Journal of Physics: Conference Series

PAPER • **OPEN ACCESS**

Dirac fermions and Kondo effect

Dirac fermions and Kondo effect

Takashi Yanagisawa

Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba Central 2, 1-1-1 Umezono, Tsukuba 305-8568, Japan

E-mail: t-yanagisawa@aist.go.jp

Abstract. In this study, we investigate the Kondo effect induced by the s-d interaction where the conduction bands are occupied by Dirac fermions. The Dirac fermion has the linear dispersion and is described typically by the Hamiltonian such as $H_k = v\mathbf{k}\cdot\sigma + m\sigma_0$ for the wave number $\mathbf{k}$ where σ_j are Pauli matrices and σ_0 is the unit matrix. We derived the formula of the Kondo temperature T_K by means of the Green's function theory for Green's functions including Dirac fermions and the localized spin. The T_K was determined from a singularity of Green's functions in the form $T_K \propto \exp(-\mathrm{const}/\rho|J|)$. The Kondo effect will disappear when the Fermi surface is point like.

1. Introduction

Recently, the Dirac electron in solid state has been investigated intensively [1-6]. It is interesting to examine how the Kondo effect occurs in a system of Dirac electrons with magnetic impurities. It is not so trivial whether the Kondo effect indeed appears there. We expect significant and interesting behaviors when the localized spin interacts with the Dirac electron through the s-d interaction. The Dirac Hamiltonian resembles the s-d model with the spin-orbit coupling of Rashba type [7]. In this paper we investigate the s-d Hamiltonian with Dirac electrons by means of the Green's function theory and evaluate the Kondo temperature T_K.

The Hamiltonian is given by $H = H_0 + H_{sd} \equiv H_m + H_K + H_{sd}$ where

$$\begin{aligned} H_m &= \sum_{\mathbf{k}}(m-\mu)(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow} + c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}\downarrow}), && (1) \\ H_K &= \sum_{\mathbf{k}}[v(k_x - ik_y)c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\downarrow} + v(k_x+ik_y)c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} \\ &+ v_z k_z(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}\downarrow})] && (2) \\ H_{sd} &= -\frac{J}{2}\frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}[S_z(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow} - c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow}) + S_+c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}'\uparrow} + S_-c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow}]. && (3) \end{aligned}$$

v and v_z are velocities of conduction electrons, μ is the chemical potential and m is the mass of the Dirac fermion. N indicates the number of sites. We set $m = 0$ so that the chemical potential μ includes m. $c_{\mathbf{k}\sigma}$ and $c^\dagger_{\mathbf{k}\sigma}$ are annihilation and creation operators, respectively. S_+, S_- and S_z denote the operators of the localized spin. The term H_{sd} indicates the s-d interaction between the conduction electrons and the localized spin, with the coupling constant J [8, 9]. J is negative, as adopted in this paper, for the antiferromagnetic interaction.

2. Green's Functions

We define thermal Green's functions of the conduction electrons

$$\begin{aligned} G_{\mathbf{k}\mathbf{k}'\sigma}(\tau) &= -\langle T_\tau c_{\mathbf{k}\sigma}(\tau) c^\dagger_{\mathbf{k}'\sigma}(0)\rangle, & (4)\\ F_{\mathbf{k}\mathbf{k}'}(\tau) &= -\langle T_\tau c_{\mathbf{k}\downarrow}(\tau) c^\dagger_{\mathbf{k}'\uparrow}(0)\rangle, & (5)\end{aligned}$$

where T_τ is the time ordering operator. We note that the spin operators satisfy the following relations:

$$\begin{aligned} S_\pm S_z &= \mp\frac{1}{2}S_z, \quad S_z S_\pm = \pm\frac{1}{2}S_\pm, & (6)\\ S_+S_- &= \frac{3}{4} + S_z - S_z^2, & (7)\\ S_-S_+ &= \frac{3}{4} - S_z - S_z^2. & (8)\end{aligned}$$

We also define Green's functions which include the localized spins as well as the conduction electron operators. They are for example, following the notation of Zubarev [10],

$$\begin{aligned} \langle\langle S_z c_{\mathbf{k}\uparrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_\tau &= -\langle T_\tau S_z c_{\mathbf{k}\uparrow}(\tau) c^\dagger_{\mathbf{k}'\uparrow}(0)\rangle, & (9)\\ \langle\langle S_- c_{\mathbf{k}\downarrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_\tau &= -\langle T_\tau S_- c_{\mathbf{k}\downarrow}(\tau) c^\dagger_{\mathbf{k}'\uparrow}(0)\rangle, & (10)\\ \langle\langle S_z c_{\mathbf{k}\downarrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_\tau &= -\langle T_\tau S_z c_{\mathbf{k}\downarrow}(\tau) c^\dagger_{\mathbf{k}'\uparrow}(0)\rangle, & (11)\\ \langle\langle S_- c_{\mathbf{k}\uparrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_\tau &= -\langle T_\tau S_- c_{\mathbf{k}\uparrow}(\tau) c^\dagger_{\mathbf{k}'\uparrow}(0)\rangle. & (12)\end{aligned}$$

The Fourier transforms are defined as usual:

$$\begin{aligned} G_{\mathbf{k}\mathbf{k}'\sigma}(\tau) &= \frac{1}{\beta}\sum_n e^{-i\omega_n\tau} G_{\mathbf{k}\mathbf{k}'\sigma}(i\omega_n), & (13)\\ F_{\mathbf{k}\mathbf{k}'}(\tau) &= \frac{1}{\beta}\sum_n e^{-i\omega_n\tau} F_{\mathbf{k}\mathbf{k}'}(i\omega_n), & (14)\\ \langle\langle S_z c_{\mathbf{k}\uparrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_\tau &= \frac{1}{\beta}\sum_n e^{-i\omega_n\tau} \langle\langle S_z c_{\mathbf{k}\uparrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_{i\omega_n}, & (15)\\ &\cdots\cdots. \end{aligned}$$

Using the commutation relations the equation of motion for $G_{\mathbf{k}\mathbf{k}'\uparrow}(i\omega_n)$ reads

$$\begin{aligned} (i\omega_n - v_z k_z - m + \mu) G_{\mathbf{k}\mathbf{k}'\uparrow}(\omega_n) &= \delta_{\mathbf{k}\mathbf{k}'} - \frac{J}{2N}\sum_q \Gamma_{\mathbf{q}\mathbf{k}'}(i\omega_n) \\ &+ v(k_x - ik_y) F_{\mathbf{k}\mathbf{k}'}(i\omega_n). & (16)\end{aligned}$$

Here we have defined

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\tau) = \frac{1}{\beta}\sum_n e^{-i\omega_n}\Gamma_{\mathbf{k}\mathbf{k}'}(i\omega_n) = \langle\langle S_z c_{\mathbf{k}\uparrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_\tau + \langle\langle S_- c_{\mathbf{k}\downarrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_\tau. \quad (17)$$

The equation of motion for $F_{kk'} = \langle\langle c_{\mathbf{k}\downarrow}; c^\dagger_{\mathbf{k}'\uparrow}\rangle\rangle_{i\omega_n}$ is also obtained in a similar way. By using the decoupling procedure for Green's functions [11-13], we can obtain a closed solution for a set of Green's functions. The Green's function $G_{\mathbf{k}\mathbf{k}'\uparrow}(i\omega_n)$ is obtained as

$$G_{\mathbf{k}\mathbf{k}'\uparrow}(\omega) = \delta_{kk'}G^0_k(\omega) - \frac{J}{2N}G^0_k(\omega)\frac{J}{2}\Gamma(\omega)G^0_k(\omega)\frac{1}{1 + JG(\omega) + \left(\frac{J}{2}\right)^2\Gamma(\omega)F(\omega)}, \quad (18)$$

where the analytic continuation $i\omega_n \to \omega$ is carried out. We defined the following functions:

$$G_k^0(\omega) = \frac{\omega+\mu}{(\omega+\mu)^2 - v^2(k_x^2+k_y^2) - v_z^2 k_z^2}, \quad (19)$$

$$F(\omega) = \frac{1}{N}\sum_k G_k^0(\omega), \quad (20)$$

$$\Gamma(\omega) = \frac{1}{N}\sum_k \left(m_k - \frac{3}{4}\right) G_k^0(\omega), \quad (21)$$

$$G(\omega) = \frac{1}{N}\sum_k \left(n_k - \frac{1}{2}\right) G_k^0(\omega), \quad (22)$$

with $m_k = 3\sum_q \langle c_{q\uparrow}^\dagger c_{k\downarrow} S_- \rangle$ and $n_k = \sum_q \langle c_{q\uparrow}^\dagger c_{k\uparrow}\rangle$.

3. Kondo Temperature

From the Green's function $G_{\mathbf{k}\mathbf{k}'\uparrow}(i\omega_n)$, the Kondo temperature T_K is determined from a zero of the denominator in this formula. We consider

$$1 + JG(\omega) = 0 \quad (23)$$

in the limit $\omega \to 0$ by neglecting higher-order term being proportional to $(J/2)^2$. Let us adopt for simplicity that $v_z = v$ and then the dispersion is $\xi_k = \pm v\sqrt{k_x^2+k_y^2+k_z^2} - \mu$ in three dimensions. We neglect the term of the order of J in $n_k = \langle c_{k\uparrow}^\dagger c_{k\uparrow}\rangle$. The equation $1 + JG(0) = 0$ results in the Kondo temperature T_K given as

$$k_B T_K = \frac{2e^\gamma D}{\pi} \exp\left(-16\pi^2 \frac{v^3}{\mu^2}\frac{1}{|J|}\right), \quad (24)$$

where D is a cutoff and γ is Euler's constant. We assumed that $|\mu| \gg k_B T_K$ to derive the above formula. The result shows that the Kondo effect indeed occurs in a Dirac system. We can consider the Kondo effect in two dimensions by setting $v_z = 0$, and also the d-dimensional case in general. In d dimensions T_K reads

$$k_B T_K = \frac{2e^\gamma D}{\pi} \exp\left(-\frac{8(2\pi)^d}{\Omega_d}\left(\frac{v}{|\mu|}\right)^{d-1}\frac{v}{|J|}\right), \quad (25)$$

where Ω_d is the solid angle in d-dimensional space, namely, the area of the $(d-1)$-sphere S^{d-1}.

In the limit $|\mu| \to 0$, the equation $1 + JG(0) = 0$ has no solution. Hence, when $|\mu|$ is small, T_K is reduced and vanishes. This measn that, when the Fermi surface is point like, the Kondo effect never appears because of the weak scattering by the localized spin. T_K shows an algebraic behavior $T_K \propto |\mu|^\alpha$ with a constant α. In three dimensions, T_K is proportional to μ^2 for small $|\mu|$:

$$k_B T_K \simeq \frac{1}{\pi^2}\sqrt{\frac{14\zeta(3)}{32}}\mu^2 \frac{1}{v}\sqrt{\frac{|J|}{v}}, \quad (26)$$

where $\zeta(3)$ is the Riemann zeta function at argument 3. In d-dimensional space, this is generalized as

$$k_B T_K \simeq \frac{1}{\pi}\sqrt{\frac{7\zeta(3)\Omega_d}{8(2\pi)^d}}|\mu|^{(d+1)/2}\sqrt{\frac{|J|}{v^d}}. \quad (27)$$

4. Summary

We investigated the s-d Hamiltonian with the localized spin interacting with the Dirac fermions. The Green's function method is applied to examine a singularity in Green's functions to determine the Kondo temperature T_K. The singularity leads to the formula of T_K as usual being proportional to $\exp(-\text{const}/\rho|J|)$ with the density of states ρ. The Kondo effect indeed occurs in the band of Dirac fermions and will produce singular properties in physical quantities. T_K vanishes when the Fermi surface is point like and shows the algebraic behavior $T_K \propto |\mu|^\alpha$ for small $|\mu|$. The term being proportional to σ_z like the magnetic field, which we did not have considered in this paper, is also important in the Kondo effect.

References

[1] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva S V, Dubonos S V and Firsov A A 2005 *Nature* **438** 197
[2] Zhang Y, Tan Y-W, Stormer H L and Kim P 2005 *Nature* **438** 201
[3] Hsieh D, Qian D, Wray K, Xia Y, Hor Y S, Cava R J and Hasan M Z 2008 *Nature* **452** 970
[4] Mitchell A K, Schuricht D, Vojta M and Fritz L 2013 *Phys. Rev.* B**87** 075430
[5] Beri B and Cooper N R 2012 *Phys. Rev. Lett.* **109** 156803
[6] Kanao T, Matsuura H and Ogata M 2012 *J. Phys. Soc. Jpn.* **81** 063709
[7] Yanagisawa T 2012 *J. Phys. Soc. Jpn.* **81** 094713
[8] Kondo J 1964 *Prog. Theor. Phys.* **32** 37
[9] Kondo J 2012 *The Physics of Dilute Mgnetic Alloys* (Cambridge University Press, Cambridge)
[10] Zubarev D 1960 *Sov. Phys. Uspekhi* **3** 320
[11] Nagaoka Y 1965 *Phys. Rev.* **138** A1112
[12] Hamann D R 1967 *Phys. Rev.* D**158** 570
[13] Zittartz J and Müller-Hartmann E 1968 *Z. Phys.* **212** 380