right) \Gamma \left( \frac{3}{4} \right), \]

where \( K_n(x) \) is the \( n \)th order modified Bessel function of the second kind. Plugging the above matrix elements \( G_{ij}^{\text{DM}} \) into equation (A8) and integrating out \( \omega \), one can obtain the analytical solutions of the RKKY interaction. The RKKY components \( J_i^{\text{DM}} \) at zero Fermi energy \( (u_F = 0) \) are given by

\[ J^x (u_F = 0) = -12 \Gamma^4 \left( \frac{3}{4} \right) + \Gamma^3 \left( \frac{3}{4} \right) \Gamma \left( \frac{1}{4} \right) \frac{1}{R^2}, \]

\[ J^y (u_F = 0) = \frac{\Gamma^2 \left( \frac{3}{4} \right) \Gamma^3 \left( \frac{3}{4} \right) \Gamma \left( \frac{1}{4} \right)}{6\pi^4 v_p}, \]

\[ J^z (u_F = 0) = -12 \frac{\Gamma^4 \left( \frac{3}{4} \right) + \Gamma^3 \left( \frac{3}{4} \right) \Gamma \left( \frac{1}{4} \right)}{6\pi^4 v_p}, \]

\[ J^{\text{OM}} (u_F = 0) = 0. \]

(A10)

For the finite Fermi energy \( (u_F \neq 0) \), utilizing the asymptotic form of the Bessel functions \( K_n(x) \approx \sqrt{\frac{\pi}{2x}} e^{-x} \) in the condition of \( x \gg 1 \), the long-range asymptotic behavior of the RKKY components \( J_i^{\text{DM}} \) \( (Ru_F/v_l \gg 1) \) are given by
\[ J^\parallel_p (u_F \neq 0) = -\frac{\Gamma^2 \left(\frac{\gamma}{2}\right)}{2\pi^3 \rho_p v^2} \frac{1}{v^2} \left[ \cos \left(\frac{2\mu_R}{v}\right) + \sin \left(\frac{2\mu_R}{v}\right) \right], \]
\[ J^\perp_p (u_F \neq 0) = -\frac{\Gamma^2 \left(\frac{\gamma}{2}\right)}{8\pi^3 \rho_p v^2} \frac{1}{v^2}, \]
\[ J^\parallel_p (u_F \neq 0) = -\frac{\Gamma^2 \left(\frac{\gamma}{2}\right)}{2\pi^3 \rho_p v^2} \frac{1}{v^2} \left[ \cos \left(\frac{2\mu_R}{v}\right) - \sin \left(\frac{2\mu_R}{v}\right) \right], \]
\[ J^{\text{DM}}_p (u_F \neq 0) = -\frac{\Gamma^2 \left(\frac{\gamma}{2}\right)}{2\pi^3 \rho_p v^2} \frac{1}{v^2} \left[ \cos \left(\frac{2\mu_R}{v}\right) - \sin \left(\frac{2\mu_R}{v}\right) \right]. \]

Note that, the above results are obtained in the condition of \( R_R / v_L \gg 1 \). If small \( R_R / v_L \) or zero Fermi energy is considered, the RKKY components \( J^\parallel \) are highly anisotropic, i.e., \( J^\parallel \neq J^\perp \neq J^\parallel_p \), which could generate the XYZ spin model.

Similarly, the matrix elements \( G^0_{i=0,1,2} \) of the Green’s function with impurities in the non-relativistic axis \((R_x \neq 0, R_z = 0)\) also can be solved according to equations (A5) and (A6), given by

\[ G^0_x = -\frac{\sqrt{\omega} e^{i R_x \sqrt{\frac{\omega}{\pi}}} \sqrt{\cos(\theta)}}{4\pi v \sqrt{\rho_p}} \int_0^\pi d\theta \left[ i e^{R_x \sqrt{\frac{\omega}{\pi}}} \sqrt{\cos(\theta)} + e^{-R_x \sqrt{\frac{\omega}{\pi}}} \sqrt{\cos(\theta)} \right], \]
\[ G^0_y = 0, \]
\[ G^0_z = -\frac{\sqrt{\omega} e^{i R_x \sqrt{\frac{\omega}{\pi}}} \sqrt{\cos(\theta)}}{4\pi v \sqrt{\rho_p}} \int_0^\pi d\theta \left[ i e^{R_x \sqrt{\frac{\omega}{\pi}}} \sqrt{\cos(\theta)} - e^{-R_x \sqrt{\frac{\omega}{\pi}}} \sqrt{\cos(\theta)} \right] \sqrt{\cos(\theta)} d\theta. \]

Due to the vanished non-diagonal matrix element \( G^0_y = 0 \), the Green’s function always satisfies \( G^0_{2D}(\mathbf{R}, \omega) = G^0_{2D}(\mathbf{R}, \omega) \), and so \( J^{\text{DM}} = 0 \). Then, the RKKY components of equations (A7) and (A8) with impurities in the non-relativistic axis can be further simplified as

\[ H^\parallel_{p, \text{RKKY}} = J^\parallel_p S_1 \cdot S_2 + J^\parallel_p S^S_1 S^S_2, \]

with

\[ J^\parallel_p = -\frac{2\lambda^2}{\pi} \int_{-\infty}^{\infty} \left[ (G^0_x)^2 - (G^0_z)^2 \right] d\omega, \]
\[ J^\perp_p = -\frac{4\lambda^2}{\pi} \int_{-\infty}^{\infty} (G^0_z)^2 d\omega. \]

After integrating out \( \omega \), the RKKY components \( J^\parallel_p (u_F = 0) \) can be solved as

\[ J^\parallel_p (u_F = 0) = \frac{3\nu_p \lambda^2 (\rho_1 + \rho_2)}{4\pi v L^2} \frac{1}{R}, \]
\[ J^\perp_p (u_F = 0) = -\frac{6\nu_p \lambda^2 \rho_2}{4\pi v L^2} \frac{1}{R^2}, \]

with

\[ \rho_1 = \int_0^\pi \int_0^\pi \frac{\cos^2(\theta) + \cos^2(\theta') - 6 \cos(\theta) \cos(\theta')}{(\cos(\theta + \cos(\theta')))^4 \sqrt{\cos(\theta) \cos(\theta')}} d\theta d\theta', \]
\[ \rho_2 = \int_0^\pi \int_0^\pi \frac{\cos^2(\theta) + \cos^2(\theta') - 6 \cos(\theta) \cos(\theta')}{(\cos(\theta + \cos(\theta')))^4 \sqrt{\cos(\theta) \cos(\theta')}} d\theta d\theta'. \]
where $\rho_1 \approx -0.27659$, $\rho_2 \approx -0.65689$. For the case of finite Fermi energy, $J^H_p (u_F \neq 0)$ have to be calculated numerically according to equations (A12) and (A14), the results are shown in figure 1 and can be fitted in the following form,

$$J^H_p (u_F \neq 0) \propto \frac{u_F^{1/2} \sin \left( \frac{2\pi \sqrt{u_F}}{\sqrt{v_F}} \right)}{R^3},$$  

(A17)

where constant coefficients are dropped.

As shown above, different from the case with impurities in the relativistic axis, the DM term with impurities in the non-relativistic axis vanishes, and the RKKY components $J^p_i (u_F \neq 0)$ exhibit a magnetic anisotropy with a spin model of $XXY$ (figures 4 and 5).

In particular, in the asymptotic form of the Bessel functions $K_\nu(x) \approx \sqrt{\pi / 2x} e^{-x}$, the long-range asymptotic behaviors of the Green’s function can be written as

$$G^l_i (\pm R, \omega) \propto \frac{1}{R^{1/4}} \omega^{1/4} e^{iR},$$  

$$G^p_i (\pm R, \omega) \propto \frac{1}{R^{1/2}} \omega^{1/4} e^{i\sqrt{R\omega}}.$$  

(A18)

Plugging the above equations into equation (A8), one can also obtain the same decaying law as that of equations (A10), (A11), (A15) and (A17).
A.2. The case of 3D-type I S-DSMs

For the case of 3D-type I S-DSMs (i.e., $\xi_1 = 0$ and $\xi_2 = 1$), the Green’s function of equation (A21) can be rewritten as

$$G_{3D,I} (\pm \mathbf{R}, \omega) = \frac{1}{(2\pi)^3} \int \int \int d\mathbf{k_r} \, d\mathbf{k}_s \, d\mathbf{k}_l \, \frac{G_{\omega_0 + \nu \mathbf{k}_s^2 \sigma_x + \nu \mathbf{k}_l^2 \sigma_z + \nu \mathbf{k}_r^2 \sigma_z}{\omega^2 - \left( \nu \mathbf{k}_r^2 + \nu \mathbf{k}_s^2 + \nu \mathbf{k}_l^2 \right)} e^{i \mathbf{k}_r \cdot \mathbf{R}_r + i \mathbf{k}_s \cdot \mathbf{R}_s + i \mathbf{k}_l \cdot \mathbf{R}_l},$$

$$= \frac{1}{4\pi^2} \int_0^\infty d\mathbf{k}_r \, \int_0^{\mathbf{k}_r} d\mathbf{k}_s \, \int_0^{\mathbf{k}_r} d\mathbf{k}_l \, \frac{G_{\omega_0 + \nu \mathbf{k}_s^2 \sigma_x + \nu \mathbf{k}_l^2 \sigma_z + \nu \mathbf{k}_r^2 \sigma_z}}{\omega^2 - \left( \nu \mathbf{k}_r^2 + \nu \mathbf{k}_s^2 + \nu \mathbf{k}_l^2 \right)} e^{i \mathbf{k}_r \cdot \mathbf{R}_r + i \mathbf{k}_s \cdot \mathbf{R}_s + i \mathbf{k}_l \cdot \mathbf{R}_l},$$

$$= \frac{1}{4\pi^2} \int_0^\infty d\mathbf{k}_r \, \int_0^{\mathbf{k}_r} d\mathbf{k}_s \, \int_0^{\mathbf{k}_r} d\mathbf{k}_l \, \left( \omega_0 + \nu \mathbf{k}_s^2 \sigma_x + \nu \mathbf{k}_l^2 \sigma_z + \nu \mathbf{k}_r^2 \sigma_z \right) J_0 \left( k_r R_r \right) \pm i \nu k_l J_1 \left( k_l R_l \right) \left[ \cos (\varphi) \sigma_x + \sin (\varphi) \sigma_y \right] e^{i \mathbf{k}_r \cdot \mathbf{R}_r + i \mathbf{k}_s \cdot \mathbf{R}_s + i \mathbf{k}_l \cdot \mathbf{R}_l},$$

where $R_l = \sqrt{R_r^2 + R_z^2}$ and tan (|$\varphi$|) = $R_z/R_r$. Using a parameter transformation ($k_s^2, \nu k_l$) = ($k_s^2, \nu k_l$), the Green’s function $G_{3D,I} (\mathbf{R}, \omega)$ can be simplified as

$$G_{3D,I} (\pm \mathbf{R}, \omega) = G_{1,0,0} + G_{1,\pm,\pm} \pm G_{1,\pm,\mp} \left[ \cos (\varphi) \sigma_x + \sin (\varphi) \sigma_y \right].$$

Plugging the Green’s function of equation (A21) into equation (2) of the main text and summing over the spin degrees of freedom, the RKKY components can be written in the form of

$$J_{RKKY}^{3D,I} = \sum_{i=x,y,z} J^i \left( S_i^1 S_i^2 + J^{DM} \mathbf{e} \cdot \left( \mathbf{S}_1 \times \mathbf{S}_2 \right) + J^e \left( S_i^1 S_i^2 + S_i^z S_i^z \right) \right),$$

with

$$J^e = \frac{-2 \lambda^2}{\pi} \Im \int_{-\infty}^{+\infty} \left[ G_{1,0,0} - G_{1,\pm,\pm} \cos (2\varphi) \right] d\omega,$$

$$J^f = \frac{-2 \lambda^2}{\pi} \Re \int_{-\infty}^{+\infty} \left[ G_{1,0,0} + G_{1,\pm,\pm} \cos (2\varphi) \right] d\omega,$$

$$J^{DM} = \frac{-4 \lambda^2}{\pi} \Re \int_{-\infty}^{+\infty} \left( G_{1,0,0} \lambda \right) d\omega,$$

$$J^e = \frac{4 \sin (\varphi) \cos (\varphi)}{\lambda^2} \Im \int_{-\infty}^{+\infty} G_{1,z}^2 d\omega,$$

where $\mathbf{e} = \left[ \cos (\varphi), \sin (\varphi), 0 \right]$. According to equation (A20), the Green’s function $G_{3D,I} (\pm \mathbf{R}, \omega)$ with impurities in the relativistic axis ($R_l \neq 0, R_z = 0$) can be solved as
For the case of finite Fermi energy ($\omega = \text{finite}$), the RKKY components $J_i$ at zero Fermi energy ($\omega = 0$) are given by

\begin{align}
J_y^f (\omega = 0) &= \frac{18 \cos (2\varphi_y)}{240\pi^3 v_p^2 / \lambda^2} - \frac{1}{R^2}, \\
J_z^f (\omega = 0) &= \frac{-18 \cos (2\varphi_z)}{240\pi^3 v_p^2 / \lambda^2} + \frac{1}{R^2}, \\
J_z^{DM} (\omega = 0) &= 0, \\
J_z^f (\omega = 0) &= \frac{3 \sin (2\varphi_z)}{40\pi^3 v_p^2 / \lambda^2}.
\end{align}

For the case of finite Fermi energy ($\omega \neq 0$), utilizing the asymptotic form of Bessel functions $J_\nu (x) \approx \sqrt{\pi / 2x} e^{-x}$ in the condition of $x \gg 1$, the long-range asymptotic behavior of the RKKY components ($R|\varphi|, v_p \gg 1$) can be solved as

\begin{align}
J_y^c (\omega \neq 0) &= \frac{\lambda^2 \Gamma^2 \left(\frac{3}{2}\right) \sin^2 \left(\varphi_y\right)}{4\pi^3 v_p^2 / \lambda^2} \frac{u_p^{3/2}}{v_p} \left[ \cos \left(\frac{2u_p R}{v_p}\right) - \sin \left(\frac{2u_p R}{v_p}\right) \right], \\
J_z^c (\omega \neq 0) &= \frac{\lambda^2 \Gamma^2 \left(\frac{3}{2}\right) \cos^2 \left(\varphi_y\right)}{4\pi^3 v_p^2 / \lambda^2} \frac{u_p^{3/2}}{v_p} \left[ \cos \left(\frac{2u_p R}{v_p}\right) + \sin \left(\frac{2u_p R}{v_p}\right) \right], \\
J_z^{DM} (\omega \neq 0) &= 0, \\
J_z^c (\omega \neq 0) &= \frac{\lambda^2 \Gamma^2 \left(\frac{3}{2}\right) \sin \left(2\varphi_y\right)}{8\pi^3 v_p^2 / \lambda^2} \frac{u_p^{3/2}}{v_p} \left[ \cos \left(\frac{2u_p R}{v_p}\right) - \sin \left(\frac{2u_p R}{v_p}\right) \right].
\end{align}
As shown above, for impurities reside on $y$ axis or $z$ axis ($\phi_{y} = 0$ or $\phi_{z} = \pi/2$), the DM term $\beta_{\text{DM}}$ survives and the frustrated term $\beta_{F}$ vanishes. Note that, the results of equation (A26) are obtained in the condition of $Ru_{I}/v_{I} \gg 1$. If small $ Ru_{I}/v_{I}$ or zero Fermi energy is considered, the RKKY interaction exhibits a strong magnetic anisotropy with a spin model of XYZ ($J_{x} \neq J_{y} \neq J_{z}$).

According to equation (A20), the Green’s function $G_{3D,I}^{p}(\pm \mathbf{R}, \omega)$ with impurities in the non-relativistic axis ($R_{y} = 0, R_{z} \neq 0$) can be solved as,

$$
G_{3D,I}^{p}(\pm \mathbf{R}, \omega) = \frac{v_{p}/v_{I}^{2}}{(4\pi)^{2}} \int_{0}^{\infty} k^{3/2} dk \int_{0}^{\infty} \sin(\theta) \frac{\omega + \sigma_{0} + \nu_{p} k \cos(\theta) \sigma_{z}}{\sqrt{\cos(\theta)}} \cos \left[ \sqrt{k \cos(\theta) R_{x}} \right],
$$

$$
= -\omega e^{-R_{x}/\sqrt{\pi}} + e^{-R_{x}/\sqrt{\pi}} \sigma_{0} + \frac{2\nu_{p}}{4\pi R_{x} v_{I}^{2}} \sigma_{0} + \frac{2\nu_{p} + R_{x} (nR_{x} + 2\sqrt{mv_{p} \omega})}{4\pi R_{x} v_{I}^{2}} e^{-R_{x}/\sqrt{\pi}} \sigma_{z},
$$

(A27)

Due to the vanished non-diagonal matrix element $G_{3D}^{p} = 0$, the Green’s function always satisfies $G_{3D,I}^{p}(\mathbf{R}, \omega) = G_{3D,I}^{p}(-\mathbf{R}, \omega)$, and so $\beta_{\text{DM}} = 0$. Then, the RKKY components of equations (A22) and (A23) with impurities in the non-relativistic axis can be further simplified as

$$
H_{p,\text{RKKY}} = \sum_{i=x,y,z} J_{p}^{i} S_{i} S_{i}^{\dagger},
$$

(A28)

with

$$
J_{p}^{x} = -\frac{2\lambda^{2}}{\pi} \text{Im} \int_{-\infty}^{\infty} \left[ (G_{3D,I}^{p})^{2} - (G_{3D,I}^{p})^{2} \right] d\omega,
$$

$$
J_{p}^{z} = -\frac{2\lambda^{2}}{\pi} \text{Im} \int_{-\infty}^{\infty} \left[ (G_{3D,I}^{p})^{2} + (G_{3D,I}^{p})^{2} \right] d\omega.
$$

(A29)

After some algebraic calculations, one can obtain the corresponding analytical solutions as

$$
J_{p}^{x} (u_{I} = 0) = -\frac{27\lambda^{2} v_{p}^{4}}{\pi^{3} v_{I}^{4}} \frac{1}{R^{8}},
$$

(A30)

$$
J_{p}^{z} (u_{I} = 0) = \frac{12\lambda^{2} v_{p}^{4}}{\pi^{3} v_{I}^{4}} \frac{1}{R^{8}},
$$

and

$$
J_{p}^{x,z} (u_{I} \neq 0) = -\frac{\lambda^{2} v_{p}^{4/3} u_{I}^{5/2} \cos \left( 2R \sqrt{\frac{u_{I}}{v_{p}}} \right)}{8\pi^{3} v_{I}^{4}}.
$$

(A31)

Here, the DM term vanishes, and the RKKY interaction of $u_{I} = 0$ exhibits a magnetic anisotropy with a spin model of XXY ($J_{x} = J_{y} \neq J_{z}$).

In particular, in the asymptotic form of the Bessel functions $K_{n}(x) \approx \sqrt{\pi/2x} e^{-x}$, the long-range asymptotic behaviors of the Green’s function are given by

$$
G_{3D,I}^{p}(\pm \mathbf{R}, \omega) \propto \frac{1}{R^{3/4}} \omega^{3/4} e^{\frac{\nu_{p} \omega}{R}},
$$

$$
G_{3D,I}^{p}(\pm \mathbf{R}, \omega) \propto \frac{1}{R} \omega e^{\frac{\nu_{p} \omega}{\sqrt{R}}},
$$

(A32)

Plugging the above equations into equation (A23), we can also obtain the same decaying law as shown in equations (A25), (A26), (A30) and (A31).
A3. The case of 3D-type II S-DSM

For the case of 3D-type II S-DSM (i.e., $\xi_1 = 1$ and $\xi_2 = 0$), the Green’s function of equation (A2) can be rewritten as

$$G_{3D,II}(\pm R, \omega) = \frac{1}{(2\pi)^4} \int_{k_x} \int_{k_y} \int_{k_z} \frac{\omega^2 + \sigma_0 + \nu_p (k_x^2 + k_y^2) \sigma_z + \nu_k k_x \tau_y}{\omega^2 - \nu_p^2 k_z^2 - \nu_k^2 k_x^2} e^{i \xi k_x R_1 + i \xi k_y R_2 + i \xi k_z R_3},$$

$$= \frac{1}{(2\pi)^4} \int_{0}^{\infty} k_x \int_{0}^{\infty} k_y \int_{0}^{\infty} k_z \int_{0}^{\infty} d\omega' \int_{0}^{\infty} \frac{\omega^2 + \sigma_0 + \nu_p k_x^2 \sigma_z + \nu_k k_x \sigma_y}{\omega^2 - \nu_p^2 k_z^2 - \nu_k^2 k_x^2} e^{i \xi k_x R_1} e^{i \xi k_y R_2} e^{i \xi k_z R_3} \cos (\omega' - \omega),$$

$$= \frac{1}{2\pi^2} \int_{0}^{\infty} k_x \int_{0}^{\infty} \int_{0}^{\infty} d\omega R_0 \int_{0}^{\infty} d\omega R_0 \int_{0}^{\infty} d\omega R_0 \left( \omega^2 + \sigma_0 + \nu_p k_x^2 \sigma_z \right) \cos (k_x R_x) \pm i\nu_k \sin (k_x R_x) \sigma_y \omega^2 - \nu_p^2 k_z^2 - \nu_k^2 k_x^2,$$  

(A33)

where $R_1 = \sqrt{R_x^2 + R_z^2}$ and $\tan (\varphi') = R_y/R_x$. Using a parameter transformation $(k_x, \nu_p k_z, \nu_k)$, the Green’s function $G_{3D,II}(\pm R, \omega)$ can be simplified as

$$G_{3D,II}(\pm R, \omega) = G_{3D,II}(\omega) = G_{III,0} \sigma_0 + G_{III,2} \sigma_z \pm G_{III,1} \sigma_y.$$  

(A35)

Plugging the Green’s function of equation (A35) into equation (2) of the main text and summing over the spin degrees of freedom, the RKKY components can be written in the form of

$$H_{3D,III}^{RKKY} = \sum_{i,s} J_s I_i S_i S_i^* e \cdot (S_i \times S_i),$$

(A36)

with

$$J^s = - \frac{2\lambda^2}{\pi} \operatorname{Im} \int_{-\infty}^{\infty} (G_{III,0}^2 + G_{III,2}^2 - G_{III,1}^2) d\omega,$$

$$J^v = - \frac{2\lambda^2}{\pi} \operatorname{Im} \int_{-\infty}^{\infty} (G_{III,0}^2 + G_{III,2}^2 - G_{III,1}^2) d\omega,$$

$$J^f = - \frac{2\lambda^2}{\pi} \operatorname{Im} \int_{-\infty}^{\infty} (G_{III,0}^2 + G_{III,2}^2 - G_{III,1}^2) d\omega,$$

$$J^{DM} = - \frac{4\lambda^2}{\pi} \operatorname{Re} \int_{-\infty}^{\infty} (G_{III,0} G_{III,1}) d\omega,$$

(A37)

where $e = (0, 1, 0)$.

According to equation (A34), the Green’s function $G_{3D,II}(\pm R, \omega)$ with impurities in the relativistic axis ($R_{||} = 0, R_{\perp} \neq 0$) can be solved as

$$G_{3D,II}^I(\pm R, \omega) = \frac{1}{2\pi^2} \int_{0}^{\infty} k_x \int_{0}^{\infty} \int_{0}^{\infty} d\omega R_0 \int_{0}^{\infty} d\omega R_0 \int_{0}^{\infty} d\omega R_0 \left( \frac{\omega}{\omega^2 - \nu_p^2 k_z^2 - \nu_k^2 k_x^2} \right) \cos (k_x R_x) \pm i\nu_k \sin (k_x R_x) \sigma_y \omega^2 - \nu_p^2 k_z^2 - \nu_k^2 k_x^2,$$  

(A38)
Plugging the above matrix elements $G_{i=0,1,2}^\parallel$ into equation (A37) and integrating out $\omega$, one can obtain the analytical solutions of the RKKY interaction. The RKKY components $f_i^p$ at zero Fermi energy ($u_F = 0$) are given by

$$f_i^p (u_F = 0) = -\frac{(4 + \pi^2) v_F \lambda^2}{256 \pi^3 v_p^2} \frac{1}{R^3}.$$  

$$f_i^p (u_F = 0) = -\frac{(\pi^2 - 8) v_F \lambda^2}{512 \pi^3 v_p^2} \frac{1}{R^3}.$$  

$$f_i^p (u_F = 0) = \frac{4 - \pi^2}{256 \pi^3 v_p^2} \frac{1}{R^3}.$$  

$$f_i^{DM} (u_F = 0) = 0.$$  

For the case of finite Fermi energy ($u_F \neq 0$), utilizing the asymptotic form of Bessel functions $K_n(x) \approx \sqrt{\pi/2} x^{-1} e^{-x}$ in the condition of $x \gg 1$, the long-range asymptotic behavior of the RKKY components ($R_{\|}/v_F \gg 1$) can be solved as

$$f_i^p (u_F \neq 0) = -\frac{\lambda^2}{64 \pi^3 v_p^2} \frac{u_F \sin \left(\frac{2 R_{\|}}{v_F}\right)}{R^2},$$  

$$f_i^p (u_F \neq 0) = -\frac{v_F \lambda^2}{64 \pi^3 v_p^2} \frac{\cos \left(\frac{2 R_{\|}}{v_F}\right)}{R^3},$$  

$$f_i^p (u_F \neq 0) = -\frac{\lambda^2}{64 \pi^3 v_p^2} \frac{u_F \sin \left(\frac{2 R_{\|}}{v_F}\right)}{R^2},$$  

$$f_i^{DM} (u_F \neq 0) = -\frac{\lambda^2}{64 \pi^3 v_p^2} \frac{u_F \cos \left(\frac{2 R_{\|}}{v_F}\right)}{R^2}.$$  

As shown above, the nonzero DM term $f_i^{DM}$ survives in the case of finite Fermi energy. Note that, the results of equation (A40) are obtained in the condition of $R_{\|}/v_\perp \gg 1$. If small $R_{\|}/v_\perp$ or zero Fermi energy is considered, the RKKY interaction exhibits a strong magnetic anisotropy with a spin model of XYZ ($f_i^\perp \neq f_i^\parallel \neq f_i^{DM}$).

According to equation (A34), the Green’s function $G_{SD,\|}^p (\pm R, \omega)$ with impurities in the non-relativistic axis ($R_\| \neq 0, R_\perp = 0$) can be solved as

$$G_{SD,\|}^p (\pm R, \omega) = \frac{v_F}{4\pi^2} \int_0^{\infty} k dk \int_0^{\pi/2} d\theta \theta \sigma_0 + \frac{\sigma_0 + v_F k \cos (\theta) \sigma_2}{\omega^2 - \frac{v_F^2}{k^2} k^2} \int_0^{\sqrt{\omega^2 - v_F^2 k^2}} j_0 \left[ \sqrt{\omega^2 - v_F^2 k^2} \right],$$  

$$= \frac{\omega^2}{4\pi^2 v_F} \int_0^{\pi/2} \theta d\theta \left[ K_0 (\theta R_\|) - K_0 (i \theta R_\|) \sigma_0 + \right. \left. K_0 (\theta R_\|) - K_0 (i \theta R_\|) \right] \cos (\theta) \sigma_2, \int_0^{\pi/2} \theta d\theta \left[ K_0 (\theta R_\|) - K_0 (i \theta R_\|) \sigma_0 + \right. \left. K_0 (\theta R_\|) - K_0 (i \theta R_\|) \right] \cos (\theta) \sigma_2,$$

$$= G_{SD,\|}^p (R_\|, \omega) + G_{SD,\|}^p (R_\|, -\omega) + G_{SD,\|}^p (R_\|, \omega) + G_{SD,\|}^p (R_\|, -\omega).$$  

where $R_\| = R \sqrt{\omega^2 (\cos (\theta))/v_F}$. Due to the vanished non-diagonal matrix element $G_{\|,\|}^p = 0$, the Green’s function always satisfies $G_{SD,\|}^p (R, \omega) = G_{SD,\|}^p (-R, \omega)$, and so $G_{SD,\|}^p = 0$. Then, the RKKY components of equations (A36) and (A37) with impurities in the non-relativistic axis can be further simplified as

$$H_{p,\|,RKKY} = f_p^H S_1 \cdot S_2 + f_p^I S_1 S_2,$$  

$$f_p^H = -\frac{2 \lambda^2}{\pi} \int_{-\infty}^{\infty} \left[ (G_{\|,\|})_0^p \right] d\omega,$$  

$$f_p^I = -\frac{4 \lambda^2}{\pi} \int_{-\infty}^{\infty} (G_{\|,\|})_0^p d\omega.$$  

(A43)
After integrating out $\omega$, the analytical solutions of the RKKY components at zero Fermi energy can be obtained,

$$f^H_p (u_F = 0) = \frac{16v_F (\rho_3 + \rho_4) \lambda^2}{\pi^4 v^4_I} \frac{1}{R^6},$$

(A44)

$$f^J_p (u_F = 0) = -\frac{32v_F \rho_4 \lambda^2}{\pi^4 v^4_I} \frac{1}{R^6},$$

with

$$\rho_3 = \int_0^{\frac{\pi}{2}} d\theta \int_0^{\frac{\pi}{2}} d\theta' \frac{[\cos^2 (\theta) + \cos^2 (\theta') - 4 \cos (\theta) \cos (\theta')]}{[\cos (\theta) + \cos (\theta')]^6},$$

(A45)

$$\rho_4 = \int_0^{\frac{\pi}{2}} d\theta \int_0^{\frac{\pi}{2}} d\theta' \frac{\cos (\theta) \cos (\theta') \left[\cos^2 (\theta) + \cos^2 (\theta') - 4 \cos (\theta) \cos (\theta')\right]}{[\cos (\theta) + \cos (\theta')]^6},$$

$\rho_3$ and $\rho_4$ are $R$-independent and can be calculated numerically with $\rho_3 = -0.062785$ and $\rho_4 = -0.130117$. For the finite Fermi energy, $f^H_p (u_F \neq 0)$ have to be calculated numerically according to equations (A41) and (A43), the results are shown in figure 2 and can be fitted in the following form,

$$f^H_p (u_F \neq 0) \propto \frac{u_F \sin \left(\frac{2R}{\sqrt{\rho_3}}\right)}{R^3},$$

(A46)

$$f^J_p (u_F \neq 0) \propto \frac{u_F^{3/2} \sin \left(\frac{2R}{\sqrt{\rho_4}}\right)}{R^3},$$

where constant coefficients are dropped. Different from the case with impurities in the relativistic axis, the DM term here vanishes, and the RKKY interaction exhibits a magnetic anisotropy with a spin model of XXY ($f^H_p = f^J_p \neq f^J_p$).

In particular, in the asymptotic form of the Bessel functions $K_n(x) \approx \sqrt{\pi/2x} e^{-x}$, the long-range asymptotic behaviors of the Green’s function are given by

$$G_{\mathrm{II},J} (\pm R, \omega) \propto \frac{1}{R^{3/2}} \omega^{1/2} e^{i k_R},$$

(A47)

$$G_{\mathrm{II},J} (\pm R, \omega) \propto \frac{1}{R} \omega^{1/2} e^{i k_R \tan (\varphi)},$$

Plugging the above equations into equation (A37), we can also obtain the same decaying law as shown in equations (A39), (A40), (A44) and (A46).

A.4. The case of 2D DSM
A 2D DSM describing the surface state of a topological insulator [50–52] is considered with its low-energy Hamiltonian reads as

$$H_{\mathrm{2D}} = v_I (k_x \sigma_x + k_z \sigma_z),$$

(A48)

where $\sigma_{p,z}$ refer to the Pauli matrices of the spin degrees of freedom. Transforming the Green’s function $G' (\mathbf{R}, \omega) = (\omega - H_{\mathrm{2D}})^{-1}$ of $k$-space into real space, one can obtain

$$G' (\pm \mathbf{R}, \omega) = \frac{1}{4\pi^2} \int \frac{\omega_+ \sigma_0 + v_I (k_x \sigma_x + k_z \sigma_z)}{\omega_+ - \nu_I (k_x^2 + k_z^2)} e^{i (k_x R_x + k_z R_z)} d k_x d k_z,$$

(A49)

$$= \frac{1}{4\pi^2} \int_0^{2\pi} d \theta \int_0^{\frac{\pi}{2}} d \theta' \omega_+ \sigma_0 + v_I k \left[\cos (\theta) \sigma_z + \sin (\theta) \sigma_y\right] e^{i k_R \cos (\theta - \nu_I)},$$

where $R = \sqrt{R_x^2 + R_z^2}$, tan $(\varphi) = R_z / R_x$. After some algebraic calculations, the Green’s function can be easily solved as

$$G' (\pm \mathbf{R}, \omega) = g_0 \sigma_0 + \cos (\varphi) g_x \sigma_x + \sin (\varphi) g_z \sigma_z,$$

(A50)

with

$$g_0 = -\frac{\omega K_0 \left(-\frac{i \nu_I}{\nu_I}\right)}{2\pi \nu_I^2},$$

(A51)

$$g_x = -\frac{\omega K_1 \left(-\frac{i \nu_I}{\nu_I}\right)}{2\pi \nu_I^2}.$$
Plugging the above analytical Green’s functions into equation (2) of the main text, the RKKY components of 2D DSM can be expressed in the following form

\[ H_{\text{RKKY}}^{2D} = \sum_{i=x,y,z} J_{2D}^{i} S_i^x S_i^z + J_{2D}^{DM} \mathbf{e} \cdot (S_1 \times S_2) + J_{2D}^{\phi} (S_1^x S_2^z + S_1^z S_2^x), \] (A52)

with

\[ J_{2D}^{x} = \frac{2 \lambda^2}{\pi} \text{Im} \int_{-\infty}^{0} (g_0^2 + g_2^2) \, d\omega, \]
\[ J_{2D}^{y} = \frac{2 \lambda^2}{\pi} \text{Im} \int_{-\infty}^{0} [g_0^2 + g_2^2 \cos (2\varphi)] \, d\omega, \]
\[ J_{2D}^{z} = \frac{2 \lambda^2}{\pi} \text{Im} \int_{-\infty}^{0} [g_0^2 - g_2^2 \cos (2\varphi)] \, d\omega, \]
\[ J_{2D}^{DM} = \frac{4 \lambda^2}{\pi} \text{Re} \int_{-\infty}^{0} g_0 g_2 \, d\omega, \]
\[ J_{2D}^{\phi} = \frac{4 \cos (\varphi_1) \sin (\varphi_1) \lambda^2}{\pi} \text{Im} \int_{-\infty}^{0} g_2^2 \, d\omega, \]

where \( \mathbf{e} = [0, \sin (\varphi_1), \cos (\varphi_1)] \). After integrating out \( \omega \) in equation (A53), all RKKY components can be solved as,

\[ J_{2D}^{x} (u_F = 0) = -\frac{\lambda^2}{16\pi v_F R^4}, \]
\[ J_{2D}^{y} (u_F = 0) = -\frac{\lambda^2}{64\pi v_F R^3} \left[ 3 \cos (2\varphi) + 1 \right], \]
\[ J_{2D}^{z} (u_F = 0) = \frac{\lambda^2}{64\pi v_F R^3} \left[ 3 \cos (2\varphi) - 1 \right], \]
\[ J_{2D}^{DM} (u_F = 0) = 0, \]
\[ J_{2D}^{\phi} (u_F = 0) = \frac{3\lambda^2}{32\pi v_F R^3} \cos (\varphi) \sin (\varphi), \]

and

\[ J_{2D}^{x} (u_F \neq 0) = -\frac{\lambda^2}{4\pi^2 v_F^2} \frac{u_F \sin (2u_F R/v)}{R^2}, \]
\[ J_{2D}^{y} (u_F \neq 0) = -\frac{\lambda^2}{8\pi^2 v_F^2} \frac{u_F \sin (2u_F R/v)}{R^2} \left[ 1 + \cos (2\varphi) \right], \]
\[ J_{2D}^{z} (u_F \neq 0) = -\frac{\lambda^2}{8\pi^2 v_F^2} \frac{u_F \sin (2u_F R/v)}{R^2} \left[ 1 - \cos (2\varphi) \right], \]
\[ J_{2D}^{DM} (u_F \neq 0) = -\frac{\lambda^2}{4\pi^2 v_F^2} \frac{u_F \cos (2u_F R/v)}{R^2}, \]
\[ J_{2D}^{\phi} (u_F \neq 0) = -\frac{\lambda^2}{4\pi^2 v_F^2} \frac{u_F \sin (2u_F R/v)}{R^2} \cos (\varphi) \sin (\varphi), \]

where the asymptotic form of the Bessel function \( K_0(x) \approx \sqrt{\pi/2x} e^{-x} (x \gg 1) \) is applied in doped case \( u_F \neq 0 \).

Note that, for impurities reside on x axis (\( \varphi = 0 \)) or z axis (\( \varphi = \pi/2 \)), the DM term \( J_{2D}^{DM} \) survives and the frustrated term \( J_{2D}^{\phi} \) vanishes, the RKKY interaction exhibits a magnetic anisotropy with a spin model of \( XXX \) \( (J_{2D}^{x} = J_{2D}^{y} \neq J_{2D}^{z} \text{ or } J_{2D}^{z} = J_{2D}^{x} \neq J_{2D}^{y}) \).

A.5. The case of 3D DSM
A 3D DSM is considered with its low-energy Hamiltonian reads as

\[ H_{3D}' = v_1 \left( k_x \sigma_z + k_y \sigma_x + k_z \sigma_y \right), \] (A56)
where $\sigma_{x,y,z}$ refer to the Pauli matrices of the spin degrees of freedom. Transforming the Green’s function $G_{3D}^{\prime}(k,\omega) = (\omega + H_{3D}^{\prime})^{-1}$ of $k$-space into real space, one can obtain

\[
G_{3D}(R,\omega) = \frac{1}{8\pi^3} \int \int \int \frac{\omega_+ \sigma_0 + v_1 (k_x \sigma_x + k_y \sigma_y + k_z \sigma_z)}{\omega_+^2 - v_1^2 (k_x^2 + k_y^2 + k_z^2)} \mathcal{G}(k_x, k_y, k_z) \, dk_x \, dk_y \, dk_z,
\]

\[
= \frac{1}{8\pi^3} \int \frac{d\vec{k}}{2\pi^2} \frac{k^2 \sin(\theta)}{\omega_+^2 - v_1^2 k^2} \int \frac{d\theta}{2\pi} + \int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin(\theta) \sin^2(\theta) \, d\theta
\]

\[
\times \int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin(\theta) \sin^2(\theta) \, d\theta \]

\[
\times \int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin(\theta) \sin^2(\theta) \, d\theta \int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin(\theta) \sin^2(\theta) \, d\theta.
\]

where $j_n(x)$ is the spherical Bessel function. After some algebraic calculations, one can obtain the analytical expressions of Green’s function of real-space,

\[
G_{3D}(R,\omega) = f_0 \sigma_0 + \sin(\theta_R) \cos(\varphi_R) f_x \sigma_x + \sin(\theta_R) \sin(\varphi_R) f_y \sigma_y + \cos(\theta_R) f_z \sigma_z,
\]

with

\[
f_0 = \frac{-\omega}{4\pi v_1^2 R} e^{iR/\omega},
\]

\[
f_i = \frac{-R \omega + i v_1}{4\pi v_1^2 R^2} e^{iR/\omega},
\]

where $R = (R_x, R_y, R_z) = R \sin(\theta_R) \cos(\varphi_R), \sin(\theta_R) \sin(\varphi_R), \cos(\theta_R)]$. Following the same process, one can also obtain

\[
G_{3D}(-R,\omega) = f_0 \sigma_0 - \sin(\theta_R) \cos(\varphi_R) f_x \sigma_x - \sin(\theta_R) \sin(\varphi_R) f_y \sigma_y - \cos(\theta_R) f_z \sigma_z.
\]

Plugging the Green’s functions of equations (A58)–(A60) into equation (2) of the main text, the RKKY components of 3D DSM can be obtained in the following form

\[
H_{RKKY}^{3D} = \sum_{i,j=x,y,z} f_{3D}^{i} S_i^j \cdot S_j + f_{3D}^{DM} \mathbf{e} \cdot (S_1 \times S_2) + \sum_{i,j=x,y,z} f_{3D}^{ij} e_i e_j \left(S_i^j S_j^i + S_j^i S_i^j\right),
\]

with

\[
f_{3D}^{x} = \frac{-2\lambda^2}{\pi} \Im \int_{-\infty}^{\infty} \left\{ f_0^x + f_x^x \left[ \cos^2(\theta_R) + \cos(2\varphi_R) \sin^2(\theta_R) \right] \right\} d\omega,
\]

\[
f_{3D}^{y} = \frac{-2\lambda^2}{\pi} \Im \int_{-\infty}^{\infty} \left\{ f_0^y - f_y^y \cos(2\theta_R) \right\} d\omega,
\]

\[
f_{3D}^{z} = \frac{2\lambda^2}{\pi} \Im \int_{-\infty}^{\infty} \left\{ f_0^z + f_z^z \left[ \cos^2(\theta_R) - \cos(2\varphi_R) \sin^2(\theta_R) \right] \right\} d\omega,
\]

\[
f_{3D}^{DM} = \frac{-4\lambda^2}{\pi} \Re \int_{-\infty}^{\infty} f_0^x d\omega,
\]

\[
f_{3D}^{0} = \frac{4\lambda^2}{\pi} \Im \int_{-\infty}^{\infty} f_x^0 d\omega,
\]
where $e = [\sin(\theta_R) \sin(\varphi_R), \cos(\theta_R), \sin(\theta_R) \cos(\varphi_R)]$. After integrating out $\omega$ in equation (A62), the RKKY components can be obtained as

$$f_{3D}^{\omega}(u \neq 0) = \frac{\lambda^2}{32\pi^2 R^3}[1 + 5 \cos^2(\theta_R) + 5 \cos(2\varphi_R) \sin^2(\theta_R)],$$

$$f_{3D}^{\varphi}(u \neq 0) = \frac{\lambda^2}{32\pi^2 R^3}[1 - 5 \cos(2\theta_R)],$$

$$f_{3D}^{J}(u \neq 0) = -\frac{\lambda^2}{32\pi^2 R^3}[1 + 5 \cos^2(\theta_R) - 5 \cos(2\varphi_R) \sin^2(\theta_R)],$$

and

$$f_{3D}^{DM}(u \neq 0) = 0,$$

$$f_{3D}^{\theta}(u \neq 0) = \frac{5\lambda^2}{16\pi^2 R^3},$$

and

$$f_{3D}^{\omega}(u \neq 0) = \frac{\lambda^2}{16\pi^2 \nu^3} u^2 \cos(2\mu R / \nu) R^3[1 + \cos^2(\theta_R) + \cos(2\varphi_R) \sin^2(\theta_R)],$$

$$f_{3D}^{\varphi}(u \neq 0) = \frac{\lambda^2}{16\pi^2 \nu^3} u^2 \cos(2\mu R / \nu) R^3[1 - \cos(2\theta_R)],$$

$$f_{3D}^{J}(u \neq 0) = \frac{\lambda^2}{16\pi^2 \nu^3} u^2 \cos(2\mu R / \nu) R^3[1 - \cos^2(\theta_R) - \cos(2\varphi_R) \sin^2(\theta_R)],$$

$$f_{3D}^{DM}(u \neq 0) = -\frac{\lambda^2}{8\pi^2 \nu^3} u^2 \sin(2\mu R / \nu) R^3,$$

$$f_{3D}^{\theta}(u \neq 0) = -\frac{\lambda^2}{8\pi^2 \nu^3} u^2 \cos(2\mu R / \nu) R^3.$$

Note that, for impurities reside on $i$ axis ($\theta_R = 0$ or $\theta_R = \pi/2$, $\varphi_R = 0$ or $\theta_R = \pi/2$, $\varphi_R = \pi/2$), the DM term $f_{3D}^{DM}$ always survives and the frustrated term $f_{3D}^{\omega}$ vanishes, the RKKY interaction exhibits a magnetic anisotropy with a spin model of XXY ($f_{3D}^{J} = f_{3D}^{J} \neq f_{3D}^{\omega}$ or $f_{3D}^{J} = f_{3D}^{\varphi} \neq f_{3D}^{J}$ or $f_{3D}^{J} = f_{3D}^{J} \neq f_{3D}^{\theta}$).

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