Theory of Vacancy-Induced Intrinsic Magnetic Impurity with Quasi-Localized Spin Moment in Graphene

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In this paper, by considering the Hubbard model on a honeycomb lattice, we developed a theory for the intrinsic magnetic impurities (MIs) with the quasi-localized spin moments induced by the vacancies in graphene. Because the intrinsic MIs are characterized by the zero modes that are orthogonal to the itinerant electrons, their properties are much different from those of Anderson MIs with the well-localized spin moments.

Graphene consists of carbon atoms organized into honeycomb lattice, coupling with each other through sp² orbitals. Since it was isolated in 2004 by A. Geim and K. Novoselov, it had been intensively studied in the last several years. The fast uptake of interest in graphene is due primarily to its exceptional properties. The magnetic impurities in the graphene becomes an interesting issue due to the possible application to the spintronics. In particular, people found that the missing atom (single vacancy) in graphene may induce a quasi-localized state (the so-called zero mode) distributed around the impurity. The induced spin moment by the lattice-defects was also observed in experiments. Based on the Anderson model or the Kondo model, the Kondo effect and the RKKY interaction between magnetic impurities have studied by variety of groups. People found that due to the linear dispersion in graphene, some features of the magnetic impurities are changed. For example, at half filling, the RKKY coupling is strictly ferromagnetic (FM) for spin moments on the same sublattice and antiferromagnetic (AFM) for spin moments on different sublattices, in both cases falling off as 1/R³. The 1/R³ decay rate differs from the usual 1/R² decay rate for the magnetic impurities in two dimensional Fermi liquid.

In this paper we study the properties of the vacancy-induced magnetic impurities of the graphene by considering the Hubbard model on a honeycomb lattice. Here, the magnetic impurities are induced by removing an atom rather than doping an extra magnetic impurity. The wave function of zero modes around the magnetic impurities is known to be eigenstates of the system and orthogonal to the itinerant electronic states. Thus, the Anderson model or its deduced Kondo model is not applicable. On the other hand, the particle density of the zero modes falls off as 1/R². The absence of a localized length indicates a quasi-localized spin moment (QLSM) rather than a well-localized spin moment (WLSM). And the QLSM will never be screened by the itinerant electrons. As a result, this type of magnetic impurities is much difference from the traditional Anderson impurities, which the itinerant electrons always try to screen. To emphasize the differences, we call it "intrinsic magnetic impurity" to distinguish the traditional Anderson impurity which can be classified to "extrinsic magnetic impurity". So one can imagine that the system turns to repel the extrinsic magnetic impurities (MIs) by screening them, while accepting the intrinsic MIs. In this paper, our task is to systematically recognize the properties of the intrinsic MIs on graphene.

Our starting point is the Hubbard model on a honeycomb lattice, of which the Hamiltonian is

\[ H = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i \sigma}^\dagger \hat{c}_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow} - \mu \sum_i \hat{c}_{i \uparrow}^\dagger \hat{c}_{i \uparrow} \] (1)

where \( t \) is the nearest neighbor hopping, \( \mu \) is the chemical potential and \( U \) is the strength of the repulsive interaction, respectively. For graphene, \( t \) is about 2.8eV, \( U \) is about 1.5t \( \approx 4.2eV \). In this paper we ignore the next nearest neighbor hopping.

Since the honeycomb lattice is a bipartite lattice, we have two sublattices, A sublattice and B sublattice. In momentum space, for free electrons, \( H \) is reduced into

\[ H_{\text{free}} = \sum_{\mathbf{k}, \sigma} (\epsilon(\mathbf{k}) \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \epsilon^*(\mathbf{k}) \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma}) \]

where \( \epsilon(\mathbf{k}) = \sum_{\delta, \mathbf{q}} |\mathbf{q} + \mathbf{K}_1| \) in momentum reduced Brillouin Zone (BZ), \( \delta \) are nearest neighbor links. After diagonalization of the Hamiltonian, the spectra become \( E_{\pm}(\mathbf{k}) = \pm |\epsilon(\mathbf{k})| \). Near the nodal points \( \mathbf{K}_1 = (0, \frac{\pi}{3\sqrt{3}}) \), \( \mathbf{K}_2 = (\frac{\pi}{3}, \frac{\pi}{3\sqrt{3}}) \), the dispersion becomes a linear one as \( E_{\pm}(\mathbf{k}) \approx v_F |\mathbf{k}| \) where \( v_F \) is the Fermi velocity of the electrons. The lattice constant is set to be unit in the following calculations.

Firstly, we study the graphene with a lattice defect on A sublattice in the presence of an on-site potential at site \( \mathbf{R} \), \( H \rightarrow H(U = 0) + V_{\mathbf{R}} \hat{c}_{\mathbf{R}}^\dagger \hat{c}_{\mathbf{R}} \). In the unitary limit, the lattice defect becomes a vacancy, of which we have an infinite on-site potential, i.e., \( V_{\mathbf{R}} \rightarrow \infty \). Two localized states that are orthogonal to the itinerant electronic states appear, one for the electrons with up spin, and the other for the electrons with down spin. Due to the particle-hole symmetry, the localized state around the vacancies have exactly zero energy, and its wave-function distributes only on B sublattice.

In the continuum limit, the wave function of the zero mode introduced by

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one vacancy has the form of $\psi_0(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{2\pi}\sigma_3(\mathbf{r})$, where $\mathbf{r} = (x, y)$. Far from the vacancy, the decay rate of the particle density is $|\psi_0(\mathbf{r})|^2 \to 1/|\mathbf{r}|^2$. So we call it quasi-localized state.

When we consider the on-site interaction, there exists effective repulsive interaction between the electrons trapped on the zero mode as $U_{\text{eff}}(\mathbf{n}_R \mathbf{n}_R)$ where $U_{\text{eff}} = U \sum_i |\psi_0(i)|^2$. $\mathbf{n}_R$ is the number operator of quasi-localized state. After considering the chemical potential term, we get the effective Hamiltonian of the electrons on the zero mode around a single vacancy $H_L = U_{\text{eff}}(\mathbf{n}_R \mathbf{n}_R) - \mu_{\text{eff}}(\mathbf{n}_R + \mathbf{n}_R)$ where $\mu_{\text{eff}} = \mu$. For the case of $U_{\text{eff}} < \mu_{\text{eff}}$, the zero mode is double occupied; For the case of $\mu_{\text{eff}} < 0$, the zero mode is empty. So the spin moment of the quasi-localized state (we call it quasi-localized spin moment) exists when a finite chemical potential is smaller than $U_{\text{eff}}$ as $U_{\text{eff}} > \mu_{\text{eff}} > 0$.

Because the wave-functions of the quasi-local states (we borrow the name ”$d$-orbitals” to label them) $|d\rangle$ and those of the itinerant electrons (we borrow the name ”$s$-orbitals” to label them) $|s, k\rangle$ are always orthogonal each other, $\langle s, k | d \rangle = 0$, there is no ”$s$-$d$ hybridization” between the zero modes and those of the itinerant electrons. Instead, when we consider the on-site particle interaction, there exists effective ”$s$-$d$ coupling” between the QLSM induced by the vacancy and the spin moments of the itinerant electrons. Such $s$-$d$ coupling between the QLSM and the itinerant electrons can be regarded as the Hund rule’s coupling for two orthogonal orbitals - an orbital of zero mode and an orbital with finite wave-vectors. As a result, the $s$-$d$ coupling is always ferromagnetic and momentum-dependence. All these features are universal for a vacancy-induced MI in graphene, a remarkable example of the intrinsic MIs.

We assume there exists QLSM on the vacancy (or $U_{\text{eff}} > \mu_{\text{eff}} > 0$). The $s$-$d$ coupling which describes the process that the itinerant electrons are scattered by the quasi-localized state from $\mathbf{k}$ to $\mathbf{k}'$ is given by the following non-local FM Kondo-like Hamiltonian

$$H_{s-d} = - \sum_{\mathbf{k}, \mathbf{k}'} J_A (\mathbf{k}' - \mathbf{k}) \hat{s}_{\mathbf{R}} \cdot \hat{s}_{A, \mathbf{k}k'} - \sum_{\mathbf{k}, \mathbf{k}'} J_B (\mathbf{k}' - \mathbf{k}) \hat{s}_{\mathbf{R}} \cdot \hat{s}_{B, \mathbf{k}k'}$$

(2)

where $\hat{s}_{\mathbf{R}}$ is the spin operator of the QLSM induced by the vacancy at site $\mathbf{R}$ and $\hat{s}_{A/B, \mathbf{k}k'}$ is the spin operator of the itinerant electrons on $A/B$ sublattice $\hat{s}_{A/B, \mathbf{k}k'} = c_{A/B, \mathbf{k}k'}^\dagger c_{A/B, \mathbf{k}k'}$. $J_A (\mathbf{k}' - \mathbf{k})$ ($J_B (\mathbf{k}' - \mathbf{k})$) is the strength of the $s$-$d$ coupling on sublattice $A$ ($B$), respectively as

$$J_{A/B} (\mathbf{k}' - \mathbf{k}) = \int \int \psi_{\mathbf{k}' A/B}^* (\mathbf{r}_1) \psi_{\mathbf{k} B} (\mathbf{r}_2 - \mathbf{R}) U (\mathbf{r}_1 - \mathbf{r}_2) \psi_{\mathbf{k}' A/B} (\mathbf{r}_2) \psi_{\mathbf{k} B} (\mathbf{r}_1 - \mathbf{R}) d\mathbf{r}_1 d\mathbf{r}_2$$

$$= \frac{U}{N} \sum_{j \in A/B} |\psi_{\mathbf{k} j}|^2 e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_j}$$

(3)

where the interaction $U (\mathbf{r}_1 - \mathbf{r}_2) = U \delta (\mathbf{r}_1 - \mathbf{r}_2)$. $\psi_{\mathbf{k} A} (\mathbf{r}_1)$ is the field of itinerant electrons with wave vector $\mathbf{k}$. We see that the $s$-$d$ coupling is induced by the on-site interaction $U$, and it is non-local. So, we call it ”nonlocal $s$-$d$ coupling” of QLSM.

Because the quasi-localized state around the vacancy at $A$ sublattice distributes only on $B$ sublattice, we have $J_A (\mathbf{k}' - \mathbf{k}) = 0$, $J_B (\mathbf{k}' - \mathbf{k}) \neq 0$. In Fig.(1) we show the non-local s-d coupling in the momentum space. Form Fig.(1), one can see that the non-local s-d coupling has a maximum value at $\mathbf{q} = \mathbf{k}' - \mathbf{k} \to 0$, $|J_B (\mathbf{q} = 0)| = U$ and then falls off as $|J_B (\mathbf{q})| \to 1/|\mathbf{q}|$. The situation of QLSM is much different from the WLSM of Anderson magnetic impurity due to the $s$-$d$ hybridization, of which the local AFM s-d coupling (the Kondo coupling) is constant in momentum space and can be written into a formulation into real space, $H_{s-d} = JS \cdot \hat{s}_i$.

Now we have a nonlocal FM Kondo model that describes coupling between the QLSM to the itinerant electrons due to the Hund rules’ coupling $H_{s-d}$. The Hamiltonian becomes

$$H_{\text{Kondo}} = H_{\text{Free}} - \mu \sum_k \hat{c}_k^\dagger \hat{c}_k + H_{s-d}.$$ 

(4)

We have used a mean-field approach to study the possible Kondo effect. From the mean-field theory, we don’t find the bound state between the QLSM and the itinerant electrons. Thus we guess that the quasi-local state has 1/2 spin moment and always decouple from the itinerant electrons.

In the following parts, we consider the case of two vacancies. Due to quasi-localization, the wave functions of the zero modes around two vacancies could overlap even when they are not close to each other. The overlap of the wave functions leads to the direct Heisenberg exchange coupling and the superexchange coupling between
the QLSMs. When the distance is too far to overlap, the coupling between QLSMs mainly comes from the RKKY interaction which is mediated by the itinerant electron.

At first step, we study the RKKY coupling between two QLSMs around the vacancies on R and R’ which is described by the following Hamiltonian

\[ J_R(R, R') \hat{S}_R \cdot \hat{S}_{R'} \]

where the RKKY interaction strength \( J_R(R, R') \) is

\[
J_R(R, R') = -\sum_q J_{A,R}(q) J_{A,R'}(-q) \chi_{AA}(q) \\
- \sum_q J_{A,R}(q) J_{B,R'}(-q) \chi_{AB}(q) \\
- \sum_q J_{B,R}(q) J_{A,R'}(-q) \chi_{BA}(q) \\
- \sum_q J_{B,R}(q) J_{B,R'}(-q) \chi_{BB}(q).
\]

\( \chi = \begin{pmatrix} \chi_{AA} & \chi_{AB} \\ \chi_{BA} & \chi_{BB} \end{pmatrix} \)

is renormalized spin susceptibility from random phase approximation (RPA) calculation. \( \chi_0(q) \) is defined by \( \chi_0(q) = \frac{1}{N} \sum_k G_\sigma(k) G_{-\sigma}(k-q) \).

In the continuum limit \( (q \to 0) \) and weak interaction case \( (U/t < 1) \), the spin susceptibility in terms of microscopical variables is \( \chi_0 \sim \frac{1}{q} \). So we can easily derive that \( J_R \sim \int \frac{1}{q^2} e^{i(q \cdot R)} d^2q \sim \frac{1}{q^2} \). The decay rate of the RKKY coupling between the intrinsic MIs is much different with \( \frac{1}{q^2} \) decay rate of the RKKY coupling for two extrinsic (Anderson) MIs.

FIG. 2: (Color online) The RKKY coupling between two QLSMs. For (a) and (c), the interaction strength is \( U/t = t \). In (b) and (d), \( J_R \) diverges at \( U_c = 2.23t \). (a) and (b) are the results for armchair direction. (c) and (d) are the results for zigzag direction. The fitted line is \( 1/R \).

FIG. 3: (Color online) The DHE coupling between two QLSMs on the same sublattice along armchair direction for the case of \( U = 1.5t \).

and armchair direction. The RKKY coupling is FM for two vacancies on the same sublattice (we denote the case by AA/BB) as \( J_R(R \in A/B, R' \in A/B) < 0 \) and AFM for two vacancies on the different sublattices (we denote the case by AB/BA) as \( J_R(R \in A/B, R' \in B/A) > 0 \) that has been predicted before [11].

For the weak interacting case, the RKKY interaction is proportion to \( U^2 \) as \( J_R \to U^2 \). On the other hand, due to the magnetic instability near \( U \to U_c = 2.23t \), the renormalized spin susceptibility \( \chi \) diverges. Thus, we found that the RKKY coupling also diverges near the quantum critical point at \( U_c \), as \( J_R \to (U_c - U)^{-1} [10] \). See the results in Fig.(2b) and Fig.(2d).

At second step, we study the direct Heisenberg exchange (DHE) coupling. The DHE coupling between two QLSMs on R and R’ is described by the following Hamiltonian

\[ J_D(R, R') \hat{S}_R \cdot \hat{S}_{R'} \]

where \( J_D(R, R') = -U \sum_i |\psi_0,R_i|^2 |\psi_0,R_i'|^2 \) is the coupling strength which is always negative (or \( J_D < 0 \)). \( \psi_0,R \) and \( \psi_0,R' \) are wave functions of the two quasi-localized states of the vacancies at R and R’.

The wave function of the quasi-localized state exactly distributes only on the opposite sub-lattices. Therefore, the DHE coupling between two QLSMs around vacancies on the different sublattices vanishes, \( J_D(R \in A/B, R' \in B/A) = 0 \). On the contrary, the DHE coupling between two QLSMs of vacancies on the same sublattice is finite, \( J_D(R \in A/B, R' \in A/B) < 0 \). In Fig.(3), we calculate the DHE coupling of two defects (see the black line). The fit decay rate from the numerical calculations for \( R < 38 \) is about \( R^{-1.412} \) along zigzag direction and \( R^{-1.644} \) along armchair direction. However, for the WLSMs of Anderson MIs, the DHE coupling between the localized spin moments can be definitely ignored.
TABLE I: The differences between intrinsic MI and extrinsic MI in graphene. ‘?’ means that we are not sure about this result from mean field calculations. $\alpha$ is about 1.412 along zigzag direction and 1.644 along armchair direction.

| Type of magnetic impurity | Vacancy-induced magnetic impurity in graphene | Anderson magnetic impurity in graphene |
|---------------------------|---------------------------------------------|----------------------------------------|
| Spin moment               | Intrinsic                                   | Extrinsic                              |
| s-d hybridization         | 0                                           | Finite                                 |
| s-d coupling              | Non-local FM Hund rule’s coupling           | Local AFM Kondo coupling               |
| Kondo effect              | No screening effect (?)                     | Kondo effect in pseudo-gap system      |
| Decay rate of RKKY coupling | $R^{-1}$                                  | $R^{-3}$                               |
| Decay rate of DHE coupling | $R^{-5}$ for AA/BB case; 0 for AB/BA case | 0                                      |
| Decay rate of SE coupling | $R^{-2}$ for AB/BA case; 0 for AA/BB case | 0                                      |

At third step, we study the superexchange (SE) coupling. When there are two vacancies on different sublattices nearby, the wave-functions of the zero modes around different vacancies may overlap and the quantum tunneling effect occurs. As a result, the energy degeneracy of the localized states is removed and we may have a finite energy level splitting. Taking the tight-binding limit, we can regard the quasi-localized states to obtain the sets of wave functions $\psi_{0,i}(\mathbf{R})$, where $\sigma = \uparrow, \downarrow$ denote spin degree of freedom and $\mathbf{R}$ denotes the position of the impurity. The quantum tunneling effect leads to an effective hopping of electrons from one quasi-localized state to another. The effective model of the zero modes becomes $t_{RR'} \left( \hat{\alpha}_{\mathbf{R},\sigma} \hat{\alpha}_{\mathbf{R'},\sigma} + h.c. \right)$ where $\hat{\alpha}_{\mathbf{R},\sigma}$ is an annihilation operator around a vacancy and the hopping strength $t_{RR'}$ is just the energy splitting $\Delta E_{RR'}$ from the quantum tunneling as $t_{RR'} \rightarrow \Delta E_{RR'}/2$. After considering the effective on-site interaction $U_{\text{eff}}$, the effective Hamiltonian of the electrons on the two quasi-localized states is given by

$$H_{\text{eff}} = -t_{RR'} (\hat{\alpha}_{\mathbf{R},\sigma} \hat{\alpha}_{\mathbf{R'},\sigma} + h.c.) - \mu_{\text{eff}} \sum_{\mathbf{R}} n_{\mathbf{R},\sigma} + U_{\text{eff}} \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}}^\uparrow \hat{n}_{\mathbf{R}}^\downarrow. \quad (8)$$

At half filling $\mu_{\text{eff}} = 0$, for the two QLSMs, there exists an energy splitting between the singlet state and the triplet states. We get an effective SE term $J_S(\mathbf{R}, \mathbf{R'}) \hat{S}_{\mathbf{R}} \cdot \hat{S}_{\mathbf{R'}}$ where $J_S(\mathbf{R}, \mathbf{R'})$ is the SE coupling strength. For two vacancies on the same sublattice, $J_S(\mathbf{R} \in A/B, \mathbf{R'} \in A/B) = 0$. For two vacancies on the different sublattices, $J_S(\mathbf{R} \in A/B, \mathbf{R'} \in B/A) = 0$. In the strong coupling limit, $U_{\text{eff}}/t_{RR'} \rightarrow \infty$, $J_S \simeq \frac{4U_{\text{eff}}t_{RR'}}{U_{\text{eff}}}$. Due to $|t_{RR'}| \rightarrow \frac{1}{R}$ for $R \rightarrow \infty$, we have $J_S(\mathbf{R}, \mathbf{R'}) \simeq \frac{4U_{\text{eff}}t_{RR'}}{U_{\text{eff}}} \rightarrow \frac{4U_{\text{eff}}}{R}$. For the weak coupling case, we calculate the SE coupling strength numerically. The results are given in Fig.(4). However, for the WLSMs of Anderson MIs, there is no SE coupling between the localized spin moments.

In summary, we derive the effective coupling between two QLSMs. For AA/BB case, the total coupling between two QLSMs is $J_D + J_R$. Now both $J_D$ and $J_R$ are negative. So we have an FM coupling. We also compare $|J_D|$ and $|J_R|$ and find that $|J_D| > |J_R|$ for short distance between two vacancies while $|J_D| < |J_R|$ for large distance. The critical distance dependents on the on-site interaction $U$. In Ref.[17], a decay rate of $R^{-1.43}$ ($R^{-1.644}$) for moments along zigzag (armchair) direction separations of up to 25Å had been extracted. Our results ($R^{-1.412}$) match their calculations. For AB/BA case, the coupling between two QLSMs is $J_S + J_R$. Now both $J_S$ and $J_R$ are positive. So we have an AFM coupling. We also compare $J_S$ and $J_R$ and find that $J_S > J_R$ for short distance between two vacancies while $J_S < J_R$ for large distance. Thus, for the case of graphene with $U = 1.5t$, from the results in Fig.(3) and Fig.(4), the RKKY coupling is always smaller than SE coupling or DHE coupling when the distance between two vacancies is short, $R < 38$. These results that seem to contradict to
people’s intuition can be naturally understood from the quasi-localization of the intrinsic MI induced by vacancies in graphene. That means people had over-estimated the contribution of RKKY coupling during studying the quantum magnetism of graphene with vacancies.

In the end we draw the conclusions. In this paper we developed a theory for the intrinsic MIs with the QLSM induced by the vacancies in graphene. Because the intrinsic MIs are characterized by the zero modes that are orthotropic to the itinerant electrons, their properties are much different to those of traditional Anderson MIs with the WLSMs. We give a table to compare the principal features of the two types (intrinsic and extrinsic) of MIs in graphene. Furthermore, the theory for the intrinsic MIs with the QLSM induced by the vacancies can be generalized to other bipartite system with particle-hole symmetry.

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