In the limit $\omega\tau_c \to 0$, Eq. (24) becomes

$$R_{LL'}(M) = -\delta_{LL'} 2v^2\tau_c \sum_\lambda [1-(-1)^{l+L+\lambda}] \times (2\lambda+1) W^2(l\lambda KK; LK) . \quad (30)$$

Noting that

$$(-1)^{l+L+\lambda} = [(2l+1)(2L+1)]^{1/2} W(llLL; 0\lambda) \quad (31)$$

and making use of the sum rules 6.13 and 11.11 of Rose,[5] we obtain (12). For the special case $l=1$, we must have $L'=\lambda=L$ in (24), since a magnetic field simply rotates the atoms of an ensemble and does not couple different multipole moments. Then one can use tabulated Clebsch-Gordan coefficients (Rose,[5] p. 225) to obtain (17) from (24).

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Conduction-Electron Spin Polarization around a Magnetic Impurity*

CHAMAN MEHROTRA†

Department of Physics, Indian Institute of Technology, Kanpur, India

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The spatial distribution of the conduction-electron spin polarization has been calculated for the Anderson model using the Hartree-Fock approximation. An expression for low temperatures has been obtained. The long-range behavior of spin polarization at absolute zero temperature is compared with the Ruderman-Kittel-Kasuya-Yosida result.

I. INTRODUCTION

THERE are two models (the Anderson and the Wolff-Clogston)[1–3] based on Friedel's picture[4] of virtual states to explain the appearance of localized magnetic moments (henceforth called local moments) in a dilute alloy of magnetic atoms in a nonmagnetic host. Both of these models are capable of predicting qualitatively the appearance of local moments in many cases. Several recent review papers[5–7] have discussed various attempts to get the exact solution of the problem of the local moments in different models.

Recently, Schrieffer, and Wolff[8] have shown that under a certain transformation the Anderson Hamiltonian goes over to the exchange Hamiltonian form, used by Kondo to show the Kondo effect.[9] The spin polarization for an exchange Hamiltonian has already been studied and the results are known as Ruderman-Kittel-Kasuya-Yosida (RKKY) polarization.[10–13] Several authors[14,15] have made calculations for spin polarization due to a magnetic impurity in different models.

The present paper is aimed at deriving conduction-electron spin polarization around a magnetic impurity in the Anderson model, under the Hartree-Fock (HF) approximation, as a function of the distance from the impurity. An expression for spin polarization at low temperatures is obtained. The long-range behavior at absolute zero temperature is compared with the RKKY result,[10–13] to see if Anderson's description of the magnetic impurity conforms to the expected exchange form of the conduction-electron-impurity interaction.

The magnitude of spin polarization is calculated for the most favorable case for the appearance of the local moments,[1] in which the levels for spin-up and spin-down electrons are close to each other and lie symmetrically about the Fermi level. A comparison of the magnitudes in our case and in the corresponding RKKY limit is made.

II. THEORY

In the Anderson model we take an extra d orbital for the impurity. The overcompleteness of the resulting set has been discussed by Anderson and McMillan.[16] They have shown that such a description gives essentially identical results with the case in which the impurity d orbital is orthogonalized to the conduction band states. In the present paper we calculate polarization in the region beyond the range of the d orbital. Irrespective of whether we start with an overcomplete set or an orthog-

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† Present address: Division of Physical Sciences, Meerut University Institute of Advanced Studies, Meerut, India.

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onal set, in this region the band states can be taken as plane waves. Therefore, the spin polarization of conduction electrons come mainly from the electron-electron Green functions. The contribution of others is small and has thus been neglected.

In the notation of Anderson,[1] the electron-electron Green functions $G_{\mathbf{kk}'}{}^{\sigma}(\mathcal{E})$, under the HF approximation, are given by

$$G_{\mathbf{kk}'}{}^{\sigma}(\mathcal{E})=\frac{\delta_{\mathbf{kk}'}}{\mathcal{E}-\mathcal{E}_{\mathbf{k}}}+\frac{V_{\mathbf{k}d}V_{d\mathbf{k}'}}{(\mathcal{E}-\mathcal{E}_{\mathbf{k}})(\mathcal{E}-\mathcal{E}_{\mathbf{k}'})(E-E_{\sigma}+i\Delta)}, \quad (1)$$

where $\mathcal{E}=E+i0^{+}$, $E_{\sigma}=E_d+U\langle n_{d-\sigma}\rangle$, and

$$\Delta=-\mathrm{Im}\sum_{\mathbf{k}}V_{\mathbf{k}d}V_{d\mathbf{k}}/(E+i0^{+}-\mathcal{E}_{\mathbf{k}});$$

Δ is taken not to be depending on E, and Im stands for imaginary part.

The number density of electrons with spin σ, at a point $\mathbf{r}$, is given by the following expression[6,15]:

$$n^{\sigma}(\mathbf{r})=\lim_{\mathbf{r}\to\mathbf{r}'}\frac{\Omega}{(2\pi)^6}\int d\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{r}}\int d\mathbf{k}'e^{-i\mathbf{k}'\cdot\mathbf{r}'}\int_{-\infty}^{\infty}dE \times f(E)\left[-\frac{\mathrm{Im}}{\pi}G_{\mathbf{kk}'}{}^{\sigma}(\mathcal{E})\right], \quad (2)$$

where $f(E)=[1+e^{(E-E_f)/k_BT}]^{-1}$ is the Fermi-Dirac energy-distribution function and Ω is the volume of the crystal. The spin polarization of conduction electrons will be given by

$$p(\mathbf{r})=\sum_{\sigma}\sigma n^{\sigma}(r)=[n^{\uparrow}(\mathbf{r})-n^{\downarrow}(\mathbf{r})]. \quad (3)$$

We calculate now the spin polarization for a case in which at a given temperature T°K, $\langle n_{d\uparrow}\rangle$ and $\langle n_{d\downarrow}\rangle$ are known through a self-consistent treatment. $V_{\mathbf{k}d}$ is assumed to depend only on the magnitude of $\mathbf{k}$ and writing $V_{\mathbf{k}d}=V_{|\mathbf{k}||d|}=V_{kd}$ we get

$$p(\mathbf{r})=-\lim_{\mathbf{r}\to\mathbf{r}'}\frac{2\Omega}{(2\pi)^7}\int d\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{r}}\int d\mathbf{k}'e^{-i\mathbf{k}'\cdot\mathbf{r}'}\int_{-\infty}^{\infty}dEf(E) \times\mathrm{Im}\sum_{\sigma}\frac{\sigma V_{kd}V_{dk'}}{(\mathcal{E}-\mathcal{E}_{\mathbf{k}})(\mathcal{E}-\mathcal{E}_{\mathbf{k}'})(E-E_{\sigma}+i\Delta)}. \quad (4)$$

Performing the angle integrations we get $[\mathcal{E}_{\mathbf{k}}=\hbar^2k^2/2m]$

$$p(\mathbf{r})=-\frac{\Omega}{4\pi^5r^2}\mathrm{Im}\sum_{\sigma}\sigma\int_{-\infty}^{\infty}dE\frac{f(E)}{(E-E_{\sigma}+i\Delta)} \times\int_0^{\infty}dk\frac{k\sin(kr)V_{kd}}{E+i0^{+}-\hbar^2k^2/2m} \times\int_0^{\infty}dk'\frac{k'\sin(k'r)V_{dk'}}{E+i0^{+}-\hbar^2k'^2/2m}. \quad (5)$$

If V_{kd} is analytic in the complex k plane, we can write

$$\int_0^{\infty}dk\frac{k\sin(kr)V_{kd}}{E+i0^{+}-\hbar^2k^2/2m}=-\frac{m\pi}{\hbar^2}e^{ir(2mE/\hbar^2)^{1/2}}V_{\surd(E)d}, \quad (6a)$$

where $V_{\surd(E)d}=V_{kd}|_{k=(2mE/\hbar^2)^{1/2}}$. In some cases V_{kd} may be peaked about $k=k_d$; $(E_d=\hbar^2k_d{}^2/2m)$. In such a case, V_{kd} will have poles in the upper half of the complex k plane. We assume them to be at $k=\pm k_d+ia$, with $a>0$. Then we have

$$\int_0^{\infty}dk\frac{k\sin(kr)V_{kd}}{E+i0^{+}-\hbar^2k^2/2m}=-\frac{m\pi}{\hbar^2}[e^{ir(2mE/\hbar^2)^{1/2}}V_{\surd(E)d}+e^{-ar}Q(E,k_d,r)], \quad (6b)$$

where Q is a function of E,k_d, and r; and is oscillatory in nature. Thus even if we start with V_{kd} having poles in the upper half of the complex k plane the terms containing Q will drop out in the large r limit and therefore, in what follows, we have not made any attempt to solve explicitly the integrals containing Q and Q^2. If the form of V_{kd} is known we can easily find Q. A convenient form of V_{kd} is

$$V_{kd}=\frac{B(|\mathbf{k}|,k_d)}{(k-k_d)^2+a^2}, \quad (7)$$

where $B(|\mathbf{k}|,k_d)$ is an analytic function of k.

The expression for $p(\mathbf{r})$ then becomes

$$p(\mathbf{r})=-\frac{\Omega}{16\pi^3r^2}(2m/\hbar^2)^2\,\mathrm{Im}\sum_{\sigma}\sigma\int_{-\infty}^{\infty}dE \times\frac{f(E)}{E-E_{\sigma}+i\Delta}[e^{i2r(2mE/\hbar^2)^{1/2}}V_{\surd(E)d}V_{d\surd(E)} +e^{ir(2mE/\hbar^2)^{1/2}}(V_{\surd(E)d}+V_{d\surd(E)})e^{-ar}Q+Q^2e^{-2ar}]. \quad (8)$$

Dependence of $V_{\surd(E)d}V_{d\surd(E)}$ on E in the first term in the expression for $p(\mathbf{r})$ can be taken into account by writing it in terms of Δ:

$$\Delta=-\mathrm{Im}\sum_{\mathbf{k}}V_{kd}V_{dk}\delta(E-\hbar^2k^2/2m) =(m/(2\pi\hbar^2))(2mE/\hbar^2)^{1/2}V_{\surd(E)d}V_{d\surd(E)}. \quad (9)$$

Equation (8) then reduces to

$$p(\mathbf{r})=-\frac{\Omega}{4\pi^2r^2}(2m/\hbar^2)^{1/2}\,\mathrm{Im}\sum_{\sigma}\sigma \times\left[\int_0^{\infty}dEf(E)\frac{e^{i2r(2mE/\hbar^2)^{1/2}}}{(E-E_{\sigma}+i\Delta)\sqrt{E}} +F_{1\sigma}e^{-ar}+F_{2\sigma}e^{-2ar}\right], \quad (10)$$

where

$$F_{1\sigma}=\int_0^\infty \frac{dEf(E)e^{ir(2mE/\hbar^2)^{1/2}}}{E-E_\sigma+i\Delta}(V_{\surd(E)d}+V_{d\surd(E)})Q$$

and

$$F_{2\sigma}=\int_0^\infty \frac{dEf(E)Q^2}{E-E_\sigma+i\Delta}.$$

$F_{1\sigma}$ and $F_{2\sigma}$ are functions of k_F, k_d, E_σ, r, and T; with $k_F=(2mE_f/\hbar^2)^{1/2}$.

In the above expression integration over the negative values has been excluded since we consider only the real values of k which correspond to $E>0$. For $E<0$, $V_{\surd(E)d}V_{d\surd(E)}=0$ from Eq. (9). Equation (10) can be rewritten as

$$p(\mathbf{r})=-\frac{\Omega}{2\pi^2r^2}(2m/\hbar^2)\ \mathrm{Im}\sum_\sigma \sigma\Bigg[\int_0^\infty dkf(k)\times\frac{e^{i2kr}}{k^2-2m(E_\sigma-i\Delta)/\hbar^2}+e^{-ar}F_{1\sigma}+e^{-2ar}F_{2\sigma}\Bigg],\quad(11)$$

where $f(k)=F(E)|_{E=\hbar^2k^2/2m}$. Writing $2m(E_\sigma-i\Delta)/\hbar^2=k_\sigma^2$, where k_σ has a negative imaginary part, we can write

$$\int_0^\infty\frac{dkf(k)e^{i2kr}}{k^2-k_\sigma^2}=-i(2k_\sigma)^{-1}\int_0^\infty dt\times e^{-ik_\sigma t}\int_0^\infty dkf(k)[e^{ik(t+2r)}-e^{ik(t-2r)}].\quad(12)$$

For integration over k we integrate the above expression by parts. Since $f(k)=0$ at $k=\infty$ and $f(k)=1$ at $k=0$ the expression for $p(\mathbf{r})$ becomes

$$p(\mathbf{r})=-\frac{\Omega}{2\pi^2r^2}(2m/\hbar^2)\ \mathrm{Im}\sum_\sigma\sigma\times\Bigg\{\Delta(2k_\sigma)^{-1}\int_0^\infty dte^{-ik_\sigma t}\Bigg[(2r+t)^{-1}+(2r-t)^{-1}+\int_0^\infty dEf'(E)\Bigg(\frac{e^{i(2r+t)(2mE/\hbar^2)^{1/2}}}{2r+t}+\frac{e^{i(2r-t)(2mE/\hbar^2)^{1/2}}}{2r-t}\Bigg)\Bigg]+e^{-ar}F_{1\sigma}+e^{-2ar}F_{2\sigma}\Bigg\}.\quad(13)$$

Now we evaluate $p(\mathbf{r})$ at low temperatures, i.e., $k_BT<E_f$. Using the well-known Sommerfeld and Bethe[17] expansion

$$\int dEf'(E)F(E)\simeq-F(E_f)-\pi^2T^2F''(E_f)/6,\quad(14)$$

we get the following expression for $p(\mathbf{r})$:

$$p(\mathbf{r})=-(\Omega/2\pi^2r^2)(2m/\hbar^2)\times\mathrm{Im}\sum_\sigma\sigma[I_\sigma(r)+e^{-ar}F_{1\sigma}+e^{-2ar}F_{2\sigma}],\quad(15a)$$

where

$$I_\sigma(r)=\Delta(2k_\sigma)^{-1}\Bigg\{e^{i2k_\sigma r}[E_1(i2k_\sigma r)-E_1(i2r(k_\sigma-k_F))]-e^{-i2k_\sigma r}[E_1(-i2k_\sigma r)-E_1(-i2r(k_\sigma+k_F))]+\frac{\pi^2T^2}{24k_F^3}(2m/\hbar^2)\Bigg[\frac{2k_Fr+i}{i(k_\sigma^2-k_F^2)}-\frac{2k_F^2}{(k_\sigma^2-k_F^2)^2}\Bigg]\Bigg\},\quad(15b)$$

where

$$E_1(z)=\int^\infty\frac{e^{-u}}{u}du,$$

and z is complex. Equations (15) give the spin polarization as a function of r at low temperatures.

Long-Range Behavior at Absolute Zero Temperature

At absolute zero temperature $p(\mathbf{r})$ is given by

$$p(\mathbf{r})=-\frac{\Omega}{2\pi^2r^2}(2m/\hbar^2)\ \mathrm{Im}\sum_\sigma\sigma\Bigg\{\Delta(2k_\sigma)^{-1}\int_0^\infty dt\times e^{-ik_\sigma t}\Bigg[\frac{1-e^{ik_F(t+2r)}}{t+2r}-\frac{1-e^{-ik_F(t-2r)}}{t-2r}\Bigg]+F_{1\sigma}{}^0e^{-ar}+F_{2\sigma}{}^0e^{-2ar}\Bigg\},\quad(16a)$$

$$=-\frac{\Omega}{2\pi^2r^2}(2m/\hbar^2)\ \mathrm{Im}\sum_\sigma\sigma\times[\Delta(2k_\sigma)^{-1}\{e^{i2k_\sigma r}[E_1(i2k_\sigma r)-E_1(i2r(k_\sigma-k_F))]-e^{-i2k_\sigma r}[E_1(-i2k_\sigma r)-E_1(-i2r(k_\sigma+k_F))]\}+e^{-ar}F_{1\sigma}{}^0+e^{-2ar}F_{2\sigma}{}^0],\quad(16b)$$

where $F_{1\sigma}{}^0=F_{1\sigma}|_{T=0°\mathrm{K}}$ and $F_{2\sigma}{}^0=F_{2\sigma}|_{T=0°\mathrm{K}}$. Since k_σ has a negative imaginary part for r large, we can write

$$\int_0^\infty dt\frac{e^{-ik_\sigma t}}{t+2r}\simeq(i2k_\sigma r)^{-1}$$

and

$$\int_0^\infty dt\frac{e^{-ik_\sigma t}}{t-2r}\simeq-(i2k_\sigma r)^{-1}-i\pi e^{-i2k_\sigma r}.\quad(17)$$

Since $a>0$ the terms containing $F_{1\sigma}{}^0$ and $F_{2\sigma}{}^0$ drop out in this limit. The spin polarization in large r limit is then given by

$$p(\mathbf{r})=\frac{\Omega\Delta}{4\pi^2r^2}\sum_\sigma\sigma\Bigg[\frac{E_\sigma}{E_\sigma^2+\Delta^2}-\frac{(E_\sigma-E_f)\cos(2k_Fr)-\sin(2k_Fr)}{(E_\sigma-E_f)^2+\Delta^2}\Bigg].\quad(18)$$

[17] F. Seitz, *The Modern Theory of Solids* (McGraw-Hill Book Co., New York, 1940), p. 146.

We see that the expression for $p(\mathbf{r})$ shows the RKKY behavior. It also has $(\cos(2k_Fr))/r^3$ and $(\sin(2k_Fr))/r^3$ terms besides an additional term which varies as $1/r^3$.

We simplify the expression for $p(\mathbf{r})$ further for a case in which localized magnetic moment is barely formed and is very small. In such a situation the energy levels for spin-up and spin-down electrons lie close to Fermi level.[1] In this limit we have $\langle n_{d\uparrow}\rangle=\frac{1}{2}(1+\delta)$ and $\langle n_{d\downarrow}\rangle=\frac{1}{2}(1-\delta)$, where $\delta\ll 1$. Conditions for self-consistency[1] of the solution give

$$E_\uparrow=E_f-\tfrac{1}{2}U\delta \quad\text{and}\quad E_\downarrow=E_f+\tfrac{1}{2}U\delta. \tag{19}$$

With these substitutions $p(\mathbf{r})$ for large r is given by

$$p(\mathbf{r})=\frac{U\delta\Delta}{4\pi^2r^3}[\cos(2k_Fr)+(\Delta/E_f)^2]. \tag{20}$$

The second term in the above expression will be small for a fairly sharp d level. The $(\cos(2k_Fr))/r^3$ term gives the RKKY polarization.[10–13] In the corresponding RKKY limit, the coefficient of $(\cos(2k_Fr))/r^3$ term is

$$9\pi n^2J\Omega I_n{}^z/(4E_fk_F{}^3)\simeq k_F{}^3\Omega J\delta/(16\pi^3E_f) \tag{21}$$

writing $I_n{}^z\simeq\delta$ and $n=k_F{}^3/(6\pi^2)$; and the various terms are in Kittel's notation.[18] As has been shown by Schrieffer and Wolff,[8] in the large U limit, we can write for small moment case $J\simeq 8|V_{kFd}|^2/U$. With this substitution the expression (21) reduces to

$$k_F{}^38|V_{kFd}|^2\delta\Omega/(16\pi^3E_fU). \tag{22}$$

If we denote by R the ratio of $(\cos(2k_Fr))/r^3$ terms in our case [Eq. (21)] and in the corresponding RKKY limit [Eq. (22)], we have

$$R=\pi U^2E_f/(2k_F{}^2\Delta|V_{kFd}|^2). \tag{23}$$

From Eq. (9),

$$|V_{kFd}|^2=2\pi\Delta\hbar^2/(mk_F). \tag{24}$$

Therefore

$$R=[U/\Delta 2\sqrt{2})]^2. \tag{25}$$

Since for local moment to appear $U/(\pi\Delta)\simeq 1$, R in Eq. (25) is close to unity. Hence the order of magnitude of spin polarization is same in both these cases.

[18] C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), p. 363.

III. CONCLUSIONS

Equations (15) give spin polarization at low temperatures as a function of distance from the impurity, in terms of $E_\uparrow$ and $E_\downarrow$ which can be found in a self-consistent manner. Knowing the form of V_{kd} expression (13) can be used directly to calculate spin polarization at any temperature. The function $E_1(z)$ for any value of z can be evaluated from a Taylor series expansion.[19] The contribution of $G_{dd}{}^\sigma$ and $G_{kd}{}^\sigma$ to spin polarization has not been included in our expression (2). Therefore it is strictly valid only beyond the range of the d orbital. From Eq. (18) we observe that at absolute zero temperature the spin polarization varies as r^{-3} and has terms like $(\cos(2k_Fr))/r^3$ and $(\sin(2k_Fr))/r^3$ in the large r limit. This is similar to RKKY result.[10–13] Expression (20) gives the long-range behavior of spin polarization for the case in which localized magnetic moment is barely formed. The magnitude of the $(\cos(2k_Fr))/r^3$ is found to be the same as in corresponding RKKY limit. The additional $1/r^3$ term is deviation from the standard RKKY result and might be attributed to polarization due to bare localized magnetic moment without electron cloud around it. This term will be small for a fairly sharp d level, i.e., $\Delta/E_f<1$.

The agreement of long-range behavior of spin polarization with the RKKY result conforms to the expected exchange mechanism for the conduction-electron–impurity interaction.

Although Schrieffer and Wolff[8] did not derive the expression $J\simeq 8|V_{kFd}|^2/U$ in the HF approximation we have used this result to get an idea of the magnitude of the spin polarization in our case.

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