RKKY interaction of magnetic impurities in multi-Weyl semimetals

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Abstract

We have systematically investigated the Ruderman–Kittel–Casuaya–Yosida (RKKY) interaction between two magnetic impurities in Weyl semimetals with arbitrary monopole charge \( Q \). We find that the RKKY interaction becomes intrinsically anisotropic for \( Q \geq 2 \), and its dependence on Fermi energy and impurity separation is directly controlled by the monopole charge. With the increase of \( Q \), the RKKY interaction becomes more long-ranged and more anisotropic, which makes interesting magnetic orders easier to form and thus may have important applications in spintronics.

Keywords: RKKY interaction, spintronics, multi-Weyl semimetal, Weyl semimetal

(Some figures may appear in colour only in the online journal)

1. Introduction

Electronic band structure plays a fundamental role in condensed matter physics because many properties of materials are directly determined by it [1]. Recently, Weyl semimetals (WSMs) have attracted major research interest because their energy bands host isolated crossing points protected by topology [2–9]. A remarkable property of the crossing points is that they carry integer Berry flux and thus can be taken as monopoles in momentum space [10]. As a direct consequence of the integer Berry flux (or the monopole charge), equal numbers of chiral Landau levels will show up in the presence of a magnetic field. If an electric field is further applied in parallel with the magnetic field, novel phenomena related to chiral anomaly will take place [11–15].

Although WSMs have been extensively studied, most works are restricted to the WSMs belonging to the class with monopole charge \( Q = 1 \) [16–19], and the classes with \( Q \geq 2 \) remain much less explored due to lack of experimentally confirmed materials. In contrast with the \( Q = 1 \) class, the classes with \( Q \geq 2 \) will inevitably show anisotropic energy dispersion away from the crossing points [20–22]. Consequently, their density of states will also show distinctive power laws, which immediately indicates that the monopole charge will affect a series of physical properties [23–33]. Motivated by these observations, in this work we give a systematic study on the Ruderman–Kittel–Casuaya–Yosida (RKKY) interaction [34–36], which is an indirect interaction between magnetic impurities induced by itinerant carriers, for WSMs with arbitrary monopole charge.

The RKKY interaction in WSMs with \( Q = 1 \) have already been investigated [37, 38]. Based on the ideal isotropic model, the authors found that the interaction is isotropic, and for the intrinsic case it decays with a power law \( H_{\text{RKKY}}(R) \propto R^{-3} \) with \( R \) the distance between two impurities; while for finite doping, the decaying power law becomes \( H_{\text{RKKY}}(R) \propto R^{-3} \), indicating that the interaction is in fact quite short-ranged [37, 38]. In this work, we generalize these studies to arbitrary large \( Q \), and find that for \( Q \geq 2 \), the interaction becomes anisotropic, with \( H_{\text{RKKY}}(z) \propto z^{-4/3}Q^{-1} \) and \( H_{\text{RKKY}}(\rho) \propto \rho^{-Q-4} \) for the intrinsic case, and \( H_{\text{RKKY}}(z) \propto z^{-2/3}Q^{-1} \) and \( H_{\text{RKKY}}(\rho) \propto \rho^{-3} \) for finite doping. Thus, for large \( Q \), the interaction becomes quasi-one-dimensional and long-ranged, which may trigger interesting magnetic orders. Besides, the power law can be utilized as a way to determine the monopole charge of WSMs.

The paper is organized as follows. In section 2, we outline the setup of our model and deduce general forms of RKKY range functions. In section 3, we present long-range asymptotic results for two most representative alignments of impurities, namely along the line connecting the multi-Weyl points.
and in the perpendicular plane. Both the dependence on impurity separation and on Fermi energy are discussed. We end with brief conclusion in section 4.

2. The setup

As Weyl points emerge from the touching of two adjacent non-degenerate bands, the low-energy effective Hamiltonian near Weyl points with monopole charge \( Q \) can be generally written down as follows:

\[
H_0(k) = \chi \lambda \left( k_+^0 \sigma_+ + k_-^0 \sigma_- \right) + \chi v(k_z - \chi k_0) \sigma_z,
\]

in which \( \sigma_\pm = \frac{1}{2} (\sigma_x \pm i \sigma_y) \) and \( k_\pm = k_x \pm ik_y \). \( \sigma \) denotes two kinds of chirality of multi-Weyl points; \( \lambda \) is a parameter with mass dimension \( (1 - Q) \), and \( v \) is the Fermi velocity in the \( z \) direction. The multi-Weyl points are located at \( \pm (0, 0, k_0) \) in momentum space. We will refer to the line connecting the multi-Weyl points as the vertical direction, and the plane perpendicular to the line as the transverse plane.

Now consider two magnetic impurities with localized spins \( S_1 \) and \( S_2 \) that are well embedded into the WSMs, such that the effect of surface states can be neglected. Besides, for simplicity of notation, the two localized spins are placed at the origin of coordinates and position \( R \). The standard \( s-d \) interaction, which describes the coupling between localized spins and itinerant electrons, is given by

\[
H_I = (J \tau_0 + \Lambda \tau_z) S_1 \cdot \sigma \delta (r - R),
\]

where \( J \) and \( \Lambda \) represent the intranode and internode coupling strength, respectively. The \( s-d \) interaction can be treated as a perturbation to the multi-Weyl Hamiltonian. At zero temperature, the RKKY interaction between these two magnetic impurities can be obtained by second order perturbation theory [34–38], which is

\[
H_{RKKY} = \sum_{\alpha = 0,1} \sum_{\alpha' = 0,1} \left[ \frac{1}{2} \delta_{\alpha \alpha'} \right] S_\alpha^0 S_\alpha'^0 \times \text{Im} \left\{ \frac{1}{\pi} \int_{-\infty}^{\infty} \text{d} \tilde{\tau} \text{Tr} [\sigma_\alpha G_\alpha (\epsilon, \mathbf{R}) \sigma_\beta G_{\alpha'} (-\epsilon, \mathbf{R})] \right\},
\]

where \( \epsilon_F \) is the Fermi energy, \( G_\alpha (\epsilon, \mathbf{R}) \) denotes the real-space Green’s function matrix in the absence of magnetic impurities.

2.1. Green’s function

In the absence of magnetic impurities, the Green’s function in momentum space takes the form of \( G_\chi^{-1} (\epsilon, \mathbf{k}) = \epsilon - H_0 (\mathbf{k}) \). To get its form in the energy-coordinate representation, we perform a Fourier transformation,

\[
G_\chi (\epsilon, \mathbf{R}) = \int \frac{d^3k}{(2\pi)^3} \frac{\epsilon + \tilde{H}_0 (\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{R}}}{\epsilon - E_k},
\]

where \( E_k = \sqrt{\lambda^2 k_0^2 + v^2 k_0^2} \) and \( \tilde{H}_0 (\mathbf{k}) = \chi \lambda \left( k_+^0 \sigma_+ + k_-^0 \sigma_- \right) + \chi v k_z \sigma_z \). Note that the energy dispersion relation is linear in the vertical direction and nonlinear in the transverse plane for \( Q \geq 2 \).

The above integration can be more conveniently solved in spherical coordinates, i.e. \( (k_x, k_y, k_z) \rightarrow (k, \phi, \psi) \), where \( \phi \) denotes the angle between the momentum vector and the \( x-y \) plane. After some straightforward calculations, we find that

\[
G_\chi (\epsilon, \mathbf{R}) = C_\epsilon e^{i\chi k_0 z} \left( g_0 \sigma_0 + \chi g_1 \sigma_1 + \chi g_3 \sigma_3 \right),
\]

where \( g_0 = \sigma \cdot \delta (\tilde{\theta}), \) with \( \delta (\tilde{\theta}) = \cos (Q \tilde{\theta}) \delta + \sin (Q \tilde{\theta}) \hat{y} \), and the constant multiplier defined as \( C_\epsilon = -\frac{1}{4\pi^2 v^2 \left( \frac{\lambda}{\chi} \right)^2 / Q} \). The dimensionless coefficients \( g_{0,1,3} (\epsilon, \rho, z) \) are complex functions of the following form:

\[
g_0 (\epsilon, \rho, z) = \frac{\epsilon}{(k_0 \alpha / \rho)^2} \int_0^{\infty} dq q^{1/2} d\phi \left[ q \cos \phi / \lambda \right]^{1/2} \cos \left( q \sin \phi / \rho \right) / q^2 - \epsilon^2,
\]

\[
g_1 (\epsilon, \rho, z) = e^{iqz} \left( \frac{1}{(k_0 \alpha / \rho)^2} \int_0^{\infty} dq q^{1/2} d\phi \left[ q \cos \phi / \lambda \right]^{1/2} \cos \left( q \sin \phi / \rho \right) / q^2 - \epsilon^2 \right),
\]

\[
g_3 (\epsilon, \rho, z) = \left( \frac{1}{(k_0 \alpha / \rho)^2} \int_0^{\infty} dq q^{1/2} d\phi \left[ q \cos \phi / \lambda \right]^{1/2} \cos \left( q \sin \phi / \rho \right) / q^2 - \epsilon^2 \right).
\]

2.2. RKKY interaction

We find that the RKKY interaction in multi-WSMs generally have four distinctive types of terms:

\[
H_{RKKY} (\epsilon, \mathbf{R}) = F_1 S_1 \cdot S_2 + F_2 (S_1 \times S_2) \cdot \hat{s} + F_3 (S_1 \cdot \hat{s}) (S_2 \cdot \hat{s}) + F_4 S_1^0 S_2^0,
\]

where the range functions \( F_{1,2,3,4} \) are defined as follows:

\[
F_1 = \frac{1}{2} \left[ G_{00} (J^2 + \Lambda^2 \cos (2k_0 z)) + (G_{33} + (-1)^Q G_{11}) (J^2 - \Lambda^2 \cos (2k_0 z)) \right],
\]

\[
F_2 = \frac{1}{2} \left[ G_{00} \Lambda^2 \sin (2k_0 z), \right]
\]

\[
F_3 = (-1)^Q G_{11} (J^2 - \Lambda^2 \cos (2k_0 z)),
\]

\[
F_4 = -G_{33} (J^2 - \Lambda^2 \cos (2k_0 z)).
\]

In the above equation, the first term is the rotation-invariant Heisenberg term, which favors either parallel or antiparallel alignment of the impurity spins depending on the sign of \( F_1 \). The second term is the Dzyaloshinsky–Moriya (DM)

term [39, 40], which favors configurations in which the impurity spins are orthogonal; this term should vanish for odd $Q$ because inversion symmetry remains intact in these cases. The third term is the so-called spin-frustrated term, which favors the (anti)parallel alignment of the impurity spins along $\hat{s}$. Importantly, for both the DM and spin-frustrated terms, the favored direction $\hat{s}$ generally does not coincide with $\hat{\rho}$ (alignment of the two magnetic impurities projected on the transverse plane) for $Q > 2$, which predicts novel spin structures for multi-WSMs. The last term is the Ising term. Note that when $Q = 1$, i.e. for single Weyl nodes, $\hat{s} = \hat{\rho}$ and equation (8) reduces to the form derived in [38].

Note that when we generalize our system to many magnetic impurities which are distributed randomly in real materials, the spin-frustrated term frustrates the spins of magnetic impurities, hence the terminology. Furthermore, the rapid oscillating terms $\lambda^2 \cos (k_0 z)$ and $\lambda^2 \sin (2k_0 z)$ should average out (over impurity positions) for large momentum separation $2k_0$ and do not contribute to net magnetization. The intranode process thus contribute predominately to the RKKY interaction [37, 41]. We will take this simplification in the following discussions.

Our main quest now reduces to calculating the $G_{ij}$ coefficients, as defined for $i, j \in \{0, 1, 3\}$,

$$G_{ij}(\varepsilon_F, R) \equiv \frac{C}{k_0 \nu} \times \text{Im} \int_{-\infty}^{\varepsilon_F} d\epsilon g_{ij},$$

$$= C \text{Im} \int_{-\infty}^{\varepsilon_F} d\tilde{\epsilon} \tilde{g}_{ij} \equiv CG_{ij},$$

(10)

with constant $C = -\frac{k_0^2}{2Q^2 \pi^2} \frac{\lambda^2}{(Q^2 \pi^2)^{1/4}}$. The momentum separation of multi-Weyl points provides a natural scale for our system. For convenience, we will switch to dimensionless variables $\tilde{\epsilon} \equiv \epsilon / (k_0 \nu)$, $\tilde{\zeta} \equiv k_0 z$ and $\tilde{\rho} \equiv (k_0 \nu / \lambda)^{1/2} \rho$. Naturally, two most interesting cases are $\tilde{\rho} = 0$ and $\tilde{\zeta} = 0$, which correspond to impurities alignment along the $z$ axis and in the transverse plane, respectively. We discuss both scenarios in details below. The $G_{ij}$’s are generally not analytically integrable. Fortunately, for large values of $\tilde{z}$ and $\tilde{\rho}$, we manage to devise analytical approximations that agree well with numerical results.

3. Results and discussions

3.1. Impurities along the vertical direction

For magnetic impurities aligned along the vertical direction, i.e. $\tilde{\rho} = 0$, as $J_0(0) = 0$ for $Q < 2^+$ and $J_0(0) = 1$, the $\tilde{g}_i$ coefficients can be simplified to

$$\tilde{g}_0 = i \int_0^{\infty} d\tilde{\epsilon} \int_{-\pi / 2}^{\pi / 2} d\phi \left( \frac{\cos(\cos(\phi) q^2 - 1)}{q^2 - \tilde{\rho}^2} \cos(\phi \sin \phi) \right).$$

$$\tilde{g}_1 = i \int_0^{\infty} d\tilde{\epsilon} \int_{-\pi / 2}^{\pi / 2} d\phi \left( \frac{\cos(\phi) q^2 - 1}{q^2 - \tilde{\rho}^2} \sin(\phi \sin \phi) \right).$$

$$\tilde{g}_1 = 0.$$  (11)

The asymptotic dependence of $\tilde{g}_i$ on $\tilde{z}$ and $\tilde{\rho}$ can be shown heuristically. For $\tilde{g}_0$, the integration of the numerator over $\phi$ has $\tilde{g}(q / \tilde{z})^{1/4} \cos(q^2 \tilde{z} - \pi / 2Q)$ as the leading term, the subsequent Cauchy integration over $q$ gives $\tilde{g}_0 \propto (\tilde{z} / 1)^{1/4} \exp(i(q^2 \tilde{z} - \pi / 2Q))$. Also, it is explicit from equation (11) that $\tilde{g}_3 = -i \frac{\partial^2}{\partial \tilde{z}^2} \tilde{g}_0$. At large distance $\tilde{z} >> 1$, it is readily seen that $\tilde{g}_0 \approx \tilde{g}_3$.

The coefficients $\tilde{g}_{ij}$ thus take the following form for finite Fermi energy and at long distance:

$$\tilde{g}_{00}(\varepsilon_F, \tilde{z}) \approx \tilde{g}_{33}(\varepsilon_F, \tilde{z}) \approx \alpha_1 \frac{\tilde{v}^2}{2Q^{1/4} \tilde{z}} \cos(2\tilde{z}^2 - \pi / Q),$$  (12)

where $\alpha_1 = \frac{2^{11/32} \pi^2}{8} \left( \Gamma \left( \frac{1}{4} \right) \right)^2$ is a real constant that only depends on chiral charge $Q$.

It is understood that the integration over occupied states in the valence band ($\int_{-\infty}^{\varepsilon_F} d\tilde{\epsilon} \tilde{g}_{ij}$) generates unphysical divergence, which can be regulated using the soft cutoff procedure [42]. Specifically, for the intrinsic case ($\epsilon_F = 0$), the corresponding form can be obtained by dimensional analysis,

$$\tilde{g}_{00}(0, \tilde{z}) \sim \tilde{g}_{33}(0, \tilde{z}) \propto \frac{1}{\tilde{z}^{Q+\epsilon}}.$$  (13)

The above terms could be safely dropped from equation (12) since we are only interested in the long range scenario. Note that the leading term argument does not apply to infinite integrals, hence the $\sim$ between $\tilde{g}_{00}(0, \tilde{z})$ and $\tilde{g}_{33}(0, \tilde{z})$ indicating different constant multipliers. The constant multipliers can in principle be worked out numerically for each chiral charge $Q$.

Finally, we have the long range asymptotic form of RKKY interaction for impurities along $z$ axis. For finite doping,

$$H_{RKKY}^{\text{LR}} \propto \left( \frac{\tilde{v}}{2Q^{1/4} \tilde{z}} \right)^2 \cos(2\tilde{z}^2 - \pi / Q) \left( \frac{S_1 \cdot S_2 - S_3^0 S_3^0}{2} \right).$$  (14)

For reference, figure 1 plots exact numerical results of RKKY range functions in double-Weyl semimetal ($Q = 2$) with vertical impurity alignment. The power law dependence on impurity separation and Fermi energy agree well with our asymptotic result. The cancellation of the Ising term and the term $\alpha_1$ is a real constant to be determined numerically for each monopole charge with vertical impurity alignment.

For the intrinsic case, the RKKY interaction becomes nonoscillatory,

$$H_{RKKY}^{\text{00}} \propto \frac{1}{\tilde{z}^{Q+\epsilon} / 2Q^{1/4} \tilde{z}} \left( \frac{S_1 \cdot S_2 - S_3^0 S_3^0}{2} \right),$$  (15)

with $\beta_1$ being a real constant to be determined numerically for given $Q$. With the increase of monopole charge, the RKKY interaction becomes more long-ranged.

3.2. Impurities in the transverse plane

For magnetic impurities aligned in the transverse plane, i.e. $\tilde{\rho} = 0$, the $\tilde{g}_i$ coefficients can be simplified to
The asymptotic RKKY interaction for impurities in the transverse plane thus reduces to
\[ H_{\text{RKKY}}^0 \sim \frac{c}{\tilde{\rho}^3} \cos(2\tilde{\epsilon}_F/\tilde{\rho}) \times sc, \]
with the spin correlator
\[ sc = \begin{cases} 
S_1 \cdot S_2 = (S_1 \cdot \hat{s})(S_2 \cdot \hat{s}), & Q \text{ odd}, \\
(S_1 \cdot \hat{s})(S_2 \cdot \hat{s}), & Q \text{ even}. 
\end{cases} \]

Analogous heuristic argument can be applied to the above equations. The coefficients \( \tilde{G}_i \) take the following form for finite Fermi energy and at long distance:
\[ \tilde{g}_0 = \int_0^{\infty} dq \int_{-\pi/2}^{\pi/2} d\phi \frac{q^2/(\cos \phi)^2}{q^2 - \tilde{\epsilon}^2}, \]
\[ \tilde{g}_1 = i \int_0^{\infty} dq \int_{-\pi/2}^{\pi/2} d\phi \frac{q^2/(\cos \phi)^2}{q^2 - \tilde{\epsilon}^2}, \]
\[ \tilde{g}_3 = 0. \] (16)

For odd \( Q \), the spin correlator term is much similar to the that derived in equation (14), only that the preferred spin alignment \( \hat{s} \) generally does not coincide with impurity alignment \( \tilde{\rho} \) when \( Q \neq 1 \). For even \( Q \), the spin-frustrated term dominates the RKKY interaction since the components of the Heisenberg term cancel out.

Figure 2 shows exact numerical results of RKKY range functions in double-Weyl semimetal (\( Q = 2 \)) for impurities in the transverse plane, the power-law dependence on impurity separation and Fermi energy agree well with our analytical result. Note that the cancellation of \( \tilde{g}_{00} \) and \( \tilde{g}_{11} \) is valid up to the leading order and leaves out a minor Heisenberg term proportional to \( \tilde{\rho}^3 \sin(2\tilde{\epsilon}_F/\tilde{\rho}) \) (see solid red lines in figure 2). Similar higher-order residual term is also present between the cancellation of \( F_1 \) and \( F_4 \) in previous section (not explicitly plotted in figure 1).

For the intrinsic case, the regulated result of the divergent integration \( \int_0^\infty d\tilde{\rho} \tilde{g}_i^2 \) gives
\[ \tilde{g}_{00}(0, \tilde{\rho}) \sim \tilde{g}_{11}(0, \tilde{\rho}) \sim \frac{1}{\tilde{\rho}^{3+\nu}}, \] (20)
and the RKKY interaction becomes non-oscillatory,
\[ H_{\text{RKKY}}^{p,0} \sim \frac{1}{\tilde{\rho}^{3+\nu}} |S_1 \cdot S_2 - \beta_2 (S_1 \cdot \hat{s})(S_2 \cdot \hat{s})|. \] (21)
with $\beta_2$ being a real constant for given $Q$. For large monopole charge, the interaction becomes quite short-ranged in planar directions.

3.3. Discussion of the results

Equations (14), (15), (18) and (21) constitute the central results of our present work. It is quick to verify that for $Q = 1$ WSMs, the RKKY interaction takes the form of

$$H_{\text{RKKY}} \propto \frac{\tau^2 \cos(2\xi_f \tilde{R})}{R^3} (S_1 \cdot S_2 - S_j \rho_j^1),$$  \tag{22}

for finite doping, and

$$H_{\text{RKKY}}^0 \propto \frac{1}{R^3} (S_1 \cdot S_2 - \beta S_j^0 \rho_j^1),$$  \tag{23}

for the intrinsic case, where $j$ denotes the direction of impurity alignment. Both formulas coincide with the results previously obtained in [37, 38].

Compared to the $Q = 1$ case, several distinctive features arise for $Q \geq 2$. First, for finite doping the RKKY interaction decays as $1/\tilde{R}^{2+Q^2+1}$ and $1/\tilde{p}^3$ for two representative impurity alignments (as $1/\tilde{R}^{2+Q^2+1}$ and $1/\tilde{p}^{Q^2+4}$ for the intrinsic case, respectively). With the increase of monopole charge $Q$, it is readily seen that the range functions become more long-ranged in the vertical direction. Second, the power-law dependence on the Fermi energy amounts to $2^{Q^2}$ for the vertical direction and $\tilde{\xi}_F^{1/2+Q^2+1}$ for the transverse directions, suggesting that the increase of Fermi energy contributes a bigger boost to the RKKY range functions in the latter case. Besides, there exists an even-odd discrepancy for impurities in the transverse plane: for odd $Q$, the Heisenberg term coexists with the spin-frustrated term; while for even $Q$ the Heisenberg term cancels out up to leading order and the spin-frustrated term dominates the RKKY interaction (see equation (19)).

Interestingly, for $Q \geq 3$, the doped $1/\tilde{R}^{2+Q^2+1}$ decay is slower than many conventional materials including ordinary metals ($R^{-3}$) [34], 2D electron gas systems ($R^{-2}$) [43], graphenes [42] and surface states of topological insulators [44] (both $R^{-2}$ for doped and $R^{-3}$ for undoped cases). This long-rangeness combined with the intrinsic anisotropy would give rise to a rich behavior of spin interactions in multi-Weyl semimetal systems.

4. Conclusion

In summary, we have studied the RKKY interactions for WSMs with arbitrary monopole charge $Q$ and analytically obtained their asymptotic expressions in the long range limit. The results indicate that the power-law dependence of the RKKY interaction on impurity separation and Fermi energy is directly controlled by the monopole charge. As the power-law dependence is tightly related to the monopole charge, it thus provides a potential way to determine the monopole charge of WSMs. More importantly, the interaction becomes quite long-ranged and quasi-one-dimensional for WSMs with large monopole charge, which may trigger interesting magnetic orders and result in applications in spintronics.

Besides the material candidates predicated by first-principle calculations [20, 22, 45], recently, several other works postulate that multi-WSMs can be dynamically created either from normal insulators [46] or from crossing nodal line semimetals [47, 48]. Considering the rapid development of this field, it is expected that our theoretical predictions can be experimentally tested in near future.

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