



Research articles

Velocity-determined anisotropic behaviors of RKKY interaction in 8-*Pmmn* boropheneShu-Hui Zhang^{a,*}, Ding-Fu Shao^b, Wen Yang^{c,*}^a College of Mathematics and Physics, Beijing University of Chemical Technology, Beijing 100029, China^b Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588-0299, USA^c Beijing Computational Science Research Center, Beijing 100193, China

A B S T R A C T

As a new two-dimensional Dirac material, 8-*Pmmn* borophene hosts novel anisotropic and tilted massless Dirac fermions (MDFs) and has attracted increasing interest. However, the potential application of 8-*Pmmn* borophene in spin fields has not been explored. Here, we study the long-range RKKY interaction mediated by anisotropic and tilted MDFs in magnetically-doped 8-*Pmmn* borophene. To this aim, we carefully analyze the unique real-space propagation of anisotropic and tilted MDFs with noncolinear momenta and group velocities. As a result, we analytically demonstrate the anisotropic behaviors of long-range RKKY interaction, which have no dependence on the Fermi level but are velocity-determined, i.e., the anisotropy degrees of oscillation period and envelop amplitude are determined by the anisotropic and tilted velocities. The velocity-determined RKKY interaction favors to fully determine the characteristic velocities of anisotropic and tilted MDFs through its measurement, and has high tunability by engineering velocities shedding light on the application of 8-*Pmmn* borophene in spin fields.

1. Introduction

The charge and spin are two intrinsic ingredients of the electron, and the success of electronics based on the charge transport lures people to develop the spin-related applications [1,2]. However, a lot of solid-state materials are nonmagnetic and/or do not show its spin properties, then hinder their applications in spin fields. One way to surmount the obstacle is through the doping of nonmagnetic materials with magnetic impurity atoms [3]. The itinerant carriers of host materials can help to couple the magnetic impurities indirectly, i.e., the Rudermann-Kittel-Kasuya-Yosida (RKKY) interaction [4–6]. The RKKY interaction is an important mechanism underlying rich magnetic phases in diluted magnetic systems [7] and giant magneto-resistance devices [2], and has potential applications in spintronics [8,1,9], and scalable quantum computation [10,11], as the RKKY interaction enables long-range coupling of distant spins [12–16].

The importance of RKKY interaction makes its research to closely accompany the advent and development of new materials. In recent years, the RKKY interaction has been widely studied in various materials such as graphene [17–21], monolayer transition-metal dichalcogenides [22–27] topological insulators [28–33], silicene [34,35], phosphorene [36–38], layered structures [39–42] and Dirac and Weyl semimetals [43–45]. Among these studies, the RKKY interaction mediated by massless Dirac fermions (MDFs) has attracted a lot of interest, which exhibits many new behaviors and brings about potential

opportunities of nonmagnetic Dirac materials for spin applications. However, previous studies are mainly limited to the Dirac materials with isotropic MDFs, this leaves the influence of novel MDFs on the RKKY interaction unexplored.

The 8-*Pmmn* borophene with the crystal structure of Fig. 1(a) is one kind of two-dimensional Dirac material, in which the novel MDFs are anisotropic and tilted as shown by Fig. 1(b) in contrast to those isotropic ones in the well-known graphene. Recently, since its seminal prediction [46], wide theoretical efforts have been paid to calculate the unprecedented electronic properties [47–50] and to construct the effective low-energy continuum Hamiltonian [48,49] which has been used to study the plasmon dispersion and screening properties [51], the optical conductivity [52], Weiss oscillations [53], and Metal-insulator transition induced by strong electromagnetic radiation [54]. The rapid experimental advances of various borophene monolayers [55–57] further boost wider research interest on 8-*Pmmn* borophene. The anisotropic exchange coupling and the magnetic anisotropy are very crucial to spin applications [1,7,58–60], so our interest is to examine the anisotropic features of RKKY interaction due to the novel MDFs. Here, we study the RKKY interaction mediated by the anisotropic and tilted MDFs by using the effective model of 8-*Pmmn* borophene. In the long range, we analytically derive the Green's function (GF) of anisotropic and tilted MDFs to show the unique real-space propagation properties, and then their mediation to RKKY interaction whose oscillation period and envelop amplitude are both anisotropic and determined by the

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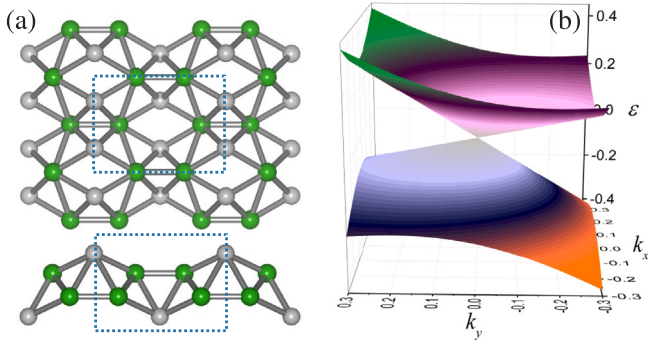


Fig. 1. (a) Crystal structure of 8-Pmmn borophene from top view (upper panel) and side view (bottom panel). The ridge boron atom (green) and the inner boron atom (gray) are nonequivalent. In each unit cell, there are eight atoms delimited by the dashed blue rectangle. (b) Anisotropic and tilted Dirac cone in 8-Pmmn borophene. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

velocities, i.e., velocity-determined RKKY interaction. As a result, our theoretical study show the potential of velocity-determined RKKY interaction in the characterization of characteristic velocities of anisotropic tilted MDFs and the application of 8-Pmmn borophene for spin fields.

This paper is organized as follows. In Section 2, we start from the intrinsic electronic properties of 8-Pmmn borophene, present the general expression of RKKY interaction, and reveal the analytical behaviors of the real-space GF including the symmetry properties, the classical trajectories and the explicit analytical expression. Then in Section 3, we perform exact numerical calculations to show the typical features of velocity-determined RKKY interaction. Most importantly, the analytical expression for RKKY is derived and is used to understand the velocity-determined RKKY interaction. Finally, we summarize this study in Section 4.

2. Theoretical formalism

In 8-Pmmn borophene, the effective Hamiltonian of anisotropic and tilted MDFs near one Dirac cone is [48,53]

$$\hat{H}_0 = (v_x \sigma_x \hat{p}_x + v_y \sigma_y \hat{p}_y + v_t \sigma_0 \hat{p}_y), \quad (1)$$

where $\hat{p}_{x,y}$ are the momentum operators, $\sigma_{x,y}$ are 2×2 Pauli matrices, and σ_0 is the 2×2 identity matrix. The anisotropic velocities are $v_x = 0.86v_F$, $v_y = 0.69v_F$, and $v_t = 0.32v_F$ with $v_F = 10^6$ m/s. In this study, we set $\hbar = v_F \equiv 1$ to favor our dimensionless derivation and calculations since they can define the length unit l_0 and the energy unit ε_0 through $\hbar v_F = l_0 \varepsilon_0$, e.g., $\varepsilon_0 = 0.66$ eV when $l_0 = 1$ nm. To solve the Schrödinger equation $\hat{H}_0 \psi = \varepsilon \psi$, the energy dispersion [see Fig. 1(b)] and the corresponding wave functions are, respectively,

$$\varepsilon_{\lambda, \mathbf{k}} = v_t k_y + \lambda \sqrt{v_x^2 k_x^2 + v_y^2 k_y^2}, \quad (2)$$

and

$$\psi_{\lambda, \mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} |u_{\lambda}(k_x, k_y)\rangle \quad (3)$$

with

$$\left| u_{\lambda} \left(\begin{matrix} k_x \\ k_y \end{matrix} \right) \right\rangle \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \frac{(v_x k_x + i v_y k_y)}{\varepsilon_{\lambda, \mathbf{k}} - v_t k_y} \end{bmatrix}.$$

Here, $\lambda = \pm$ denotes the conduction (valence) band, $\mathbf{k} = (k_x, k_y)$ and $\mathbf{r} = (x, y)$ are, respectively, the momentum and position vectors, and $|u_{\lambda}(k_x, k_y)\rangle$ is the spinor part of the wave function.

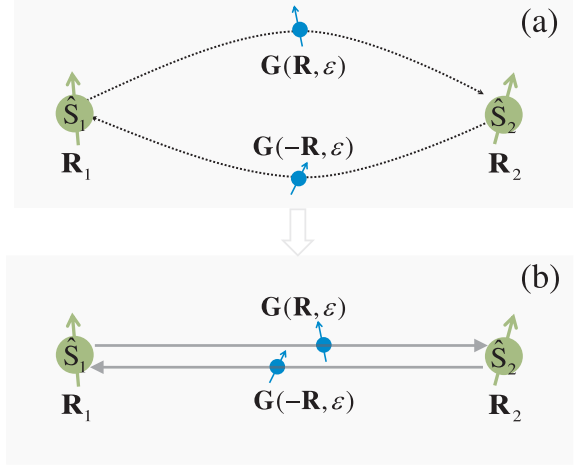


Fig. 2. Schematic diagram of RKKY interaction of two localized spins $\hat{S}_{1,2}$ at $\mathbf{R}_{1,2}$ mediated by the propagation Green's functions $\mathbf{G}(\mathbf{R}, \varepsilon)$ and $\mathbf{G}(-\mathbf{R}, \varepsilon)$ of itinerant carriers between them. Generally, all quantum states below the Fermi level ε_F (see Eq. (4)) contribute to the Green's functions as shown by the curved dotted lines in (a), and then the RKKY interaction. However, at large distances, the Green's functions are dominated by the states with group velocities parallel to $\mathbf{R}$ (i.e., the classical trajectories as shown by the straight solid lines in (b)), and then RKKY interaction is determined by the limited momentum states on the Fermi surface (see Eq. (27)).

2.1. Expression for the RKKY interaction

In the uniform 8-Pmmn borophene, as shown by Fig. 2(a), for two local spins $\hat{S}_{1,2}$ at $\mathbf{R}_{1,2}$ coupled to the carrier spin density $\hat{\mathbf{s}}(\mathbf{x}) = \hat{\mathbf{s}}(\hat{\mathbf{r}} - \mathbf{x})$ via the s-d exchange interaction $-J_0 \hat{S}_1 \cdot \hat{\mathbf{s}}(\mathbf{R}_1) - J_0 \hat{S}_2 \cdot \hat{\mathbf{s}}(\mathbf{R}_2)$, the carrier-mediated RKKY interaction assumes the isotropic Heisenberg form due to the absence of spin-orbit coupling, i.e., $\hat{H}_{\text{RKKY}} = J_{jj'} \hat{S}_1 \cdot \hat{S}_2$, where the range function [20,61,62]

$$J_{jj'}(\varepsilon_F, \mathbf{R}) = -\frac{J_0^2}{2\pi} \text{Im} \int_{-\infty}^{\varepsilon_F} F_{jj'}(\varepsilon, \mathbf{R}) d\varepsilon \quad (4)$$

is determined by the intrinsic real-space GF of carriers, i.e.,

$$F_{jj'}(\varepsilon, \mathbf{R}) = G_{jj'}(\mathbf{R}, \varepsilon) G_{jj'}(-\mathbf{R}, \varepsilon). \quad (5)$$

Due to the integral forms of Eq. (4) over the energy and of Eq. (7) over the momentum (see the subsequent subsection), all quantum states propagating between $\mathbf{R}_1$ and $\mathbf{R}_2$ below the Fermi level ε_F contribute to the RKKY interaction as shown by the curved dotted line in Fig. 2(a). In addition, $j, j' \in \{1, 2\}$ label the orbitals used in the basis for the Hamiltonian of 8-Pmmn borophene. Until now, the respective contribution of different orbitals to form the Dirac states of 8-Pmmn borophene is still in debate [48] and the interaction properties between magnetic impurity and the borons' orbitals call for further density functional calculations, so we focus on the long-range behaviors of RKKY interaction in our model study.

2.2. Real-space GF

The real-space GF is the key to understand the spatial propagation of carries and their mediation to the RKKY interaction, which is defined by

$$\mathbf{G}(\mathbf{R}, \varepsilon) \equiv \langle \mathbf{R}_2 | (\varepsilon + i0^+ - \hat{H}_0)^{-1} | \mathbf{R}_1 \rangle. \quad (6)$$

Here, $\mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1$ accounts for the translational invariance in uniform system and is the connecting vector for two magnetic impurities, and $\mathbf{G}$ is one 2×2 matrix expressed in the orbital basis instead of the spin basis originating from the spin-degenerate Hamiltonian of 8-Pmmn borophene in the orbital basis [48]. The real-space GF can be obtained from the Fourier transformation

$$\mathbf{G}(\mathbf{R}, \varepsilon) = \frac{1}{4\pi^2} \iint d^2\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{R}} \mathbf{G}(\mathbf{k}, \varepsilon), \quad (7)$$

of the momentum-space GF

$$\mathbf{G}(\mathbf{k}, \varepsilon) \equiv [z - H_0(\mathbf{k})]^{-1} = -\frac{2(\varepsilon - \gamma_2 k_y)}{v_x} \frac{|u_\lambda(k_x, k_y)\rangle \langle u_\lambda(k_x, k_y)|}{(k_x - k_{x,+})(k_x - k_{x,-})}. \quad (8)$$

with

$$k_{x,\pm}(k_y) = \pm \sqrt{(\varepsilon - \gamma_2 k_y)^2 - \gamma_1^2 k_y^2}. \quad (9)$$

Here, $\gamma_1 = v_y/v_x$, $\gamma_2 = v_t/v_x$, $\varepsilon = z/v_x$ with $z = \varepsilon + i0^+$, and $\lambda = \text{sgn}(\varepsilon)$ conforms to the energy dispersion. In the definition of momentum-space GF, we have used the form of $\hat{H}_0$ in the momentum space, i.e., $H_0(\mathbf{k}) = \langle \mathbf{k} | \hat{H}_0 | \mathbf{k} \rangle$. To perform the contour integral over k_x straightforwardly:

$$\mathbf{G}(\mathbf{R}, \varepsilon) = \frac{\text{sgn}(x)}{2\pi} \int dk_y e^{i\phi_s} \frac{\varepsilon - \gamma_2 k_y}{iv_x k_{x,s}} \left| u_\lambda(k_x, k_y) \right\rangle \left\langle u_\lambda(k_x, k_y) \right|, \quad (10)$$

where $s = \text{sgn}(x)\text{sgn}(\varepsilon - \gamma_2 k_y)$, and $\phi_s(k_y, \mathbf{R}) = k_{x,s}x + k_y y$ is the propagation phase factor which has an energy dependence but is omitted for conciseness. And noting here, we always adopt $x = 0^+$ to replace $x = 0$ when we consider $\mathbf{R}$ along the y -axis. Later, we firstly discuss the symmetry properties of GF, then derive the dominant contributing states (namely, the classical trajectories) to real-space GF and their features, which help us to derive the analytical expression of real-space GF.

2.2.1. Symmetry properties of GF

From the Eq. (10), the symmetry properties of GF can be derived, which determines the RKKY properties. On one hand, we have $G_{11}(\mathbf{R}, \varepsilon) = G_{22}(\mathbf{R}, \varepsilon)$, this is identical to the case of graphene with isotropic MDFs [20]. However, there is no symmetrical relation between $G_{12}(\mathbf{R}, \varepsilon)$ and $G_{21}(\mathbf{R}, \varepsilon)$ in contrast to $G_{12}(\mathbf{R}, \varepsilon) = G_{21}(\mathbf{R}, \varepsilon)$ in graphene [62]. On the other hand, one can arrive at

$$\mathbf{G}(\mathbf{R}, -\varepsilon) = -(\mathbf{G}^*(\mathbf{R}, \varepsilon))^T. \quad (11)$$

Here, T denotes the transpose operation of a matrix. Eq. (11) is also applicable to isotropic MDFs in graphene as expected from the electron-hole symmetry [62], so its origin can be seen as a generalized electron-hole symmetry for anisotropic and tilted MDFs. The symmetry properties is beneficial to the discussions of the RKKY interaction and reduces the numerical calculations as shown in the next section, e.g., our focus can be mainly on the electron-doped case by using Eq. (11).

2.2.2. Classical trajectory: traveling nature and group velocity

The integral form of Eq. (10) over k_y shows that in general all momentum states should contribute together to the real-space GF. For convenience, we can separate these momentum states into two classes: traveling states and evanescent states. For the conductance (valence) band with $\lambda = +$ ($\lambda = -$), we have traveling states with $\gamma_2 k_y < \varepsilon$ ($\gamma_2 k_y > \varepsilon$) and evanescent states with $\gamma_2 k_y > \varepsilon$ ($\gamma_2 k_y < \varepsilon$). To identify the dominant contributing states to GF, we use the saddle point approximation. According to the saddle point approximation [63–66], the dominant contribution to Eq. (10) is the classical trajectory from $\mathbf{R}_1$ to $\mathbf{R}_2$, which is determined by the first order derivative of propagation phase factor ϕ_s :

$$\frac{\partial \phi_s}{\partial k_y} = 0. \quad (12)$$

Eq. (12) leads to the identity:

$$\frac{\gamma_2(\varepsilon - k_{y,s}^c \gamma_2) + \gamma_1^2 k_{y,s}^c}{k_{x,s}^c} = \tan\theta, \quad (13)$$

with $\tan\theta = y/x$ and θ being the azimuthal angle of $\mathbf{R}$ relative to the x

axis. Eq. (13) can be rewritten as a quadratic equation with one unknown:

$$\left(\gamma_1^2 - \gamma_2^2 \right) (k_{y,s}^c)^2 + 2\varepsilon \gamma_2 k_{y,s}^c + \frac{\varepsilon^2 (\gamma_2^2 - \tan^2 \theta)}{\gamma_1^2 - \gamma_2^2 + \tan^2 \theta} = 0. \quad (14)$$

Once $k_{y,s}^c$ are derived, one can obtain $k_{x,s}^c = k_{x,s}(k_{y,s}^c)$ for the classical trajectory. In other words, the classical trajectory has the momentum $\mathbf{k}_s^c = (k_{x,s}^c, k_{y,s}^c)$, in which the components have explicit analytical expressions:

$$k_{x,s}^c = \frac{s|\varepsilon|\gamma_1}{\sqrt{\gamma_1^2 - \gamma_2^2 + \tan^2 \theta}}, \quad (15a)$$

$$k_{y,s}^c = -\frac{1}{\gamma_1^2 - \gamma_2^2} \left(\varepsilon \gamma_2 - \frac{s|\varepsilon|\gamma_1 \tan\theta}{\sqrt{\gamma_1^2 - \gamma_2^2 + \tan^2 \theta}} \right). \quad (15b)$$

So one can arrive at $\varepsilon - \gamma_2 k_{y,s}^c = \varepsilon f(\gamma_1, \gamma_2, \theta)$ with

$$f(\gamma_1, \gamma_2, \theta) = \frac{\gamma_1^2}{\gamma_1^2 - \gamma_2^2} - \frac{s\lambda\gamma_1\gamma_2}{\gamma_1^2 - \gamma_2^2} \frac{\tan\theta}{\sqrt{\gamma_1^2 - \gamma_2^2 + \tan^2 \theta}}. \quad (16)$$

For the anisotropic and tilted MDFs with $\gamma_1 > \gamma_2$ in 8-*Pmmn* borophene, $f(\gamma_1, \gamma_2, \theta) > \gamma_1/(\gamma_1 + \gamma_2) > 0$ leads to $\text{sgn}(\varepsilon - \gamma_2 k_{y,s}^c) = \lambda$ or $s = \lambda \text{sgn}(x)$ for the classical trajectory. Therefore, the classical trajectory is always of traveling nature.

Turning to the group velocity $\mathbf{v}_\lambda(\varepsilon, \mathbf{k}) = (v_{\lambda,x}, v_{\lambda,y})$ of anisotropic tilted MDFs, which has the components

$$v_{\lambda,x} \equiv \frac{\partial \varepsilon_{\lambda,\mathbf{k}}}{\partial k_x} = \frac{\lambda v_x k_x}{\sqrt{k_x^2 + \gamma_1^2 k_y^2}}, \quad (17a)$$

$$v_{\lambda,y} \equiv \frac{\partial \varepsilon_{\lambda,\mathbf{k}}}{\partial k_y} = v_t + \frac{\lambda v_x \gamma_1^2 k_y}{\sqrt{k_x^2 + \gamma_1^2 k_y^2}}. \quad (17b)$$

Eq. (17) shows that the electron and hole group velocities are related to each other through $\mathbf{v}_\lambda(\varepsilon, \mathbf{k}) = \mathbf{v}_\lambda(-\varepsilon, -\mathbf{k})$. In Fig. 3, we show the texture of electron (red color) and hole (blue color) group velocities on the Fermi surfaces with $\varepsilon_{+,\mathbf{k}} = 0.1$ and $\varepsilon_{-,\mathbf{k}} = -0.1$. Due to the anisotropy and tilt, the Fermi surface is a shifted ellipse with its semimajor (semiminor) axis parallel to $\mathbf{e}_y$ ($\mathbf{e}_x$) of the Cartesian coordinate system $x - y$, and has noncolinear momenta and group velocities [67]. The velocity textures for electrons and holes shown by Fig. 3 have the inversion symmetry in the momentum space consistent with Eq. (17).

On the classical trajectory with the momentum $\mathbf{k}_s^c = (k_{x,s}^c, k_{y,s}^c)$, one can obtain

$$\frac{v_{\lambda,y}^c}{v_{\lambda,x}^c} = \tan\theta. \quad (18)$$

As a result, $\mathbf{v}_\lambda^c(\varepsilon, \mathbf{k}_s^c) \parallel \mathbf{R}$ for the classical trajectory, this implies $\mathbf{G}(\mathbf{R}, \varepsilon)$ are mainly contributed by the states with the group velocities parallel to the connecting vector $\mathbf{R}$. For convenience, we introduce $\mathbf{v}_\lambda^c(\varepsilon, \mathbf{R}) \equiv \mathbf{v}_\lambda^c(\varepsilon, \mathbf{k}_s^c)$. $\mathbf{v}_\lambda^c(\varepsilon, \mathbf{R}) \parallel \mathbf{R}$ for the classical trajectory provides one principle to identify the dominant momentum states contributing to real-space GF $\mathbf{G}(\mathbf{R}, \varepsilon)$, i.e., through comparing the direction of the group velocity of each state on the Fermi surface and that of $\mathbf{R}$. As an application of this skill, we give an example to consider $\mathbf{G}(\mathbf{R}, \varepsilon)$ for electrons without loss of generality. According to the velocity texture shown in Fig. 3, the dominant contributing momentum states on the electron Fermi surface lie on the right (left) vertex of semiminor axis for $\mathbf{G}(\mathbf{R}, \varepsilon)$ along the positive (negative) x -axis which is consistent with Eq. (15) with $\theta = 0$ and π :

$$k_{x,\pm}^c = \pm \frac{\varepsilon \gamma_1}{\sqrt{\gamma_1^2 - \gamma_2^2}}, \quad (19a)$$

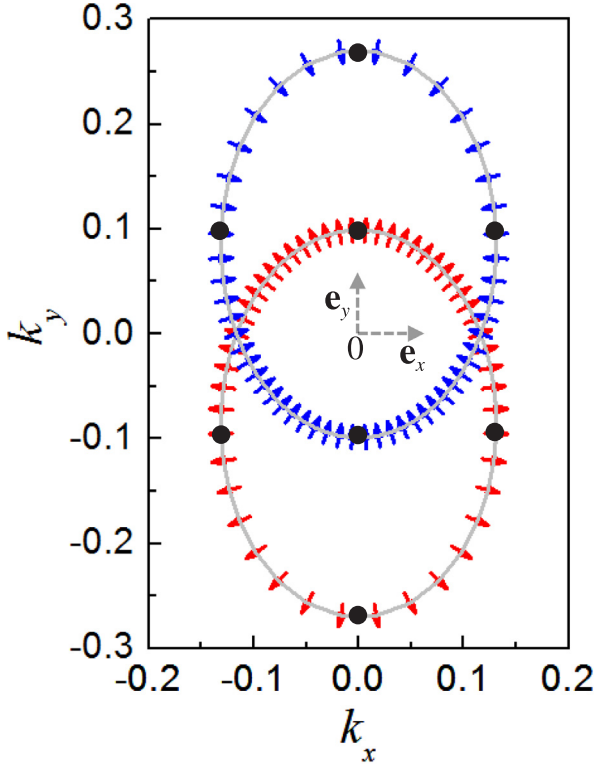


Fig. 3. Texture of electron (red) and hole (blue) group velocities on the Fermi surfaces with $\varepsilon_{+,k} = 0.1$ and $\varepsilon_{-,k} = -0.1$. The Fermi surfaces are shifted ellipses with noncolinear momenta and group velocities, and the group velocities (black dots) on the vertices of semimajor (semiminor) axis are parallel to $\mathbf{e}_y$ ($\mathbf{e}_x$) of the Cartesian coordinate system $x-y$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$$k_{y,\pm}^c = -\frac{\varepsilon \gamma_2}{\gamma_1^2 - \gamma_2^2}. \quad (19b)$$

Noting here $k_{y,\pm}^c$ adopt one value and equal to the shifted momentum of the center of the elliptical Fermi surface away from the coordinate origin [67], which helps to determine the momentum position of semiminor axis in the y direction. Similarly, the dominant contributing momentum states on the electron Fermi surface lie on the upper (bottom) vertex of semimajor axis for $\mathbf{G}(\mathbf{R}, \varepsilon)$ along the positive (negative) y -axis, which is consistent with Eq. (15) with $\theta = \pm\pi/2$:

$$k_{x,\pm}^c = 0, \quad (20a)$$

$$k_{y,\pm}^c = \frac{\varepsilon}{\gamma_2 \pm \gamma_1}. \quad (20b)$$

Therefore, it is an effective principle to identify the dominant contributing momentum states to GF by using the velocity texture on the Fermi surface, and this principle should be very useful for the complex Fermi surfaces without analytical solutions.

2.2.3. Analytical GF

Near the classical trajectory, the Taylor expansion of $\phi_s(k_y)$ is

$$\phi_s(k_y, \mathbf{R}) = \phi_s^c(\mathbf{R}) - \alpha_s(k_y - k_{y,s}^c)^2 + o(k_y), \quad (21)$$

where $\phi_s^c(\mathbf{R}) \equiv \phi_s^c(k_{y,s}^c, \mathbf{R})$ since the $\mathbf{R}$ determines $k_{y,s}^c$ for a fixed Fermi surface, $o(k_y)$ is the high-order small quantity as the function of k_y and

$$\alpha_s = -\frac{1}{2} \frac{\partial^2 \phi_s}{\partial k_y^2} \bigg|_{k_{y,s}^c} = \frac{x \varepsilon^2 \gamma_1^2}{2(k_{x,s}^c)^3}. \quad (22)$$

In light of the stationary phase approximation, the real-space GF at the

large distance is contributed mainly by the electron propagation along the classical trajectory. As a result, the real-space GF can be expressed analytically as:

$$\mathbf{G}(\mathbf{R}, \varepsilon) \approx \frac{\text{sgn}(x) e^{i\phi_s^c} \varepsilon - \gamma_2 k_{y,s}^c}{2\pi i v_x k_{x,s}^c} \sqrt{\frac{\pi}{i\alpha_s}} \left| u_l(k_{x,s}^c, k_{y,s}^c) \right\rangle \left\langle u_l(k_{x,s}^c, k_{y,s}^c) \right|, \quad (23a)$$

$$= \frac{e^{i\phi_s^c - \lambda\pi/4} \varepsilon - \gamma_2 k_{y,s}^c}{2\pi i \lambda v_x |k_{x,s}^c|} \sqrt{\frac{\pi}{|\alpha_s|}} \left| u_l(k_{x,s}^c, k_{y,s}^c) \right\rangle \left\langle u_l(k_{x,s}^c, k_{y,s}^c) \right|, \quad (23b)$$

Here, the Gaussian formula $\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\pi/\alpha}$ has been used. And α is a complex variable with the angle $\arg(\alpha) \in (-\pi, \pi]$, so $\sqrt{\alpha} = \sqrt{|\alpha|} e^{i\arg(\alpha)/2}$. It is worthy to emphasize that Eq. (23) is consistent with Eq. (11) and has a clear symmetry origin, i.e., the inversion symmetry of velocity textures for electrons and holes as shown by Fig. 3.

3. Results and discussions

In order to clearly present the numerical and analytical results for the RKKY interaction in 8-*Pmmn* borophene, we introduce the scaled RKKY range function $\mathcal{J}_{ij} = J_{ij} R^2 / J_0^2$ with $R = |\mathbf{R}|$. Fig. 4(a) and (b) show the RKKY range function $\mathcal{J}_{11}$ for the connection vector $\mathbf{R}$ between two impurities along x -axis and y -axis, in which the red dashed lines are plotted by using the results of exact numerical calculations based on the Eqs. 4 and 10.

3.1. Negligible sublattice and valley effect

In the unit cell of 8-*Pmmn* borophene, there are 8 boron atoms, among which two are nonequivalent and maybe regarded as the sublattice degree of freedom in analogy to graphene [20,68]. Now, the respective contribution of different orbitals of different atoms to form the Dirac states of 8-*Pmmn* borophene is still in debate [48]. The low-energy spectrum of 8-*Pmmn* borophene is expressed in a proper basis, which has no clear connection with the nonequivalent atoms in contrast to the case in graphene. So using the low-energy spectrum of 8-*Pmmn* borophene, we can just discuss the orbital-dependent RKKY interaction as done in three-dimensional Dirac semimetals [45].

The carrier-mediated RKKY interaction is determined by the GF of carriers (cf. Eq. 4). The 8-*Pmmn* borophene has two inequivalent Dirac cones which can be included in the calculation of GF by combing two valley-dependent GFs. The combination should be a sum of valley-dependent GFs weighed by proper phase factors [69,20]. The phase factors can be identified through the low-energy expansion of the lattice model. At present, the lattice model for 8-*Pmmn* borophene is very

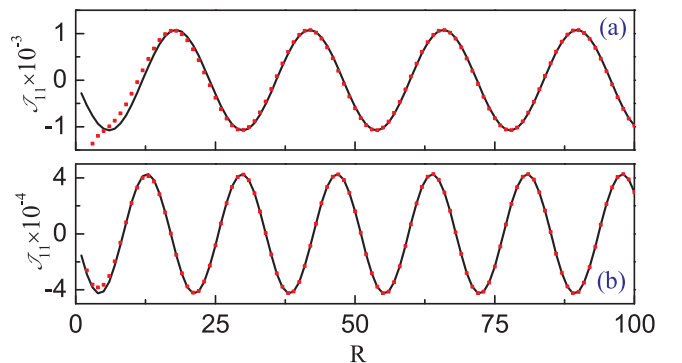


Fig. 4. RKKY range function $\mathcal{J}_{11}$ for the connection vector between two impurities along x -axis (a) and y -axis (b). In the plots, we have used the analytical formula (black solid lines) and numerical calculations (red dotted lines) for the electron doping $\varepsilon_F = 0.1$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

tedious [48], so the phase factors are not known. Even if two valleys can be included properly, their interference only cause the short-range oscillation decorated on the RKKY interaction as a function of impurity distance. Due to the large momentum spacing between two valleys [48], the short-range oscillation is on the atomic scale.

Here, we consider the RKKY interaction in the doped 8-*Pmmn* borophene, and focus its long-range oscillation determined by the Fermi wavelength on the nanometer scale, decay rate determined by the system dimension and the envelop amplitude without dependence on the oscillation detail. Therefore, the sublattice effect and valley effect are negligible in our study.

3.2. Analytical expressions for RKKY interaction

To understand the unique behaviors of RKKY interaction mediated by anisotropic and tilted MDFs in 8-*Pmmn* borophene, we derive the analytical formula for $J_{jj'}$. At large distances, the integrand in Eq. (4) can be rewritten as

$$F_{jj'}(\epsilon, \mathbf{R}) = F_{jj'}^0(\epsilon, \mathbf{R}) e^{i\phi_s(\mathbf{R}) + i\phi_{-s}(-\mathbf{R})} \quad (24)$$

where $F_{jj'}^0(\epsilon, \mathbf{R})$ is a slowly-varying function of the energy. Due to the rapid oscillation of the phase factor $e^{i\phi_s(\mathbf{R}) + i\phi_{-s}(-\mathbf{R})}$, the integral over energy in Eq. 4 is dominated by the contributions near the Fermi energy ϵ_F , so we can perform the expansion as follows:

$$\phi_s(\mathbf{R}) + \phi_{-s}(-\mathbf{R}) \approx \phi_s^c(\mathbf{R}) + \phi_{-s}^c(-\mathbf{R}) + \frac{R}{v_\lambda^c(\epsilon_F)} (\epsilon - \epsilon_F), \quad (25)$$

with

$$\frac{1}{v_\lambda^c(\epsilon_F)} = \frac{1}{v_\lambda^c(\epsilon_F, \mathbf{R})} + \frac{1}{v_\lambda^c(\epsilon_F, -\mathbf{R})}. \quad (26)$$

Here, we have used $v_\lambda^c(\epsilon_F, \pm\mathbf{R}) \parallel (\pm\mathbf{R})$ on the classical trajectories (cf. classical trajectories in Section 2.2). We further make the approximation $F_{jj'}^0(\epsilon, \mathbf{R}) = F_{jj'}^0(\epsilon_F, \mathbf{R})$ for the slowly-varying function, then the RKKY range function becomes

$$J_{jj'}(\epsilon_F, \mathbf{R}) \approx \frac{J_0^2 v_\lambda^c(\epsilon_F)}{2\pi R} \text{Re} \left[F_{jj'}^0(\epsilon_F, \mathbf{R}) e^{i\phi_s^c(\mathbf{R}) + i\phi_{-s}^c(-\mathbf{R})} \right]. \quad (27)$$

The analytical formula Eq. (27) implies that the RKKY interaction is determined by the momentum states with group velocities parallel to the connection vector $\mathbf{R}$ between two magnetic impurities and with the energies equal to Fermi level ϵ_F as shown by the straight solid lines in Fig. 2(b). In contrast, Eq. (4) has an explicit integral over energy and an implicit integral over momentum for GF, so the contributions of all momentum states below ϵ_F to the RKKY interaction should be considered. Therefore, Eq. (27) provides a simplified version and a physically transparent expression of Eq. (4). Eq. (27) has an immediate application, which leads to

$$\mathbf{J}(\epsilon_F, \mathbf{R}) = (\mathbf{J}(-\epsilon_F, \mathbf{R}))^T. \quad (28)$$

with the range function matrix

$$\mathbf{J} = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} \quad (29)$$

by recalling Eq. (11) (cf. symmetry discussions in Section 2.2). This range function relation originates from the inversion symmetry of velocity textures for electrons and holes as shown by Fig. 3, which favors our discussions limited to electron doping case in our study. Eq. (27) is also used to plot the black solid lines in Fig. 4. At large distances, the results of analytical formula and numerical calculations agree very well with each other, so Eq. (27) can capture the main features of long-range RKKY interaction.

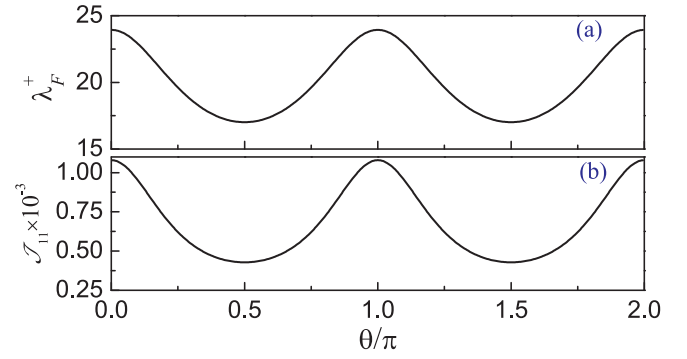


Fig. 5. The oscillation period λ_F^+ (a) and the envelop amplitude (b) of RKKY range function. Here, $\epsilon_F = 0.1$.

3.3. Velocity-determined RKKY interaction and its implications

Firstly, the decay rate of RKKY interaction is $J_{jj'}(\epsilon_F, \mathbf{R}) \propto 1/R^2$ since $F_{jj'}(\epsilon_F, \mathbf{R}) \propto 1/R$ by referring to Eqs. (5) and (23), this dimension-determined decay behavior is as that in conventional two-dimensional electron gases [70,71] and in other doped Dirac materials with two-dimensional isotropic MDFs [17–21,28–30].

Secondly, the oscillation period of $J_{jj'}(\epsilon_F, \mathbf{R})$ is determined by the phase factor $\phi_s^c(\mathbf{R}) + \phi_{-s}^c(-\mathbf{R})$, which is given by

$$\lambda_F^s = \frac{2\pi R}{|\phi_s^c(\mathbf{R}) + \phi_{-s}^c(-\mathbf{R})|} \quad (30)$$

for the fixing Fermi level ϵ_F . To consider $\epsilon_F = 0.1$, we use Eq. (30) to plot the oscillation period in Fig. 5(a) as the function azimuthal θ of the connection vector $\mathbf{R}$. Fig. 5(a) has the mirror symmetry about y-axis originating from the symmetry of Hamiltonian [51], and shows two peaks (valleys) along $\pm x$ -axis ($\pm y$ -axis). We defines the peak-valley ratio as the anisotropy degree of the oscillation period. Referring to Eq. (15), for $\epsilon_F > 0$, one can obtain $\lambda_F^+(\theta = 0) = \pi(\gamma_1^2 - \gamma_2^2)^{1/2}/(\epsilon_F \gamma_1)$ and $\lambda_F^+(\theta = \pi/2) = \pi(\gamma_1^2 - \gamma_2^2)/(\epsilon_F \gamma_1)$, which both show the inverse linear energy dependence of the oscillation period identical to the case for the isotropic MDFs [20,29]. In particular, in Fig. 5(a), $\lambda_F^+(\theta = 0) = 24$ and $\lambda_F^+(\theta = \pi/2) = 17$ when $\epsilon_F = 0.1$ for the RKKY range function along x-axis and y-axis, respectively. As a result, the anisotropy degree of the oscillation period is a constant $v_x/(v_y^2 - v_t^2)^{1/2} \approx 1.4$ independent of the Fermi energy ϵ_F .

Thirdly, the envelope amplitude of the oscillating RKKY interaction is another important feature beyond the decay rate and oscillation period. The envelope amplitude depends linearly on Fermi level ϵ_F by combing Eqs. (23) and (27) and by using $\alpha_s \propto \epsilon^2$ in Eq. (22). In Fig. 5(b), Eqs. (23) and (27) are used to plot the envelope amplitude of RKKY interaction J_{11} as the function azimuthal θ of $\mathbf{R}$. In analogy to the oscillation period, we also define peak-valley ratio as the anisotropy degree for the envelope amplitude, which can be extracted analytically from Eqs. (23) and (27) and is a constant $v_x^2 v_y^2 / (v_y^2 - v_t^2)^2 \approx 2.5$ independent of the Fermi energy ϵ_F .

As a result, the RKKY mediated by the anisotropic and tilted MDFs has anisotropic features in its oscillation period and envelop amplitude but does not change its decay rate. The spatial anisotropy is an usual feature of RKKY interaction, at least on the atomic scale considering the discrete lattice nature of host materials, and the spatially anisotropic RKKY interaction has been reported in experiment [72,73]. Theoretically, there are quite a few studies on the close relation between anisotropic RKKY interaction in long range (on the scale of Fermi wavelength) and band features of various materials, e.g., III-V diluted magnetic semiconductors [74], semiconductor quantum wires [75], surface states on Pt(111) [76], the surface of the topological insulator Bi₂Se₃ [77], spin-polarized graphene [78], three-dimensional Dirac semimetals [45], three-dimensional electron gases with linear spin-orbit coupling [79], and phosphorene with [36] and without

mechanical strain [80], and so on. However, comparing to the other materials, the anisotropic RKKY interaction in 8-*Pmmn* borophene is independent of the Fermi energy ε_F but is velocity-determined, which has two significant implications. On one hand, the velocity-determined RKKY interaction fully determines the band dispersion described by three velocities $v_{x,y,t}$ (cf. band dispersion of Eq. (2)), this provides an alternative way to characterize the band dispersion. And the RKKY interaction has also proposed to probe the topological phase transition in silicene nanoribbon [34] and quasiflat edge modes in phosphorene nanoribbon [37,38]. On the other hand, the anisotropy of RKKY interaction is expected to be tunable by choosing other Dirac materials with different $v_{x,y,t}$ (e.g., quinoid-type graphene and α -(BEDT-TTF)₂I₃[81]) and even by tuning $v_{x,y,t}$ in the same Dirac material (e.g., graphene under strain [82]). In Dirac materials, the RKKY interaction leads to the ordering of magnetic impurities as discussed theoretically [28,83–85] and demonstrated experimentally [86–88]. Based on the velocity-determined RKKY interaction mediated by anisotropic tilted MDFs, new anisotropy-induced magnetic properties are expected and has high tunability. Therefore, we hope this study is helpful to the physical understanding of 8-*Pmmn* borophene and its possible applications in spin fields.

4. Conclusions

In this study, we investigate the RKKY interaction mediated by the anisotropic and tilted MDFs in 8-*Pmmn* borophene. In the long range, the RKKY interaction is mainly contributed by the limited momentum states with group velocities parallel to the connection vector $\mathbf{R}$ between two magnetic impurities and with the energies equal to Fermi level ε_F . As a result, we analytically demonstrate that the RKKY interaction in 8-*Pmmn* borophene has the usual decay rate as in the other two-dimensional materials, but is anisotropic in its oscillation period and envelop amplitude with the explicit velocity dependence $v_x/(v_y^2 - v_t^2)^{1/2}$ and $v_x^2 v_y^2 / (v_y^2 - v_t^2)^2$. The velocity-determined RKKY interaction implies its usefulness to fully characterize the band dispersion of 8-*Pmmn* borophene and other similar Dirac materials, and its tunability by engineering the anisotropic tilted MDFs. In addition, the velocity-determined RKKY interaction should be observable in present experiment since the evidence of RKKY interaction mediated by anisotropic MDFs on surface Mn-doped Bi₂Te₃ has been reported through focusing interference patterns observed by scanning tunneling microscopy [73]. This study is relevant to spatial propagation properties of novel anisotropic tilted MDFs, and shows the potential spin application of 8-*Pmmn* borophene.

Note added. Recently, we became aware of a related preprint [89], which studies the RKKY interaction in 8-*Pmmn* borophene along two specific directions.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at <https://doi.org/10.1016/j.jmmm.2019.165631>.

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