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Phys. Rev. B **101**, 155421 — Published 21 April 2020

DOI: [10.1103/PhysRevB.101.155421](https://doi.org/10.1103/PhysRevB.101.155421)

Long range and tunable RKKY interaction in topological channel of gated bilayer graphene

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Abstract

Two separate gate electrodes with opposite gate voltages can drive an AB-stacked bilayer graphene(BLG) under them into different quantum valley Hall states. And between the two topological domains there appears a one-dimensional(1D) boundary, dubbed as the topological channel(TC). By means of the Lanczos method, we theoretically study the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between two magnetic impurities in such a TC of BLG. We find that the RKKY interaction is long-range with R^{-1} decay rate as the distance R between two magnetic impurities increases, whereas the slowest decay rate in any graphene structure is R^{-2} according to previous literature. Moreover, we also find that the strength and sign of the RKKY interaction in the TC can be readily controlled by altering gate voltage or carrier doping. Such a tunable and R^{-1} decaying RKKY interaction implies the possibility to establish and control a long-range magnetic ordering state in a dilute magnetic impurity-doped BLG.

I. INTRODUCTION

Since the successful fabrication of first experimental sample of graphene, such a two dimensional(2D) carbon material has long been the hot research topic in condensed matter physics and relevant fields in nearly the past two decades¹⁻¹⁰. In contrast to conventional quasi-2D materials, due to that the low-lying conduction electron behaves like the massless Dirac Fermion, graphene exhibits many peculiar electronic properties such as the RKKY interaction. The so-called RKKY interaction is an indirect exchange interaction between two magnetic impurities mediated by the conduction electrons of the host material such as graphene¹¹⁻¹³. In charge-neutral graphene, the RKKY interaction obeys the so-called Saremi's rule. Namely, it is ferromagnetic(anti-ferromagnetic) if the two magnetic impurities are located on the same(opposite) sublattice of graphene¹⁴⁻¹⁶. Such a characteristic is due to the electron-hole symmetry which graphene possesses. Furthermore, with the increase of the distance R between two magnetic impurities, the RKKY interaction in graphene decays as R^{-3} , rather than the R^{-2} decay rate expected for conventional 2D materials¹⁶⁻¹⁹. This result arises from the linear dispersion of 2D massless Dirac Fermion obeyed by the low-lying electronic states around the Fermi level in graphene.

Recently, the investigation on the RKKY interaction in graphene is extended to graphene bilayer, multilayers and other graphene derivatives. In contrast to exchange or super-exchange interactions, the RKKY interaction has relatively long range. And its sign can be inverted by changing the distance R or other factors such as Fermi level²⁰. Thus, when the RKKY interaction predominates, the result is long-range magnetic ordering, as found in many heavy-Fermion materials. Analogously, in dilute magnetic impurity-doped graphene systems, the long-range RKKY interaction is of key importance for establishing a new regime of magnetic ordering phase. And it is desirable for the purposes of manipulating the spin to realize some device functions in graphene. However, according to previous theoretical studies, the slowest spatial decay of RKKY interaction in graphene systems is R^{-2} , occurring in BLG or multilayers²¹. This is attributed to the nonlinear dispersion of conduction electrons near Fermi level in these graphene structures. Furthermore, unlike the monolayer graphene, there are more degrees of freedom to manipulate the electronic states in BLG or multilayers. For example, a vertical electric field exerted to an AB-stacked BLG can yield a topological nontrivial band gap²²⁻²⁵. Consequently, the BLG becomes a quantum valley

Hall insulator²⁵. And the valley Chern number C_v can be readily changed by inverting the direction of the vertical electric field²⁵.

In this work, we propose a theoretical model to realize a long-range RKKY interaction in BLG which decays as R^{-1} . In so doing, we apply to the BLG two separate gate electrodes with opposite gate voltages which yield a kink potential for the carbon atoms in the top and bottom layers of graphene^{26,27}. As a result, a 1D infinite topological domain wall appears between two gates under which the BLG is in distinct topological states of opposite valley Chern number. The 1D domain wall is also called the TC since it hosts 1D gapless topological boundary states^{26–29}. We find that such topological boundary states can mediate the R^{-1} decaying RKKY interaction. Moreover, our theoretical result indicates that the strength and sign of such a RKKY interaction can be readily controlled by altering the gate voltage or carrier doping.

The rest of the present work is organized as follows. In section II, our model and the corresponding tight-binding Hamiltonian are introduced, and the Lanczos method we use to obtain the retarded Green's function, further to calculate the RKKY interaction, is presented. This is the critical theoretical trick to study the RKKY interaction in aperiodic systems developed in our previous work. In section III, the numerical results about the RKKY interaction in the TC of a bipartite gated BLG are shown and discussed. Finally, in section IV the main results are summarized briefly.

II. MODEL AND METHODS

We consider a 2D infinite sheet of AB-stacked BLG where the conduction electron is subject to an antisymmetric gate potential. As shown in Fig.1(a) and (b), such an antisymmetric gate potential can be introduced by applying two semi-infinite plate capacitors in opposite charging states^{26,27}. Between the two plate capacitors there is a narrow channel(infinite along y direction). We are concerned with the RKKY interaction between two magnetic impurities absorbed on two carbon atoms in this channel. To begin with, we employ a tight-binding Hamiltonian to describe the electronic states in the BLG in the presence of the antisymmetric gate potential, which is formally written as

$$\hat{H} = \hat{H}_t + \hat{H}_b + \hat{H}_i, \quad (1)$$

where $\hat{H}_t$ and $\hat{H}_b$ denote the interaction between the atomic orbitals in the top and bottom layers respectively, and $\hat{H}_i$ for the inter-layer interaction. They are given by

$$\hat{H}_t = \sum_{\mathbf{r}} U(x) (c_{A1, \mathbf{r}+\boldsymbol{\tau}_1}^\dagger c_{A1, \mathbf{r}+\boldsymbol{\tau}_1} + c_{B1, \mathbf{r}}^\dagger c_{B1, \mathbf{r}}) + t \sum_{\mathbf{r}, \boldsymbol{\tau}_j} (c_{B1, \mathbf{r}}^\dagger c_{A1, \mathbf{r}+\boldsymbol{\tau}_j} + h.c.), \quad (2)$$

$$\hat{H}_b = - \sum_{\mathbf{r}} U(x) (c_{A2, \mathbf{r}}^\dagger c_{A2, \mathbf{r}} + c_{B2, \mathbf{r}-\boldsymbol{\tau}_1}^\dagger c_{B2, \mathbf{r}-\boldsymbol{\tau}_1}) + t \sum_{\mathbf{r}, \boldsymbol{\tau}_j} (c_{A2, \mathbf{r}}^\dagger c_{B2, \mathbf{r}-\boldsymbol{\tau}_j} + h.c.), \quad (3)$$

$$\hat{H}_i = t_1 \sum_{\mathbf{r}} c_{A2, \mathbf{r}}^\dagger c_{B1, \mathbf{r}} + t_2 \sum_{\mathbf{r}, \boldsymbol{\tau}_j} c_{A1, \mathbf{r}+\boldsymbol{\tau}_1}^\dagger c_{B2, \mathbf{r}+\boldsymbol{\tau}_1+\boldsymbol{\tau}_j} + h.c., \quad (4)$$

where $A1, B1, A2$ and $B2$ stand for the A/B sublattices of top or bottom layer of BLG, respectively, as labeled in Fig.1(c). The lattice vector $\mathbf{r}$ specifies a unit cell of BLG. And the three vectors, $\boldsymbol{\tau}_j$ with $j = 1, 2, 3$, define intra-layer C-C bonds, as explained in Fig.1(d). Thus, each creation or annihilation operator in the Hamiltonian above, written generally as $c_{\alpha, \mathbf{R}}^\dagger$ or $c_{\alpha, \mathbf{R}}$ with $\alpha = A1, B1, A2$ and $B2$, corresponds to an atomic orbital localized at the position $(\alpha, \mathbf{R})$. The intra- and inter-layer hopping parameters are marked in Fig.1(c), and they take values as $t = -2.7eV$, $t_1 = -0.4eV$ and $t_2 = -0.3eV$ respectively^{30,31}. The antisymmetric gating yields an atomic coordinate- x dependent on-site energy of electron in the TB Hamiltonian, denoted as $\pm U(x)$ for the atomic orbitals in top/bottom layer. Without loss of generality, we adopt a function

$$U(x) = V \left[\frac{2}{\exp(\beta x) + 1} - 1 \right] \quad (5)$$

to describe the antisymmetric gate potential appropriately. As illustrated in Fig.1(b), the top and bottom antisymmetric potentials form a kink potential around $x = 0$. The parameter V defines the strength of the potential and β^{-1} is viewed as the nominal width of the TC between two capacitors shown in Fig.1(a).

Following the original RKKY theory, two magnetic impurities of spin $\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$, settled upon the lattice points $(\alpha, \mathbf{R})$ and $(\alpha', \mathbf{R}')$ respectively, can establish an indirect exchange interaction mediated by the conduction electrons of the BLG subject to the kink potential. It reads

$$\hat{H}_{RKKY} = J_{\alpha-\alpha'}(\mathbf{R}, \mathbf{R}') \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2. \quad (6)$$

And the strength of RKKY interaction is given by^{16,21}

$$J_{\alpha-\alpha'}(\mathbf{R}, \mathbf{R}') = -\frac{\hbar^2 J^2}{2\pi} \int_{-\infty}^{E_F} d\varepsilon \text{Im}[G_{\alpha\mathbf{R}, \alpha'\mathbf{R}'}^r(\varepsilon) G_{\alpha'\mathbf{R}', \alpha\mathbf{R}}^r(\varepsilon)], \quad (7)$$

where J denotes the exchange energy between a magnetic impurity and the carbon atom it sits right on, E_F is the Fermi energy of the system. In the above equation, $G_{\alpha\mathbf{R},\alpha'\mathbf{R}'}^r(\varepsilon)$ is the retarded lattice Green's function. We must point out that the RKKY interaction defined herein is only a single-particle approximation of a many-body problem concerning the interaction between the local magnetic moment and conduction electrons. It is only valid for the case of weak coupling between the local magnetic moment and the spin of the conduction electron. In terms of the eigen-expansion of the Green's function and by a straightforward derivation we can obtain an alternative expression of the RKKY interaction which is helpful for us to understand the numerical result of the RKKY interaction shown below. It is given by

$$J_{\alpha-\alpha'}(\mathbf{R}, \mathbf{R}') = \hbar^2 J^2 \sum_{m,n} \text{Re} [\langle \alpha\mathbf{R} | \psi_m \rangle \langle \psi_m | \alpha'\mathbf{R}' \rangle \langle \alpha'\mathbf{R}' | \psi_n \rangle \langle \psi_n | \alpha\mathbf{R} \rangle] \times \frac{\theta(E_F - E_n)\theta(E_m - E_F)}{E_n - E_m}, \quad (8)$$

where $\theta(x)$ is the conventional step function; and $|\psi_i\rangle$ and E_i represent, respectively, the eigenstate and the corresponding eigen-energy of BLG subject to the kink potential as shown in Fig.1(b). Although it is rather difficult to get the complete set of the eigen solution, the above expression tells us that the RKKY interaction is mainly determined by the occupied and unoccupied states near Fermi level.

As seen from Eq.(7) the retarded Green's function between the two lattice points where the magnetic impurities are positioned is the critical quantity for us to work out the RKKY interaction. In this work we employ the Lanczos method in real space to numerically obtain Green's functions $G_{\alpha\mathbf{R},\alpha'\mathbf{R}'}^r(\varepsilon)$ and $G_{\alpha'\mathbf{R}',\alpha\mathbf{R}}^r(\varepsilon)$ occurring in Eq.(7). More details about the Lanczos procedure are presented in the Appendix. In addition, with the obtained retarded lattice Green's function, we can readily get the local density of states(LDOS) at an arbitrary lattice point, which is given by

$$\rho_{\alpha\mathbf{R}}(\varepsilon) = -\frac{1}{\pi} \text{Im} G_{\alpha\mathbf{R},\alpha\mathbf{R}}^r(\varepsilon). \quad (9)$$

We also define the so-called local spectral function from which we can extract the information

about the band structure together with the projections onto a given lattice point:

$$\begin{aligned}
A(R_x, k_y, \varepsilon) &= -\frac{1}{\pi} \sum_{\alpha} \text{Im} \langle \alpha, R_x, k_y | (\varepsilon - \hat{H} + i\eta)^{-1} | \alpha, R_x, k_y \rangle \\
&= -\frac{1}{\pi} \sum_{\alpha, \mathbf{R}, \mathbf{R}'} \text{Im} [\langle \alpha, R_x, k_y | \alpha, \mathbf{R} \rangle G_{\alpha \mathbf{R}, \alpha \mathbf{R}'}^r(\varepsilon) \langle \alpha, \mathbf{R}' | \alpha, R_x, k_y \rangle] \\
&= -\frac{1}{\pi} \text{Im} \sum_{\alpha} \sum_{n=0, \pm 1 \dots} G_{\alpha(R_x, n\sqrt{3}a), \alpha(R_x, 0)}^r e^{in\sqrt{3}ak_y}.
\end{aligned} \tag{10}$$

In the above expression, η is a positive infinitesimal and k_y is the Bloch wavevector along y direction which is a good quantum number due to the remaining translational symmetry in y direction of the system. The state vector $|\alpha, R_x, k_y\rangle$ is extended in y direction characterized by k_y and localized in x direction centred at R_x . The inner product between it and an atomic orbital is $\langle \alpha, \mathbf{R} | \alpha, R_x, k_y \rangle = e^{ik_y R_y} / \sqrt{N_y}$ with N_y being the number of unit cell in y direction. If we write the eigen wavefunction and energy formally as Ψ_{λ, k_y} and E_{λ, k_y} with λ as the band index, then the local spectral function can be expanded as

$$A(R_x, k_y, \varepsilon) = -\frac{1}{\pi} \sum_{\alpha, \lambda} |\langle \alpha, R_x, k_y | \Psi_{\lambda, k_y} \rangle|^2 \delta(\varepsilon - E_{\lambda, k_y}) \tag{11}$$

From such an expression we can readily infer that the band structure of the system can be visualized by a 2D plot of $A(R_x, k_y, \varepsilon)$ versus (ε, k_y) weighted by the projection of each band to the atomic orbitals at R_x . In particular, if R_x is fixed in the TC, we can readily identify the 1D boundary states from the 2D bulk states by the projection strength.

III. NUMERICAL RESULTS

When a uniform vertical electric field exerted to the AB-stacked BLG, a nonzero potential gradient V appears between layers, though the gate potential in each layer is a constant. As a result, a band gap in the magnitude of V is induced between the conduction and valence bands of the BLG, which was experimentally demonstrated in previous work^{32,33}. In Fig.1(e) and (f), we have reproduced the band profiles of the AB-stacked BLG in the presence of such a uniform gate voltage V , which is calculated by the tight-binding Hamiltonian given above except that the on-site energies of the top and bottom layers are set as $\pm V$ respectively, instead of the kink potential. One can see that a band gap appears indeed. And it increases with the gate voltage V . More importantly, such a gated BLG is a quantum valley Hall

insulator, characterized by a nonzero valley Chern number which is defined as the difference between the Chern numbers of the valence band electron at two Dirac valleys²²⁻²⁵. Following such a physical picture, the kink potential as shown in Fig.1(b) establishes different valley topological phases in both sides of the channel. In other words, the narrow channel is just the topological domain wall. Accordingly, a gapless topological boundary occurs inevitably in such a TC²⁶⁻²⁹. To expose the detail of the topological boundary state, we calculate the local spectral function as defined by Eq.(10). The numerical results of $A(R_x, k_y, \varepsilon)$ versus (ε, k_y) with given R_x are shown in Fig.2 for various cases. At first, let us look at the case of $R_x = 0$ and the kink potential strength takes a relatively large value, say $V = 0.5eV$, which, according to the aforementioned argument, can open a sizable band gap. As shown in Fig.2(a) and (b), around $\varepsilon = 0$, i.e. the Fermi level of charge-neutral system, there appears midgap states which form two linear crossings at $\varepsilon = 0$. We can see from Fig.2(a) that in contrast to bulk bands outside of the bandgap, these midgap states have much larger projections at $R_x = 0$, in particular, in the vicinity of $\varepsilon = 0$. When R_x takes a value far away from the TC, e.g. $R_x = 50a$, as shown in Fig.2(c) these midgap states disappear. This indicates the 1D characteristic of these midgap states. Namely, these midgap states are localized around the TC. Moreover, when we change the potential strength and the width of TC(the parameter β^{-1}), the bands formed by the midgap states remain gapless, see the results in Fig.2(d) and (e). All these features demonstrate unambiguously that the midgap state is just the topological boundary state around the TC. The linear crossing of topological boundary state at $\varepsilon = 0$ can be viewed as the 1D Dirac point. As seen from Fig.2(d) and (e), the interval between the two 1D Dirac points increases with the parameter V and β . It will be seen below that the topological boundary state plays a dominative role for the RKKY interaction between two magnetic impurities in the TC, which is obviously different from that in pristine BLG.

We now start to investigate the RKKY interaction in the 1D TC of BLG produced by the kink potential. For such a purpose, we put the two magnetic impurities on the central line of the TC, i.e. at $x = 0$. But they are allowed to separate from each other along the channel, i.e. y -direction. In view of the spatial inversion symmetry, we only need to consider the case of the two magnetic impurities on the top layer of the BLG. In addition, owing to the translational symmetry in y direction, we can fix one magnetic impurity, say the one labeled as α , at origin. Thus, the RKKY interaction $J_{\alpha-\alpha'}(\mathbf{R}, \mathbf{R}')$ can be written

compactly as $J_{\alpha-\alpha'}(R)$ with R being the distance between the two magnetic impurities put along y -direction. Unless claimed otherwise, we consider the charge neutral case, i.e. the Fermi level is aligned with the Dirac point of graphene.

As previously reported in relevant literature, the RKKY interaction in pristine BLG follows R^{-2} , R^{-4} and R^{-6} decay rates, respectively, for $\alpha-\alpha' = A1-A1$, $A1-B1$ and $B1-B1$ couplings²¹. Moreover, unique to graphene, the RKKY interaction obeys the so-called Saremi's rule. Namely, the RKKY interaction is ferromagnetic(anti-ferromagnetic) if the carbon atoms under two magnetic impurities belong to the same(opposite) sublattice¹⁴⁻¹⁶. It is necessary to check whether these features of the RKKY interaction remain in the kink potential induced TC of BLG. The numerical results of $J_{\alpha-\alpha'}(R)$ in the TC are shown in Fig.3. These results indicate that even in the TC, Saremi's rule still holds true, but all the aforementioned decay rates found in pristine BLG break down. Instead of that, the RKKY interaction in the TC decays as R^{-1} , regardless of the sublattice attribution of α and α' atoms. Such a feature can be unambiguously seen from the results in the insets of Fig.3(a)-(c). The R^{-1} decay indicates that the magnetic impurities can establish a long-range RKKY interaction in the TC of BLG, which is lacking in monolayer, bilayer and even multilayer graphene. Furthermore, we find that such a long-range RKKY interaction exhibits spatial oscillations with sizable period. The long-range and oscillating RKKY interaction is attributed to the presence of 1D topological boundary states in the TC. As seen from Eq.(8), the occupied and unoccupied states in the vicinity of Fermi level play the dominant role to mediate RKKY interaction. From the spectral functions shown in Fig.2 one can readily find that the 1D topological boundary states are gapless around the Fermi level(Dirac point). In contrast, the bulk states are gapped away from the Dirac point by the gate potential. Therefore, we can readily draw a conclusion that the 1D topological boundary states, dominating over the bulk states, control the behaviour of the RKKY interaction in the TC. In fact, following the theoretical treatment given in Ref.[16], we can give a more convincing explanation on the R^{-1} decay rate and spatial oscillation of RKKY interaction in the TC of BLG. We sketch our argument as follows. Firstly, according to the numerical results of local spectral function shown in Fig.2, we can assume that the topological boundary states around the 1D Dirac point have linear dispersion. According to Eq.(8), these topological boundary states act as the occupied and unoccupied states which are relevant to the RKKY interaction. Therefore, for the eigen-energies in Eq.(8) we have $E_n \sim k$ and

$E_m \sim k'$ with k and k' being the wave vectors measured from either of the two 1D Dirac points denoted as $\pm\tilde{K}$ respectively. Secondly, it is reasonable for us to presume that the electronic probability amplitude $\langle\alpha'R|\psi_l\rangle$ with $l = n, m$ differ from $\langle\alpha'0|\psi_l\rangle$ only by a phase factor $\exp[i(k \pm \tilde{K})R]$ for all the low-lying topological boundary states around the two 1D Dirac points. Putting all these approximations into Eq.(8) and then altering the summation over n and m into integrals with respect to k and k' , after a straightforward derivation, we obtain $J_{\alpha-\alpha'}(R) \sim [1 + \cos(2\tilde{K}R)]/R$ which demonstrates the R^{-1} decay with an oscillating period of $(2\tilde{K})^{-1}$. Such an analytical result agrees well with the numerical results shown in Fig.3. As shown in Fig.2, the interval between the two 1D Dirac points, i.e. $2\tilde{K}$, increases with the gate voltage V . Accordingly, the oscillation period of the RKKY interaction versus R shown in Fig.3 decreases with the increase of V .

Besides the decay rate and the spatial oscillation as discussed above, the variation of RKKY interaction in the TC with the kink potential strength can also be observed from Fig.3. As shown in Fig.3(a), we find that the variation of V has not nontrivial effect on J_{A1-A1} . In contrast, as shown in Fig.3(b) and (c), J_{B1-B1} and J_{A1-B1} increase appreciably with V . Considering that the RKKY interaction is mainly determined by the occupied and unoccupied states near the Fermi level, we should calculate and analyze the sublattice-resolved LDOS spectrum around Fermi level which is defined by Eq.(9). It can help us to understand the different dependence of RKKY interactions on V for various $\alpha-\alpha'$ couplings. The numerical results of LDOS of sublattice $A1$ and sublattice $B1$ on the central line of the TC are shown in Fig.4. As shown in Fig.4(a) and (b), the occupation of the low-lying state around the Dirac point on the sublattice $A1$ is almost unaffected by V . However, it is not such a case of the LDOS of the sublattice $B1$, which increases with V remarkably. These features of sublattice-resolved LDOS can well account for the aforementioned dependence of $J_{\alpha-\alpha'}$ on V as shown in Fig.3.

In Fig.5 the RKKY interaction as a function of R for the cases of different values of β are compared. As mentioned above, β^{-1} can be understood as the nominal width of the TC. Numerical results of $J_{A1-A1}(R)$, $J_{B1-B1}(R)$ and $J_{A1-B1}(R)$ corresponding to three typical values of β are shown in Fig.5(a), (b) and (c) respectively. The common feature of these results is that $J_{\alpha-\alpha'}$ as a function of R oscillates faster as β increases. This is because the interval between the two 1D Dirac points increases with β , which can be clearly seen in Fig.2(b) and (e). Besides, J_{A1-A1} decreases with β , although it is not obvious in Fig.5(a).

Such a result can be found by comparing the enveloping curves connecting the periodic peaks among the cases of different β values. In contrast, it is easy to find in Fig.5(b) that J_{B1-B1} increases with β . These results can also be explained by the distinct response to the variation of β of sublattice occupations of the topological boundary state in the vicinity of the Fermi level. As seen from the LDOS shown in Fig.4(c) and (d), the occupation of the sublattice $A1$ decreases with β , whereas the occupation of the sublattice $B1$ increases with β . These results are consistent with the RKKY interaction as shown in Fig.5 for different values of β . Moreover, as β increases, the enhancement of $B1$ -sublattice occupation and the suppression of $A1$ -sublattice occupation almost cancel each other out. Therefore, as shown in Fig.5(c), J_{A1-B1} hardly changes with β .

As discussed above, two separate plate capacitors in opposite charging states as sketched in Fig.1 produce kink potential, hence giving rise to long-range RKKY interaction in BLG. But we would like to point out that the gate voltages produced by two plate capacitors can be adjusted independently, which provides us with additional degree of freedom to manipulate the RKKY interaction in the TC. Before ending this work, it is significant to explore the tunability of the RKKY interaction in the TC by altering the gate voltage or carrier doping. For such a purpose, we let the on-site energy in the TB Hamiltonian of top(bottom) layer still be described by the potential function as given by Eq.(5). But in the region of $x > 0$, the potential strength is fixed, say $V = V_r$. And in the region of $x < 0$, the potential strength denoted as $V = V_l$, is allowed to be adjustable. Then we calculate $J_{\alpha-\alpha'}(R)$ as a function of V_l for the cases of two magnetic impurities fixed at some specific positions in TC. The numerical results are shown in Fig.6(a), from which we can see that with the increase of V_l , both $J_{A1-A1}(R)$ and $J_{B1-B1}(R)$ change from a weak anti-ferromagnetic to a strong ferromagnetic coupling. In contrast, $J_{A1-B1}(R)$ shows a transition from ferromagnetic to anti-ferromagnetic coupling as V_l increases.

What we can see further from Fig.6(a) is the breakdown of the Saremi's rule when $V_l \leq 0$. This is due to that in the case of $V_l \leq 0$ the on-site energy in the TB Hamiltonian of top(bottom) layer of BLG is always negative(positive). Consequently, the left and right regions of BLG are in the same topological state. Hence the topological boundary states disappear. Such a situation is verified by the numerical result shown in Fig.2(f). According to the result in previous work²⁰, in BLG under such an ordinary inter-layer bias, the RKKY interaction no longer follows Saremi's rule. In contrast, when $V_l > 0$, namely, the left and

right regions of BLG are in distinct topological states. Then, the 1D midgap state appears which retrieves the Saremi's rule. The above results and discussions are restricted within the case of charge-neutrality. If we shift the Fermi level slightly from the Dirac point, which implies carrier doping, as shown by the numerical results in Fig.6(b), the sign of the RKKY interaction can also be altered. In summary, these results shown in Fig.6 indicate that both the strength and the sign of the RKKY interaction in the 1D TC can be readily tuned by altering the gate voltage or carrier doping.

IV. CONCLUSIONS

By means of the Lanczos method to solve the retarded Green's functions, a numerical approach suitable especially for systems without translational symmetry, we study the RKKY interaction in 1D TC of BLG formed by a kink potential. We suggest such a kink potential can be actually produced by imposing two separate gate electrodes with opposite gate voltage on the BLG. We find that when two magnetic impurities are put in the TC of BLG, the RKKY interaction between them is long-range with R^{-1} decay rate, which is distinctly different from the cases in pristine graphene or BLG where RKKY interaction decays much more rapidly. Such a long-range RKKY interaction implies distinct magnetic ordering or magnetic phase transition when the BLG is doped by magnetic impurities, in contrast to conventional dilute magnetic semiconductors. Moreover, our theoretical result indicates that the strength and magnetic ordering of RKKY interaction in the TC of BLG can be readily controlled by altering gate voltage or introducing carrier doping.

ACKNOWLEDGMENTS

This work was financially supported by the National Natural Science Foundation of China (Grant No. 11774123 and 11474122) and the National Science Foundation for Young Scientists of China (Grant No. 11404132, No. 11504125 and No. 11504319). We thank the High Performance Computing Center of Jilin University for their calculation resource.

Appendix: Lanczos method

In this work we employ the Lanczos method in real space by which we can obtain numerically the lattice Green's function³⁴. The key procedure of the Lanczos method is to find out a basis set in which the tight-binding Hamiltonian of the system becomes a tridiagonal matrix. In so doing, we firstly choose a normalized seed state $|f_0\rangle$, then construct a new state orthogonal with $|f_0\rangle$ using the following formulas:

$$|F_1\rangle = \hat{H}|f_0\rangle - |f_0\rangle\langle f_0|\hat{H}|f_0\rangle = \hat{H}|f_0\rangle - a_0|f_0\rangle, \quad (\text{A.1})$$

$$|f_1\rangle = \frac{1}{b_1}|F_1\rangle, \quad (\text{A.2})$$

where $a_0 = \langle f_0|\hat{H}|f_0\rangle$, and $b_1 = \langle f_0|\hat{H}|f_1\rangle$ is the normalization coefficient of the state $|f_1\rangle$. Apparently, $|f_1\rangle$ is orthogonal to $|f_0\rangle$. It is easy to get the recursive relation when $n \geq 2$

$$|F_n\rangle = \hat{H}|f_{n-1}\rangle - a_{n-1}|f_{n-1}\rangle - b_{n-1}|f_{n-2}\rangle, \quad (\text{A.3})$$

$$|f_n\rangle = \frac{1}{b_n}|F_n\rangle, \quad (\text{A.4})$$

with the recursive coefficients:

$$a_n = \langle f_n|\hat{H}|f_n\rangle \quad (\text{A.5})$$

$$b_n = \langle f_{n-1}|\hat{H}|f_n\rangle. \quad (\text{A.6})$$

We can prove that every new state obtained by Eqs. (A.3) and (A.4) is normalized and orthogonal to the preceding ones.

On the basis of $\{|f_0\rangle, |f_1\rangle, |f_2\rangle, \dots\}$ the tight-binding Hamiltonian of the system becomes a tridiagonal matrix which takes a form as

$$H = \begin{bmatrix} a_0 & b_1 & 0 & \cdots \\ b_1 & a_1 & b_2 & \cdots \\ 0 & b_2 & a_2 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{bmatrix}. \quad (\text{A.7})$$

The retarded Green's function matrix is then defined as $G^r(\varepsilon) = (\varepsilon - H + i\eta)^{-1}$. In the numerical calculations we set the infinitesimal $\eta = 0.001|t|$ which is small enough to guarantee the convergence of the calculated Green's functions. The first diagonal element of such a Green's function can be written as

$$G_{00}^r(\varepsilon) = \langle f_0|\hat{G}^r(\varepsilon)|f_0\rangle = \frac{D_1}{D}, \quad (\text{A.8})$$

where D is the determinant of the matrix $[\varepsilon - H + i\eta]$. And D_i for $i \geq 1$ is the determinant of the matrix by taking out both the first i rows and first i columns of $[\varepsilon - H + i\eta]$. We can expand D by using Laplace theorem, i.e.

$$D = (\varepsilon + i\eta - a_0)D_1 - b_1^2 D_2. \quad (\text{A.9})$$

So we can express $G_{00}^r(\varepsilon)$ as

$$G_{00}^r(\varepsilon) = \frac{1}{\varepsilon + i\eta - a_0 - b_1^2 \frac{D_2}{D_1}}. \quad (\text{A.10})$$

Analogously, D_i can be expanded in terms of D_{i+1} and D_{i+2} as

$$D_i = (\varepsilon + i\eta - a_i)D_{i+1} - b_{i+1}^2 D_{i+2}. \quad (\text{A.11})$$

Then we can get $G_{00}^r(\varepsilon)$ by using the continued fraction expansion method. In actual calculations, we have to take a cutoff of the tridiagonal Hamiltonian matrix as long as the retarded Green's function is converged. Namely, a_∞ and b_∞ are terminated at a_N and b_N respectively, with a sufficiently large N . Then we have

$$G_{00}^r(\varepsilon) = \frac{1}{\varepsilon + i\eta - a_0 - \frac{b_1^2}{\varepsilon + i\eta - a_1 - \frac{b_2^2}{\varepsilon + i\eta - a_2 - \dots - b_{N-1}^2 \Sigma(\varepsilon)}}}, \quad (\text{A.12})$$

where

$$\Sigma(\varepsilon) = \frac{\varepsilon - i\sqrt{4b_N^2 - (\eta - a_N)^2} - a_N}{2b_N^2}. \quad (\text{A.13})$$

If we construct the seed state in the manner $|f_0\rangle = c_1|\alpha\mathbf{R}\rangle + c_2|\alpha'\mathbf{R}'\rangle$ with c_1 and c_2 being the arbitrary normalized coefficients, the obtained Green's function $G_{00}^r(\varepsilon)$ is associated with the ones used in Eq.(7), i.e.

$$G_{00}^r(\varepsilon) = |c_1|^2 G_{\alpha\mathbf{R},\alpha\mathbf{R}}^r(\varepsilon) + |c_2|^2 G_{\alpha'\mathbf{R}',\alpha'\mathbf{R}'}^r(\varepsilon) + c_1^* c_2 G_{\alpha\mathbf{R},\alpha'\mathbf{R}'}^r(\varepsilon) + c_1 c_2^* G_{\alpha'\mathbf{R}',\alpha\mathbf{R}}^r(\varepsilon), \quad (\text{A.14})$$

Then, by altering the normalized coefficients and repeating the above Lanczos procedure, we can finally obtain the Green's functions $G_{\alpha\mathbf{R},\alpha'\mathbf{R}'}^r(\varepsilon)$ and $G_{\alpha'\mathbf{R}',\alpha\mathbf{R}}^r(\varepsilon)$.

Finally, it is necessary to check the convergence of the numerical results of RKKY interaction with respect to N , the recursion cutoff in Lanczos method. If the numerical results always depend on N sensitively, it means that a result with any given N still suffer from the finite cluster effect. Hence the Lanczos method fails to study numerically the RKKY interaction of the system under our consideration. We have already checked the convergence.

Fortunately, we find that in any case the cutoff $N = 3000$ is large enough to result in a convergent result of RKKY interaction which is almost independent of the further increase of N . Such a convergence is exemplified by the numerical results in Fig.A1 where the dependence of the calculated RKKY interaction on N is shown for two typical cases of different parameter values.

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- ¹ Wallace P. R., The Band Theory of Graphite, Phys. Rev. **71**, 622 (1947).
- ² J. C. Slonczewski and P. R. Weiss, Band Structure of Graphite, Phys. Rev. **109**, 272 (1958).
- ³ Yisong Zheng and Tsuneya Ando, Hall conductivity of a two-dimensional graphite system, Phys. Rev. B **65**, 245420 (2002).
- ⁴ K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, Electric Field Effect in Atomically Thin Carbon Films, Science **306**, 666 (2004).
- ⁵ K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos and A. A. Firsov, Two-dimensional gas of massless Dirac fermions in graphene, Nature **438**, 197 (2005).
- ⁶ Dmitry A. Abanin, Patrick A. Lee and Leonid S. Levitov, Spin-Filtered Edge States and Quantum Hall Effect in Graphene, Phys. Rev. Lett. **96**, 176803 (2006).
- ⁷ M. I. Katsnelson, K. S. Novoselov and A. K. Geim, Chiral tunnelling and the Klein paradox in graphene, Nature Physics **2**, 620 (2006).
- ⁸ K. S. Novoselov, Z. Jiang, Y. Zhang, S. V. Morozov, H. L. Stormer, U. Zeitler, J. C. Maan, G. S. Boebinger, P. Kim and A. K. Geim, Room-Temperature Quantum Hall Effect in Graphene, Science **315**, 1379 (2007).
- ⁹ A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, The electronic properties of graphene, Rev. Mod. Phys **81**, 109 (2009).
- ¹⁰ S. Das Sarma, Shaffique Adam, E. H. Hwang, and E. Rossi, Electronic transport in two-dimensional graphene, Rev. Mod. Phys **83**, 407 (2011).
- ¹¹ Ruderman M A and Kittel C, Indirect Exchange Coupling of Nuclear Magnetic Moments by Conduction Electrons, Phys. Rev. **96**, 99 (1954).

- ¹² Kasuya T, A Theory of Metallic Ferro- and Antiferromagnetism on Zener's Model, *Prog. Theor. Phys.* **16**, 45 (1956).
- ¹³ Yosida K, Magnetic Properties of Cu-Mn Alloys, *Phys. Rev.* **106**, 893 (1957).
- ¹⁴ V. K. Dugaev, V. I. Litvinov and J. Barnas, Exchange interaction of magnetic impurities in graphene, *Phys. Rev. B* **74**, 224438 (2006).
- ¹⁵ Saremi S, RKKY in half-filled bipartite lattices: Graphene as an example, *Phys. Rev. B* **76**, 184430 (2007).
- ¹⁶ E. Kogan, RKKY interaction in graphene, *Phys. Rev. B* **84**, 115119 (2011).
- ¹⁷ Sherafati M and Satpathy S, RKKY interaction in graphene from the lattice Greens function, *Phys. Rev. B* **83**, 165425 (2011).
- ¹⁸ Black-Schaffer, A. M., RKKY coupling in graphene, *Phys. Rev. B* **81**, 205416 (2010).
- ¹⁹ Stephen R. Power and Mauro S. Ferreira, Indirect Exchange and Ruderman-Kittel-Kasuya-Yosida (RKKY) Interactions in Magnetically-Doped Graphene, *CRYSTALS* **3**, 49 (2013).
- ²⁰ F. Parhizgar, M. Sherafati, R. Asgari, and S. Satpathy, Ruderman-Kittel-Kasuya-Yosida interaction in biased bilayer graphene, *Phys. Rev. B* **87**, 165429 (2013).
- ²¹ Liwei Jiang, Xiaoling Lv, Wenzhu Gao, Guodong Yu, Zhe Liu and Yisong Zheng, RKKY interaction in AB-stacked multilayer graphene, *J. Phys.: Condens. Matter* **24**, 206003 (2012).
- ²² Wang Yao, Shengyuan A. Yang, and Qian Niu, Edge States in Graphene: From Gapped Flat-Band to Gapless Chiral Modes, *Phys. Rev. Lett.* **102**, 096801 (2009).
- ²³ Fan Zhang, Jeil Jung, Gregory A. Fiete, Qian Niu, and Allan H. MacDonald, Spontaneous Quantum Hall States in Chirally Stacked Few-Layer Graphene Systems, *Phys. Rev. Lett.* **106**, 156801 (2011).
- ²⁴ Wang-Kong Tse, Zhenhua Qiao, Yugui Yao, A. H. MacDonald and Qian Niu, Quantum anomalous Hall effect in single-layer and bilayer graphene, *Phys. Rev. B* **83**, 155447 (2011).
- ²⁵ Zhenhua Qiao, Wang-Kong Tse, Hua Jiang, Yugui Yao and Qian Niu, Two-Dimensional Topological Insulator State and Topological Phase Transition in Bilayer Graphene, *Phys. Rev. Lett.* **107**, 256801 (2011).
- ²⁶ Ivar Martin, Ya.M. Blanter and A. F. Morpurgo, Topological Confinement in Bilayer Graphene, *Phys. Rev. Lett.* **100**, 036804 (2008).
- ²⁷ M. Zarenia, J. M. Pereira Jr., G. A. Farias and F. M. Peeters, Chiral states in bilayer graphene: Magnetic field dependence and gap opening, *Phys. Rev. B* **84**, 125451 (2011).

- ²⁸ Hui Pan, Xin Li, Fan Zhang, and Shengyuan A. Yang, Perfect valley filter in a topological domain wall, *Phys. Rev. B* **92**, 041404(R) (2015).
- ²⁹ Yafei Ren, Zhenhua Qiao and Qian Niu, Topological phases in two-dimensional materials: a review, *Rep. Prog. Phys.* **79** 066501 (2016).
- ³⁰ Brandt N B *et al*, Modern Problems in Condensed Matter Sciences vol 20.1, ed V M Agranovich and A A Maradudin (Amsterdam: North-Holland) (1988).
- ³¹ Dresselhaus M S and Dresselhaus G, Intercalation compounds of graphite, *Adv. Phys.* **51**, 1 (2002).
- ³² Edward McCann, Asymmetry gap in the electronic band structure of bilayer graphene, *Phys. Rev. B* **74**, 161403(R) (2006).
- ³³ Castro, Eduardo V. and Novoselov, K. S. and Morozov, S. V. and Peres, N. M. R. and dos Santos, J. M. B. Lopes and Nilsson, Johan and Guinea, F. and Geim, A. K. and Neto, A. H. Castro, Biased Bilayer Graphene: Semiconductor with a Gap Tunable by the Electric Field Effect, *Phys. Rev. Lett.* **99**, 216802 (2007).
- ³⁴ E. Dagotto, Correlated electrons in high-temperature superconductors, *Rev. Mod. Phys.* **66**, 763 (1994).

FIG. 1. (Color online) (a) Schematic illustration of an AB-stacked BLG sheet subject to two separate gate electrodes with opposite gate voltages which yield a kink potential on the carbon atoms in the top and bottom layers. (b) The profile of the kink potential plotted in terms of Eq.(5). The solid and dashed lines stand for the potentials upon the top and bottom layers of BLG. (c) Side-view and (d) top-view of the lattice structure of BLG. τ_1 , τ_2 and τ_3 are three vectors labeling the intra-layer $C-C$ bonds. Band structure of BLG with a band gap induced by a uniform gate voltage V for the cases of (e) $V = 0.25\text{eV}$ and (f) $V = 0.5\text{eV}$.

FIG. 2. (Color online) The local spectral function $A(R_x, k_y, \varepsilon)$ of BLG subject to a kink potential for various cases. (a) $V = 0.5\text{eV}, \beta = 0.1a^{-1}, R_x = 0$; (b) $V = 0.5\text{eV}, \beta = 0.1a^{-1}, R_x = 0$; (c) $V = 0.5\text{eV}, \beta = 0.1a^{-1}, R_x = 50a$; (d) $V = 0.25\text{eV}, \beta = 0.1a^{-1}, R_x = 0$; (e) $V = 0.5\text{eV}, \beta = a^{-1}, R_x = 0$; (f) $V_r = 0.5\text{eV}, V_l = -0.5\text{eV}, \beta = 0.1a^{-1}, R_x = 0$.

FIG. 3. (Color online) The RKKY interactions in the TC of BLG as a function of R for different couplings. (a) $J_{A1-A1}(R)$, (b) $J_{B1-B1}(R)$ and (c) $J_{A1-B1}(R)$. The corresponding result of pristine BLG is also plotted for comparison. The insets are the result in main panel for $V = 0.5\text{eV}$ which is replotted together with the R^{-1} fitting curve in order to show clearly the R^{-1} decay rate in the large- R limit. The corresponding results of graphene monolayer are also plotted in the insets for comparison which follows the R^{-3} decay rate.

FIG. 4. (Color online) The sublattice-resolved LDOS spectrum on the central line of the TC. (a) and (c) are the results of sublattice $A1$; (b) and (d) are the results of sublattice $B1$. In (a) and (b), $\beta = 0.1a^{-1}$ is fixed, the results of $V = 0.1, 0.25$ and 0.5eV are compared. In (c) and (d), $V = 0.5\text{eV}$ is fixed, the results of $\beta = 1.0, 0.2$ and $0.1a^{-1}$ are compared.

FIG. 5. (Color online) The RKKY interactions in the TC of BLG as a function of R . (a) $J_{A1-A1}(R)$, (b) $J_{B1-B1}(R)$ and (c) $J_{A1-B1}(R)$ for different values of the parameter β with the potential strength fixed at $V = 0.5eV$.

FIG. 6. (Color online) The RKKY interactions in the TC of BLG as a function of (a) V_l and (b) E_F . For all results the distance between the magnetic impurities is specified at some appropriate values, in order to show clearly the adjustability of the sign and strength of RKKY interaction by kink potential strength or carrier doping.

FIG. A1. (Color online) Illustration of the convergence of the calculated RKKY interaction in the TC of BLG with respect to the recursion cutoff N . (a) $J_{A1-A1}(R)$ with the relevant parameters fixed at $V = 0.1eV$, $\beta = 0.1a^{-1}$, $R = 173.2a$ and (b) $J_{B1-B1}(R)$ with $V = 0.5eV$, $\beta = a^{-1}$ and $R = 1.732a$. In both cases convergence is well achieved at $N = 3000$.