Spin–orbit coupling [1], the interaction between a quantum particle’s spin and its motion, has attracted much attention in condensed matter physics. The spin–orbit coupling is crucial to the quantum spin Hall effect [2, 3] and topological insulators [4–6]. It is reported that magnetic doping is an efficient method to tune and control the transport properties of these systems [7]. Magnetic doping is a feasible method to break the time reversal symmetry on the surface of topological insulators [8–11], so that one may observe very interesting physical phenomena in such materials [4, 5]. It has also been demonstrated experimentally and theoretically that magnetic doping is a straightforward approach to generating the quantum anomalous Hall effect in topological insulator thin films [12, 13].

However, as far as we know, magnetic impurity problems, i.e. Kondo problems [14], in spin–orbit coupled systems are far from clear up to now. A clear understanding of the Kondo problem is essential to studying low temperature transport properties and magnetic ordering problems in these systems. In this paper, we study the most fundamental quantity of Kondo problems, the Kondo temperature, in a two dimensional electron gas with Rashba spin–orbit coupling. Some previous works have studied the Kondo temperature of spin–orbit coupled systems [15–19]. A unitary transformation is applied to demonstrate [15] that the spin–orbit coupling can be absorbed into the effective hopping amplitudes with no effect on the Kondo temperature. Mean-field calculations based on variational wave functions show [16] that the Kondo temperature is exponentially altered by the spin–orbit coupling, because the density of state on the Fermi surface is changed by spin–orbit coupling. Perturbation renormalization group analysis based on the Schrieffer–Wolff transformation shows [17] that...
the Kondo temperature is exponentially enhanced by the Dzyaloshinskii–Moriya (DM) interaction between the local moment and the itinerant electrons. Numerical renormalization group (NRG) calculations show [18] that the Kondo temperature is almost a linear function of Rashba spin–orbit coupling energy. Dependence of the Kondo temperature on the spin–orbit coupling is also expected for quantum dots [19], where due to additional parameters like left–right asymmetries in the tunneling couplings or magnetic fields more complicated behaviour including suppression may appear. These qualitatively different results show that the variation of Kondo temperature as a function of spin–orbit coupling in this system is still an open question.

In this work, we use the Hirsch–Fye quantum Monte Carlo (HFQMC) simulation to study the problem. HFQMC is a numerically accurate method. It has been widely used to study magnetic impurity problems in normal metals, i.e. the local moment of magnetic impurity [20, 21], the Kondo effect [22], the Ruderman–Kittel–Kasuya–Yosida interaction between magnetic impurities [23], etc. Recently the HFQMC technique has been applied to study the local moment formation of Anderson impurities in dilute magnetic semiconductors [24] and graphene [25], and the interaction between magnetic impurities in the bulk of topological insulators [26].

Let us present the model Hamiltonian here—the total Hamiltonian has three different terms: the bulk state of two-dimensional electron gas with Rashba spin–orbit coupling [1, 17, 18], the magnetic impurity with strong on-site Coulomb interaction, and the hybridization between the electron gas and the impurity states,

\[
\mathcal{H} = \mathcal{H}_b + \mathcal{H}_d + \mathcal{H}_{hyb},
\]

\[
\mathcal{H}_b = \sum_{k,s} \psi_{k,s}^\dagger \left[ \frac{k^2}{2m^*} - \mu + \alpha (k_\sigma_1 - k_\sigma_2) \right] \psi_{k,s},
\]

\[
\mathcal{H}_d = \sum_{s} d_\uparrow^\dagger (\epsilon_d - \mu) d_\uparrow + U d_\uparrow^\dagger d_\uparrow^\dagger d_\downarrow d_\downarrow,
\]

\[
\mathcal{H}_{hyb} = \sum_{k,s} (V_k \psi_{k,s} d_\uparrow + V_k^* \psi_{k,s}^\dagger d_\downarrow),
\]

where \(\psi_{k,s}^\dagger\) and \(\psi_{k,s}\) are creation and annihilation operators of two-dimensional electron gas with momentum \(k\) (the Planck constant \(\hbar\) has been set to be 1) and spin \(s = \uparrow, \downarrow\), \(m^*\) is the effective mass of two-dimensional electron gas, \(\mu\) is the chemical potential, \(\alpha\) is the strength of Rashba spin–orbit coupling, \(\sigma_{x,y,z}\) are the spin Pauli matrices, \(d_\uparrow^\dagger\) (\(d_\uparrow\)) and \(d_\downarrow^\dagger\) (\(d_\downarrow\)) are creation and annihilation operators, respectively, of spin-up (spin-down) impurity states. \(\epsilon_d\) is the energy level of the impurity state. \(U\) is the on-site Coulomb interaction. \(V_k\) is the hybridization between itinerant electrons and impurity states. We set the hybridization to be short range coupled, so that the hybridization function \(V_k\) is independent of momentum \(k\).

Here we make a note on the units and parameters used in this paper. In the continuum limit, the summation over momentum is approximated by an integration, \(\Sigma_k = \frac{4\pi N_0}{\xi^2} \int_0^{\infty} dk \frac{e^{ik\xi}}{(2\pi)^2}\), where

\[
\Sigma_d(i\omega_n) = \frac{2\Gamma}{\pi} \left[ \log\left(\frac{i\omega_n + \mu}{4\pi}\right) + 2\zeta \tanh^{-1} \zeta + \gamma \right],
\]

where \(\zeta = \frac{\omega_n}{2\Gamma}\).
where $\zeta = \tilde{\alpha} \sqrt{\tilde{\alpha}^2 + 2i(\omega + \mu)}$, $\tilde{\alpha} = \sqrt{m^*} \alpha$, and $\gamma = 0.5772$ is the Euler–Mascheroni constant. The DOS of bulk electrons is proportional to the imaginary part of $\Sigma^+ + i0$.

In HFQMC simulation, the Hubbard interaction is simulated by the statistical average over auxiliary Ising spin configurations. One can calculate many important static quantities, i.e. the local charge, the local moment, the spin susceptibility, etc, from the imaginary-time Green’s function. The dynamical quantities, i.e. the spectral function, can be obtained from HFQMC by the maximal entropy method [27]. The spin susceptibility $\chi$ is an important quantity to describe the Kondo problem,

$$\chi = \int_0^{\beta} d\tau \langle S_\uparrow(\tau) S_\uparrow(0) \rangle,$$

where $S_\uparrow = d_\uparrow^\dagger d_\uparrow - d_\downarrow^\dagger d_\downarrow$. At very high temperature (i.e. $T \geq 10$ in figure 1(a)), the total system behaves like a free electron gas, which satisfies the Curie–Weiss law and $T\chi = 1/2$ [20]. At the intermediate region ($0.1 < T < 1$ in figure 1(a)), the impurity behaves as a local moment state. Our numerical simulations show that the square of the local moments, $m^2$, are enhanced.

**Figure 2.** The product $T\chi$ for different impurity energies and different spin–orbit couplings. (a), (c) and (e) are the original data for impurity energies $\varepsilon_\uparrow - \mu = -0.3$, $\varepsilon_\uparrow - \mu = -0.5$ and $\varepsilon_\uparrow - \mu = -0.7$ respectively. (b), (d) and (f) are the corresponding rescaled curves of (a), (c) and (e). Hubbard interaction $U = 1.0$ and chemical potential $\mu = 0.2$ are chosen.

**Figure 3.** Kondo temperature as a function of spin–orbit coupling for different impurity energies. Hubbard interaction $U = 1.0$ and chemical potential $\mu = 0.2$.

In this intermediate region (the inset in figure 1(a) shows $m^2$ at different temperatures for $U = 1$). At very low temperature,
the local moment state is screened by the itinerant electrons, and the product of temperature and spin susceptibility satisfies the following universal relationship [28],

$$\Phi(4T\chi(T) - 1) = \ln(T/T_K),$$

(9)

where $\Phi$ is a universal function and $T_K$ is the Kondo temperature. We can use this relationship to fit the variation of the Kondo temperature as a function of different parameters, i.e. Hubbard interaction, spin–orbit coupling, chemical potential, hybridization, etc, by HFQMC simulations. In the following numerical simulations, all of the points are averaged over 20 independent samples, and every sample run over 2000 HFQMC loops after warm-up. The statistical errors are calculated over the 20 samples, and they are plotted as error bars in the figures. Most of them are too small to be visible.

Before a more detailed discussion about the effect of spin–orbit coupling, we show the universal curves of spin susceptibility for different Hubbard interactions, shown in figure 1. One can see that the curves in figure 1(a) are almost equal-spacing under the logarithmic coordinate of temperature, which demonstrates that the Kondo temperature is exponentially altered by the Hubbard interaction. We can use the following formula to fit the Kondo temperature,

$$T_K(U) = T_K^{(0)}e^{-aU},$$

(10)

Figure 1(b) is the numerical fitting of the universal relationship equation (9) about figure 1(a), where the vertical coordinate is fixed and the horizontal coordinate is rescaled for different Hubbard interactions. We find that the fitting result $a = 1.11572$. This value is different from the one estimated from the ‘flat band’ results,

$$T_K = D\sqrt{\rho I} \exp(-1/\rho I),$$

(11)

where $\rho I = 8U/\pi U$ and $D$ is the effective bandwidth. Equation (11) gives $a = 2.5$ for the hybridization $\Gamma = 0.05\pi$ used here. This result demonstrates that the density of states near the band edge is important to altering the Kondo temperature.

Now we study the Kondo temperature for different spin–orbit couplings. There are three important aspects which may change the Kondo temperature: (1) The DM interaction between the local moment of the impurity and the itinerant electrons, which may exponentially enhance the Kondo temperature; (2) The spin–orbit coupling can split the two-fold spin degeneracy of the Fermi energy, so that the DOS on the two separated Fermi surfaces may change the Kondo temperature; and (3), although the total DOS of the Fermi energy is not changed by the spin–orbit coupling (see figure 4 for more details), the divergence of DOS near the band edge may change the Kondo temperature. We find that our results support case (3). Now we show the numerical results.

Figure 2 gives the product of temperature and spin susceptibility as a function of temperature for different spin–orbit couplings and different impurity energy levels. Figures 2(a), (c) and (f) are original data for impurity energies $\epsilon_d - \mu = -0.3$, $\epsilon_d - \mu = -0.5$ and $\epsilon_d - \mu = -0.7$ respectively. Figures 2(b), (d) and (f) are the rescaled curves. The numerical fitting of the Kondo temperatures are given in figure 3. We find that our HFQMC results are qualitatively consistent with those from NRG calculations [18]. The Kondo temperatures are almost linear functions of the Rashba energy $E_R = m^*\alpha^2/2$. Interestingly, one can find that, when the temperature is in the intermediate region (i.e. $0.1 < T < 1$), all of the three cases ($\epsilon_d - \mu = -0.3, -0.5, -0.7$) have the same tendency that the Kondo temperature is enhanced by the spin–orbit coupling. This demonstrates that maybe the perturbative renormalisation analysis is valid in this parameter region. However, when the temperature comes into the Kondo region, i.e. $T < 0.1$, the perturbative renormalisation analysis breaks down, and there may exist some crossover from the enhancement to the depression, i.e. $T \approx 0.1$ in figure 2(e). In addition, we find that there are some differences between our HFQMC simulations and the NRG calculations: (1) when the impurity energy $\epsilon - \mu = -0.5 = -U/2$, the NRG calculations show that the Kondo temperature is enhanced by the spin–orbit coupling, our HFQMC simulations show that it is suppressed; (2) the effect of spin–orbit coupling in HFQMC simulation is much
smaller than those given in NRG. These small differences may be induced by the different definitions of spin susceptibility in HFQMC and NRG. In HFQMC [20], it is defined as the susceptibility of local spin. In NRG [29], it is defined as the total susceptibility of the electron gas plus the local spin minus the susceptibility of the normal electron gas and the universal relationship (9) is based on the NRG definition. It is difficult to give an analytical estimation of the small difference between these two definitions.

These analyses show that the effect of DM interaction can be neglected at very low temperature. There are two other important effects which can change the Kondo temperature: the difference of the two Fermi surfaces and the divergence of the DOS near the band edge. Now we discuss the results when the chemical potential is far away from the band edge. The numerical results are shown in figure 4, we calculate the product of temperature and the spin susceptibility as a function of temperature for various values of spin–orbit coupling from 0.1 to 3.0. In figure 4(b), we can see that the difference between the DOS of the two bands is dramatically enhanced. However, the universal curves in figure 4(a) are slightly changed and the Kondo temperature is almost unchanged by the spin–orbit coupling.

So we conclude that the exponential enhancement of the Kondo temperature from perturbative renormalisation group analysis of the DM interaction between the impurity state and the bulk electrons breaks down in the low temperature Kondo region. Kondo temperature is almost a linear function of Rashba spin–orbit energy when the chemical potential is far away from the band edge, the Kondo temperature is independent of the spin–orbit coupling. We further conclude that divergence of the DOS near the band edge is the most important factor altering the Kondo temperature.

Acknowledgment

This work is supported by NSAF (Grant No. U1230202), Special Foundation for theoretical physics Research Program of China (Grant No. 11447167), and CAEP.

References

[1] Winkler R 2003 Spin–Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems (Berlin: Springer)
[2] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 226801
[3] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 146802
[4] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82 3045–67
[5] Qi X L and Zhang S C 2011 Rev. Mod. Phys. 83 1057–110
[6] Moore J E 2010 Nature 464 194–8
[7] Caler D 2012 Physica E 44 860–84
[8] Chen Y L et al 2010 Science 329 659–62
[9] Wray L A, Xu S Y, Xia Y, Hisieh D, Fedorov A V, Hor Y S, Cava R J, Bansil A, Lin H and Hasan M Z 2011 Nat. Phys. 7 32–7
[10] Okada Y et al 2011 Phys. Rev. Lett. 106 206805
[11] Valla T, Pan Z H, Gardner D, Lee Y S and Chu S 2012 Phys. Rev. Lett. 108 117601
[12] Yu R, Zhang W, Zhang H J, Zhang S C, Dai X and Fang Z 2010 Science 329 61–4
[13] Chang C Z et al 2013 Science 340 167–70
[14] Hewson A C 1997 The Kondo Problem to Heavy Fermions (Cambridge: Cambridge University Press)
[15] Paaske J, Andersen A and Flensberg K 2010 Phys. Rev. B 82 081309
[16] Isaev L, Agterberg D F and Vekhter I 2012 Phys. Rev. B 85 081107
[17] Zarea M, Ulloa S E and Sandler N 2012 Phys. Rev. Lett. 108 046601
[18] Žitič R and Bonča J 2011 Phys. Rev. B 84 193411
[19] Pletyukhov M and Schuricht D 2011 Phys. Rev. B 84 041309
[20] Hirsch J E and Fye R M 1986 Phys. Rev. Lett. 56 2521–4
[21] Fye R M and Hirsch J E 1988 Phys. Rev. B 38 433–41
[22] Fye R M, Hirsch J E and Scalapino D J 1987 Phys. Rev. B 35 4901–8
[23] Hirsch J E and Lin H Q 1987 Phys. Rev. B 35 4983–7
[24] Bulut N, Tanikawa K, Takahashi S and Maekawa S 2007 Phys. Rev. B 76 045220
[25] Hu F M, Ma T, Lin H Q and Gubernatis J E 2011 Phys. Rev. B 84 075414
[26] Sun J, Chen L and Lin H Q 2014 Phys. Rev. B 89 115101
[27] Silver R N, Sivia D S and Gubernatis J E 1990 Phys. Rev. B 41 2380–9
[28] Krishna-murthy H R, Wilkins J W and Wilson K G 1980 Phys. Rev. B 21 1003–43
[29] Wilson K G 1975 Rev. Mod. Phys. 47 773–840