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# Temperature-dependent Ruderman-Kittel-Kasuya-Yosida interaction

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We develop a method that provides an analytical expression of the free-electron spin susceptibility for arbitrary temperature. The result can be further reduced by using the low-temperature approximation, which shows that the oscillation decays exponentially as $\exp(-\pi T' k_F r)$ in the long-range limit, and the wave number of the oscillation varies as $k_0 \sim k_F[1-(\pi^2/12)T'^2]$, where $T'$ is the normalized temperature with respect to the Fermi energy. The result contradicts what Darby has proposed, especially in the long-range region. On the other hand, in the short-range region, where the Sommerfeld expansion method is valid, numerical study shows that Darby's result agrees with ours fairly well.

In the Ruderman-Kittel-Kasuya-Yosida[1] (RKKY) interaction, the variation of the form of the interaction with temperature is of interest, especially in the long-range limit. The original development of the RKKY interaction was based on the assumption of a perfect Fermi gas with no lattice effects and no other polarizing moment present. In such an ideal system, the coupling constant between local spins in the RKKY interaction is proportional to the itinerant spin susceptibility, if the interaction between itinerant and local spins is treated as a point interaction. In the long-range limit at $T=0$, the free-electron spin susceptibility $\chi(r)$, which represents the spin polarization due to a point interaction, has an oscillatory decaying form $\cos(2k_F r)/r^3$. At nonzero $T$, the long-range oscillation of the free-electron spin polarization, and therefore the interaction between local spins, is damped as the Fermi surface becomes blurred with increasing temperature. In his earlier work,[2] Darby has proposed that the temperature-dependent $\chi(r)$ is proportional to

$$\frac{j_1(2k_F r)}{r^2}\exp\left[-\frac{\pi^2}{6}\left(\frac{k_B T}{\epsilon_F}\right)^2 (k_F r)^2\right], \tag{1}$$

in three dimensions at low temperature. This expression was derived from March and Murray's work[3] on the spatial electronic charge distribution around perturbations. March and Murray used the Sommerfeld expansion to derive numerically the temperature dependence of the asymptotic form of the potential which results in

$$\frac{\cos(2k_F r)}{r^3}\left[1-\frac{\pi^2}{6}\left(\frac{k_B T}{\epsilon_F}\right)^2 (k_F r)^2\right], \tag{2}$$

and suggested the above Gaussian form from this approximate result. In the Sommerfeld expansion, it is assumed that the integrand multiplied by the Fermi distribution function is nonsingular and not too rapidly varying in the neighborhood of $\epsilon=\mu$. This condition cannot be satisfied in the derivation of the long-range behavior of $\chi(r)$ because the amplitude of the spin oscillation at long range is very sensitive to the distribution near the Fermi surface. Therefore, this kind of approach is not applicable for the study of the long-range behavior.

In the present study, we propose a method that properly elucidates the effect of temperature on $\chi(r)$. Our method does not require any restrictions on the property of the integrand as the Sommerfeld expansion does. The analytical low-temperature approximation reveals that the amplitude decay of $\chi(r)$, which is algebraic at $T=0$, becomes an exponential form in the long-range limit as a function of both temperature and distance, and the oscillation period varies with temperature.

Earlier work[4] done by de Gennes has shown that the spin-spin coupling of the RKKY interaction, which is reduced to the free-electron susceptibility $\chi(r)$ in an ideal system, becomes damped exponentially due to finite electron mean free path effect by elastic, pure potential scattering in a randomly disordered system. More recently, Shegelski and Geldart[5] extended this study to the more general system which includes an $sd$ spin-exchange scattering and have found that, in this system, this $sd$ spin-exchange scattering at finite temperature does also lead to a damping in the effective spin-spin coupling.

We start out with the real space representation of $\chi(r)$ of the free-electron gas employing the linear response assumption, and $\chi(r)$ becomes

$$\chi(r)=\frac{1}{(2\pi)^3}\int d\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}\chi(\mathbf{q}) = \frac{m\mu_B^2}{2\pi^4\hbar^2 r}\int_0^\infty dq\sin(qr)\int_0^\infty dk k f(k)\ln\left|\frac{q+2k}{q-2k}\right|, \tag{3}$$

where $f(k)$ is the Fermi distribution function. By changing the order of integration, the above equation becomes

$$\chi(r)=\frac{m\mu_B^2}{(2\pi)^3\hbar^2 r^2}\int_0^\infty dk k f(k)\sin(2kr). \tag{4}$$

 

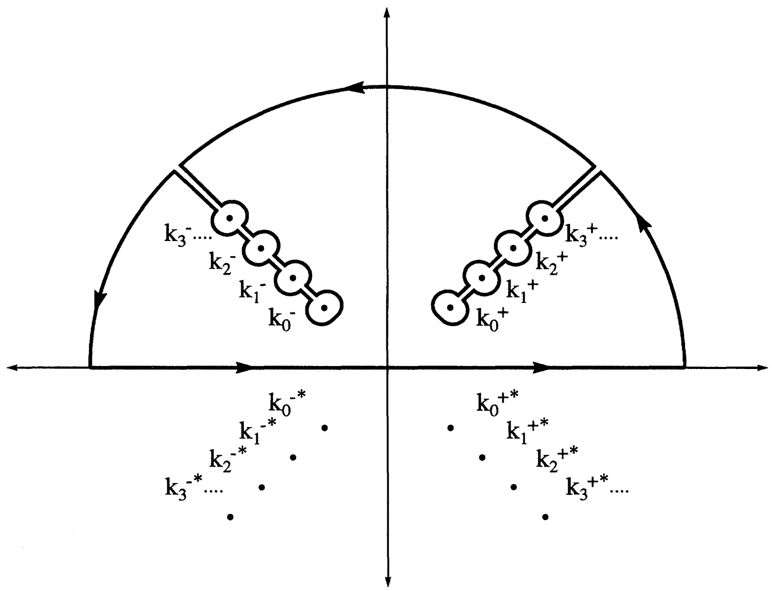


FIG. 1. The schematic representation of the poles of the Fermi distribution function of the free electron and the contour for the integral in the complex $k$ plane.

This result obtained under the linear response assumption is identical with that of Darby's first-order perturbation in real space. The order of integration cannot be interchanged in one dimension because the singularities at $q=0$ and $k=0$ contribute differently depending on the order of the integration.[6] However, in three dimensions, the singularities are at $q=\pm 2k$ only and they do not make any differences even though the order of integration is interchanged.

At $T=0$, it is easy to show that $\chi(r)$ is reduced to the usual RKKY interaction,

$$\chi(r,T=0)=\frac{m\mu_B^2}{(2\pi)^3\hbar^2}\frac{1}{r^4}[\sin(2k_Fr)-2k_Fr\cos(2k_Fr)] \tag{5}$$

from Eq. (4) as has been discussed in Kittel.[7] For finite temperature, we begin by rewriting Eq. (4) as

$$\chi(r)=\frac{m\mu_B^2}{2(2\pi)^3\hbar^2r^2}\,\mathrm{Im}\left[\int_{-\infty}^{\infty}dkkf(k)e^{2ikr}\right]$$
$$=\frac{m\mu_B^2}{2(2\pi)^3\hbar^2r^2}\,\mathrm{Im}(J). \tag{6}$$

The lower bound of the integration is extended to $-\infty$ using the symmetry of the integrand and compensated by an additional factor $\frac{1}{2}$. In the complex plane, the free-electron gas Fermi distribution function $f(k)=1/\{1+\exp[(\beta\hbar^2/2m)(k^2-k_F^2)]\}$ has poles at the points

$$k_n^+=\eta_n e^{i\varphi_n},\quad k_n^{+}{}^*=\eta_n e^{i(-\varphi_n)}, \tag{7}$$

$$k_n^-=\eta_n e^{i(\pi-\varphi_n)},\quad k_n^{-}{}^*=\eta_n e^{i(-\pi+\varphi_n)}, \tag{8}$$

where $\eta_n=(k_f^4+\{[2(2n+1)/\beta']\pi\}^2)^{1/4}$, $\varphi_n=1/2\arctan[2\times(2n+1)\pi/\beta' k_F^2]$, $\beta'=\beta\hbar^2/m$, and $n$ is an integer. Notice that $k_n^\pm$ and $k_n^{\pm}{}^*$ are complex conjugates of each other. These are simple poles, since, by expanding $1+e^{\beta'(k^2/2-k_F^2/2)}$ in a series around the pole $k_n$, we get

$$1+e^{\beta'(k^2/2-k_F^2/2)}=(k-k_n)(-k_n\beta'+\cdots). \tag{9}$$

The schematic representation of the locations of the poles in the complex planes are shown in Fig. 1. Each of these poles approaches the real axis as $T$ goes to zero. The integral in Eq. (6) can be calculated by moving the contour of integration in the upper half plane as shown in Fig. 1. The contribution from the semicircle vanishes when the contour is shifted out to infinity. Therefore the contour integral is reduced to the integral along the real axis and the sum of residues at the poles in the upper half plane. Since each of the poles is simple, the integral along the real axis $J$ becomes

$$J=-\sum_{n=0}^{\infty}\left(\oint\frac{ke^{2ikr}}{(k-k_n^+)(k_n^+\beta'+\cdots)}dk+\oint\frac{ke^{2ikr}}{(k-k_n^-)(k_n^-\beta'+\cdots)}dk\right)$$
$$=-\frac{2\pi i}{\beta'}\sum_{n=0}^{\infty}(e^{2irk_n^+}+e^{2irk_n^-}). \tag{10}$$

This form guarantees that $J$ is real because $k_n^+$'s and $k_n^-$'s are symmetric about the imaginary axis. It is an exact result for arbitrary $T$ and $r$. Analytical summation is not possible because of complicated form of $k_n^+$'s and $k_n^-$'s, but the numerical evaluation of the above equation can be done in a straightforward manner. The summation converges quite fast especially for large $r$. The resulting free-electron spin susceptibility is an oscillatory decaying function which decays faster at finite temperature than that for $T=0$. The envelopes of $\chi(r)$ for two temperatures are plotted in Fig. 2. Figure 2 shows that the decay of $\chi(r)$ is exponential asymptotically, but it is neither a simple algebraic nor exponential function in the intermediate $r$.

For low enough temperature, the summation can be substituted by integration

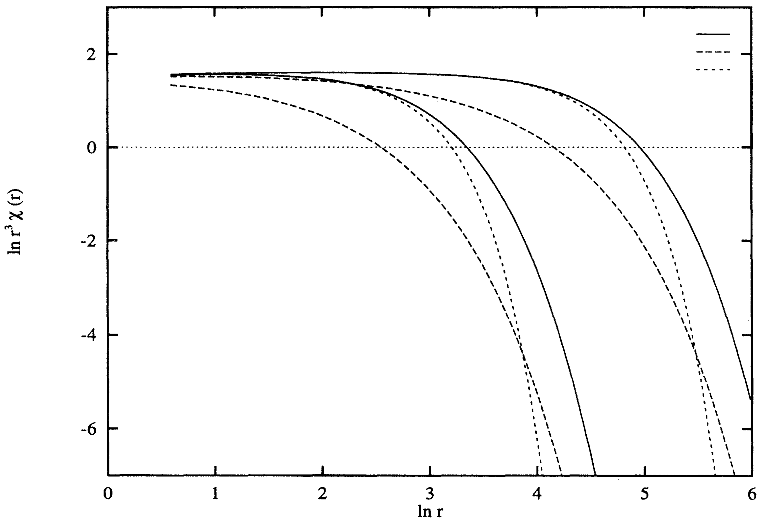


FIG. 2. Envelopes of $\chi(r)$ at two different temperatures, $T'=0.01$ and 0.05. The upper three curves are those for $T'=0.01$ and the lower three curves are those for $T'=0.05$. The dotted line represents Eq. (1), the dashed line represents Eq. (16), and the solid line represents Eq. (10).

$$J=-\frac{2\pi i}{\beta'}\left[\int_0^\infty e^{2irk_n^+}dn^+ + \int_0^\infty e^{2irk_n^-}dn^-\right], \qquad (11)$$

where $n^\pm = \pm(\beta' i/4\pi)(k_F^2-k_n^{\pm 2})-\frac{1}{2}$, or equivalently,

$$J=-\int_{k_0^+}^{k_\infty^+} k_n^+ e^{2irk_n^+}dk_n^+ + \int_{k_0^-}^{k_\infty^-} k_n^- e^{2irk_n^-}dk_n^- . \qquad (12)$$

The integrands in Eq. (12) satisfy the Cauchy-Riemann condition. So the integration is straightforward and the result is

$$J=\left(\frac{k_0^+e^{2irk_0^+}}{2ri}+\frac{e^{2irk_0^+}}{4r^2}\right)-\left(\frac{k_0^-e^{2irk_0^-}}{2ri}+\frac{e^{2irk_0^-}}{4r^2}\right). \qquad (13)$$

Here $k_0^+=k_0e^{i\varphi_0}$ and $k_0^-=k_0e^{i(\pi-\varphi_0)}$ where $k_0=(k_F^4+4\pi^2/\beta'^2)^{1/4}$ and $\tan 2\varphi_0=2\pi/\beta' k_F^2$, or using the normalized temperature $T'=k_BT/\varepsilon_F$,

$$k_0=k_F(1+\pi^2T'^2)^{1/4} \qquad (14)$$

and

$$\tan 2\varphi_0=\pi T'. \qquad (15)$$

By taking the imaginary part of the integral $J$, finally we get

$$\chi(r)=\frac{m\mu_B^2}{(2\pi)^3\hbar^2}\,e^{-2k_0r\sin\varphi_0}\times\left[\frac{\sin(2k_0r\cos\varphi_0)-2k_0r\cos(2k_0r\cos\varphi_0+\varphi_0)}{r^4}\right]. \qquad (16)$$

This equation can be reduced to zero-temperature expression Eq. (5) as $T\rightarrow 0$, since $\lim_{T\rightarrow 0}k_0=k_F$ and $\lim_{T\rightarrow 0}\varphi_0=0$. At finite temperature, both the amplitude and the period change according to temperature. The susceptibility at finite temperature cannot be expressed as a simple product of the temperature-dependent damping factor and zero-temperature susceptibility like $F(T',r)j_1(r)$, but it can be shown that the asymptotic form of the damping factor in the long-range limit can be factored out as an exponential form, which is contrary to Darby's prediction. For $2k_Fr<1$, the integrand in Eq. (4) does not vary rapidly near $\epsilon=\mu$, so the Sommerfeld expansion can be useful for the approximate derivation of the integral. In fact, the Sommerfeld expansion predicts the temperature dependence of the amplitude quite well in the low-temperature region and at short range. However, in the region where the condition $2k_Fr<1$ is not valid, the Sommerfeld expansion method cannot predict the long-range behavior properly, as can be seen in Fig. 2 in which $\ln[r^3\chi(r)]$ obtained from Eqs. (1), (10), and (16) are plotted against $\ln(r)$ for two different temperatures.

The exponential damping factor in the lowest order of temperature is

$$e^{-\pi T' K_F r} \qquad (17)$$

since $k_0\sim k_F(1+\pi^2T'^2/4)$ and $\sin\varphi_0\sim(\pi/2)T'$ at low temperature. Figure 2 shows that the decay of $\chi(r)$ obeys an exponential form in the long-range limit. Kohn and Vosco[8] remarked that if the width of the Fermi distribution function in $k$ space near the Fermi surface is $\Delta k$, the amplitude of the oscillation decays by an extra factor $e^{-\Delta kr}$ for large $r$. The diffuseness of the Fermi surface $\Delta k$ at finite temperature may be defined as $f'(k_F)\Delta k\sim 1$. Since $f'(k_F)=\beta\hbar^2k_F/4m$ in the free-electron gas, $\Delta kr=2T'k_Fr$, which is qualitatively consistent with the exponent in Eq. (16). The exponential decay in the long-range limit was also found in the one-dimensional case numerically.[9]

The wave number depends on temperature to the second order as $k_0\cos\varphi_0\sim k_F[1+(\pi^2/8)T'^2]$. The magnitude of the temperature-dependent variation of the wave number is the same order of magnitude as that of the difference between the chemical potential and the Fermi energy. If the chemical potential is used for the Fermi distribution function instead of the Fermi energy, $k_F$ in Eq. (14) should be replaced by $k_F[1-\frac{1}{6}(\pi/2)^2T'^2]$. Then the wave number in the second order becomes

$$k_0\sim k_F[1-(\pi^2/12)T'^2]. \qquad (18)$$

This variation of period with respect to temperature is only order of 0.01 percent even at room temperature.

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