One-dimensional free-electron spin susceptibility at finite temperature

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The analytical expression of the free-electron spin susceptibilities $\chi(q)$ and $\chi(r)$ in one dimension are derived at finite temperature, where the Sommerfeld expansion is not applicable near $q=2k_F$, by a series expansion method which does not require the restriction of the Sommerfeld method. The main results are (i) the oscillation of the range function decays exponentially as $\exp(-\pi k_F r k_B T/\varepsilon_F)$ in the long-range limit and (ii) the logarithmic divergence of $\chi(q)$ at $q=2k_F$ near $T=0$ is in the form of $[N(0)\mu_B^2/2]\ln(4\varepsilon_F/\pi k_B T)$. [S0163-1829(96)05133-8]

In the long-range limit, the free-electron spin susceptibility $\chi(r)$, which represents the spin polarization due to a point interaction, shows an oscillatory decaying behavior. It is well known that its envelope falls off as $1/r^d$ at zero temperature in the long range limit in the d-dimensional free-electron gas model.[1] The long-range behavior of the free-electron susceptibility is important in determining several physical properties. The Ruderman-Kittel-Kasuya-Yosida[2] (RKKY) interaction of which the coupling constant is proportional to the itinerant spin susceptibility $\chi(r)$ in the linear response assumption is one example. The pure one-dimensional RKKY interaction has the potential to produce the phase transition to spin ordering because phase transition can take place at finite temperature even in one dimension if the interaction falls off not faster than $1/r$.[2,3]

At nonzero temperature, however, the long-range oscillation of the free-electron spin polarization and thereby the RKKY interaction between local spins are damped as the Fermi surface becomes blurred with increasing temperature. Our study in three dimensions[4,5] showed that $\chi(r)$ decay is proportional to the exponential form, $e^{-\pi k_F r T'}$, in low temperature where $T'=k_BT/\varepsilon_F$. Another factor which makes the algebraically decaying long-range oscillation exponentially damped is the effect of finite electron mean free path. It was shown that the RKKY interaction is exponentially damped due to the effect of the finite electron mean free path in a randomly disordered system.[6] The temperature dependent decay length becomes comparable with the electron mean free path at high temperature.[7,8]

Traditionally, the temperature dependent behavior of the Fermi gas has been studied by use of the Sommerfeld expansion method. The Sommerfeld expansion is applicable to the derivation of $\int f(\varepsilon)h(\varepsilon)d\varepsilon$, or $\int f(k)h(k)dk$ where f is the Fermi distribution function and h is nonsingular and not too rapidly varying in the neighborhood of $\varepsilon=\mu$. But, this kind of approach is not applicable for the derivation of temperature dependent $\chi(q)$, since, in this case, $h(k)$ becomes singular at $k=\pm q/2$. As an alternative, we can approximate $f(\varepsilon)$ to a simple form instead of $h(\varepsilon)$ if $h(\varepsilon)$ is rapidly varying near Fermi surface.[9] In this approach, any type of approximations of $f'(\varepsilon)$ having finite numbers of nondifferentiable points show a beat structure in the envelope of $\chi(r)$ because of the characteristic wave numbers corresponding to these nondifferentiable points. The lowest order of approximation which is differentiable and analytically solvable $f'(\varepsilon)$ would be a cubic approximation. This form produces a monotonically decaying envelope, but its decaying behavior is different from the true one. It is worthwhile to note that higher order approximations do not necessarily give better results as far as the approximate functions are made to depend on only one parameter corresponding to temperature by the normalization and differentiability conditions.

The analytical method we proposed in the previous work[5] neither approximates $h(x)$ as the Sommerfeld method does nor approximates Fermi distribution $f(x)$ in the derivation of $\int f(x)h(x)dx$. Our method does not require the restriction of the Sommerfeld method. The general formalism gives the temperature-dependent susceptibility which can be improved systematically by considering higher order terms successively by using Euler-Maclaurin series. This series gives the result identical to the one obtained by the Sommerfeld method in the low temperature limit when expanded with respect to the powers of temperature, though its precision is not sensitively dependent on temperature because basically this series is not an expansion in terms of the powers of temperature. In this work, we apply this method to the calculation of $\chi(q)$ and $\chi(r)$ in one dimension at finite temperature. The resulting analytical low temperature expression shows that the amplitude decay of $\chi(r)$ in one dimension, which is algebraic at zero temperature, becomes exponential in the long-range limit as a function of both temperature and distance.

A physical quantity of the Fermi gas written as[5]

$$A(x,T)=\int_{-\infty}^{\infty} f(k,T)h(k,x)dk, \tag{1}$$

where $f(k,T)$ represents the Fermi distribution function emphasizing its temperature dependence explictly, can be calculated using the contour integral along the infinite semicircle in the upper half complex plane. As far as the increase of $h(k,x)$ is slower than exponential with respect to k, i.e., $\lim_{\epsilon\to 0}\lim_{|k|\to\infty}|e^{i\varepsilon k}h(k,x)/k|\to 0$, the result becomes

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$$A(x,T)=2\pi i\sum Res[f(k,T)h(k,x)]_{k*}+\int_{k_0^-}^{k_0^+}h(k,x)dk-\frac{i\pi T'k_F^2}{2}\left[\frac{h(k_0^+,x)}{k_0^+}+\frac{h(k_0^-,x)}{k_0^-}\right]$$
$$+i\pi T'k_F^2\sum_{j=1}^{\infty}\frac{B_{2j}}{(2j)!}\left[\frac{d^{(2j-1)}}{dn^{(2j-1)}}\left(\frac{h(k_n^+,x)}{k_n^+}+\frac{h(k_n^-,x)}{k_n^-}\right)\right]_{n=0}, \tag{2}$$

where

$$k_n^+=\eta_n e^{i\varphi_n}, \quad k_n^-=\eta_n e^{i(\pi-\varphi_n)}, \tag{3}$$

are the poles of the Fermi distribution function $f(k,T)=1/[1+\exp((\hbar^2/2mk_BT)(k^2-k_F^2))]$ in the upper half plane and k^*'s are the poles of $h(k,x)$. Here, B_{2j}'s are the Bernoulli numbers and

$$\eta_n=k_F(1+(\pi T_n')^2)^{1/4},$$
$$\varphi_n=\frac{1}{2}\arctan\pi T_n',$$
$$T_n'=(2n+1)k_BT/\varepsilon_F, \tag{4}$$

where n is an integer. The detailed description of this derivation can be found in Ref. 5. In this calculation, the chemical potential at finite temperature was approximated to the Fermi energy for the simplicity of calculation. This approximation affects the period of the oscillation only, and this period change is only order of 0.01% even at room temperature.[5]

In the linear response assumption, the free-electron susceptibility $\chi(q)$ for one dimension can be written

$$\chi(q)=\frac{4mL\mu_B^2}{\pi\hbar^2}\int_{-\infty}^{\infty}f(k)h(k)dk, \tag{5}$$

where $h(k)=1/q^2-4k^2$. In the above equation, $h(k,q)$ is algebraic and the residues from $k=\pm q/2$ cancel each other since $f(k)$ is an even function with respect to k. Using the general formula equation (2) it is straightforward to show that the result up to the second order, which includes $j=1$ term in the Eq. (2), is

$$\chi(q)=\frac{mL\mu_B^2}{\pi\hbar^2}\left[\frac{1}{q}\ln\frac{(q+2\eta_0\cos\varphi_0)^2+(2\eta_0\sin\varphi_0)^2}{(q-2\eta_0\cos\varphi_0)^2+(2\eta_0\sin\varphi_0)^2}-\frac{\pi T'k_F^2}{\eta_0\eta_q^2}\sin(\varphi_0-2\varphi_q)+\frac{1}{24}\frac{(\pi T'k_F^2)^2}{\eta_0^3\eta_q^4}(q^2\cos(3\varphi_0-4\varphi_q)\right.$$
$$\left.-12\eta_0^2\cos(\varphi_0-4\varphi_q))\right], \tag{6}$$

where $\eta_0=k_F(1+(\pi T')^2)^{1/4}$, $\varphi_0=1/2\arctan\pi T'$ and η_q and φ_q are defined respectively as

$$\eta_q=k_F\left|\left(1-\frac{q^2}{4k_F^2}\right)^2+(\pi T')^2\right|^{1/4}$$
$$\varphi_q=\varphi_q^* \quad (q^2>4k_F^2),$$
$$\frac{\pi}{2}-\varphi_q^* \quad (q^2<4k_F^2), \tag{7}$$

φ_q^* being $1/2\arctan(\pi T'/|1-q^2/4k_F^2|)$. At zero temperature, the second and third terms become zero and the first term reduces to the well known form,

$$\chi(q)=\frac{2mL\mu_B^2}{\pi\hbar^2 q}\ln\left|\frac{q+2k_F}{q-2k_F}\right|. \tag{8}$$

At finite temperature, Rice and Strässler showed that $\chi(2k_F)$ diverges with temperature logarithmically near $T\sim 0$ as $[N(0)\mu_B^2/2]\ln(1.14\varepsilon_B/k_BT)$ in one dimension,[10] where $N(0)$ is the density of states at the Fermi surface. This expression was obtained on the assumption that the energy near Fermi surface is linear as $\varepsilon_k=\varepsilon_F+(|k|-k_F)\hbar^2k_F/m$ for $|\varepsilon_k-\varepsilon_F|<\varepsilon_B$. This logarithmic divergence at $q=2k_F$ near $T\sim 0$ appears naturally from the first term of Eq. (6) without any assumptions. From Eq. (6), it is shown that in the low temperature limit, it becomes $[N(0)\mu_B^2/2]\ln(4\varepsilon_F/\pi k_BT)$.

The range function $\chi(r)$ is given by the Fourier transform of $\chi(q)$[11]

$$\chi(r)=\frac{1}{2\pi}\int dq e^{iqr}\chi(q)$$
$$=\frac{2mL{\mu_B}^2}{\pi^2\hbar^2}\int_{-\infty}^{\infty}dq e^{iqr}\int_{-\infty}^{\infty}dk\frac{f(k)}{q^2-4k^2}. \tag{9}$$

Since

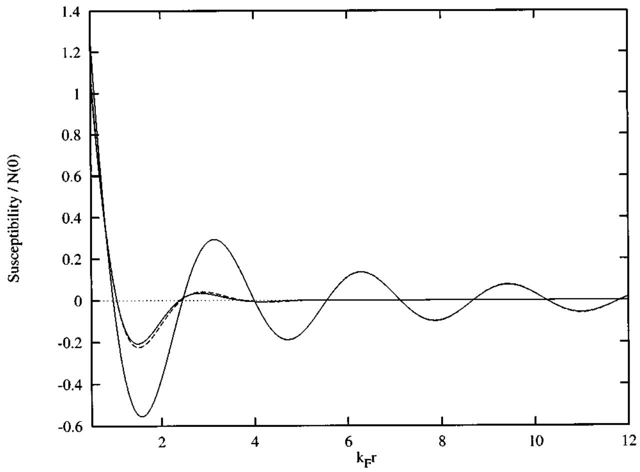

FIG. 1. The $\chi(r)$ for $T'=0.05$ and 0.5. The solid lines represent the exact results obtained numerically from (11) and the dashed ones represent Eq. (12). Notice that, for $T'=0.05$, the solid and dashed line coincide with each other.

$$\int_{-\infty}^{\infty} dk \frac{f(k)}{q^2-4k^2} = -i\pi T' k_F^2 \sum_{m=0}^{\infty} \left(\frac{1}{k_m^+(q^2-4k_m^{+2})} + \frac{1}{k_m^-(q^2-4k_m^{-2})} \right), \tag{10}$$

if we apply Euler-Maclaurin formula to Eq. (10) and calculate up to $j=1$, Eq. (6) is obtained. Direct Fourier transform of Eq. (6) can be done as shown in the next paragraph. However, a more convenient way to obtain $\chi(r)$ is to take Fourier transform term by term first, then the following form of $\chi(r)$ is obtained:

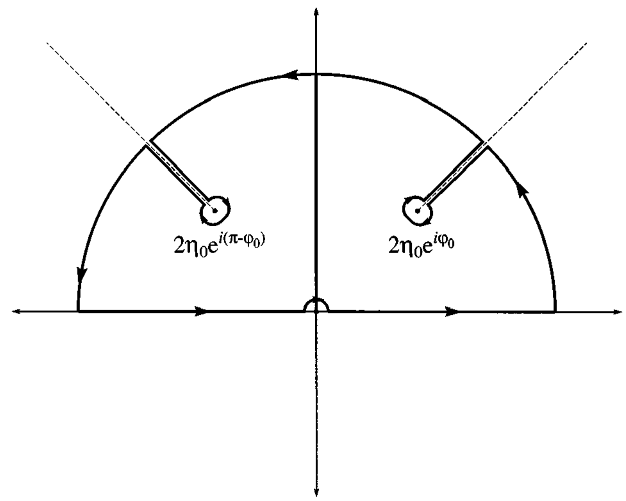

FIG. 2. The contour for the integral in Eq. (13) in the complex plane.

$$\chi(r) = \frac{mL\mu_B^2 T' k_F^2}{\hbar^2} \sum_{m=0}^{\infty} \left(\frac{e^{2ik_m^+ r}}{k_m^{+2}} + \frac{e^{2ik_m^- r}}{k_m^{-2}} \right). \tag{11}$$

Applying Euler-Maclaurin formula at this stage and calculating up to $j=1$, $\chi(r)$ becomes

$$\chi(r) = \frac{m\mu_B^2 L}{\pi\hbar^2} \left[2\int_{2\eta_0}^{\infty} \frac{e^{-kr\sin\varphi_0}}{k} \sin(kr\cos\varphi_0)dk + \frac{\pi T' k_F^2}{\eta_0^2} e^{-2\eta_0 r\sin\varphi_0} \cos(2\eta_0 r\cos\varphi_0 - 2\varphi_0) + \frac{(\pi T' k_F^2)^2}{3\eta_0^4} e^{-2\eta_0 r\sin\varphi_0} (\eta_0 r\cos(2\eta_0 r\cos\varphi_0 - 3\varphi_0) - \sin(2\eta_0 r\cos\varphi_0 - 4\varphi_0)) \right]. \tag{12}$$

The exact $\chi(r)$'s are obtained numerically from Eq. (11) by directly summing up until $|e^{2irk_m^{\pm}}/(k_m^{\pm}/k_F)^2|$ becomes less than 10^{-25} and they are compared with analytical ones in Eq. (12) for $T'=0.05$ and 0.5, respectively, in Fig. 1. It shows that analytical form of $\chi(r)$ truncated at $j=1$ is virtually exact in the range of temperature where the quantum effect is dominant.

The Fourier transform of the second order truncated $\chi(q)$ in Eq. (6) results in $\chi(r)$ of Eq. (12) also. The Fourier transform of the zeroth order term of $\chi(q)$ [the first term of Eq. (6)] is written as

$$\chi^{(0)}(r) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \chi^{(0)}(q) e^{iqr} dq = \frac{mL\mu_B^2}{2\pi^2\hbar^2} \int_{-\infty}^{\infty} \frac{1}{q} \ln \frac{(q-2\eta_0 e^{i(\pi+\varphi_0)})(q-2\eta_0 e^{i(\pi-\varphi_0)})}{(q-2\eta_0 e^{i\varphi_0})(q-2\eta_0 e^{-i\varphi_0})} e^{iqr} dq. \tag{13}$$

The integrand in Eq. (13) has four singular points $\sigma_i (i=1,2,3,4)$ which are $2\eta_0 e^{i\varphi_0}$, $2\eta_0 e^{i(\pi-\varphi_0)}$, and their complex conjugate. Each conjugate pair approaches $2k_F$ and $-2k_F$, respectively, as T goes to zero. Defining a contour as shown in Fig. 2, $\chi^{(0)}(r)$ becomes the same as the first line in Eq. (12). The calculation was based on the fact that (1) the contribution from the infinite semicircle vanishes, (2) the contribution from two branch cuts is $4\pi\int_{2\eta_0}^{\infty} dk e^{-kr\sin\varphi_0} \sin(kr\cos\varphi_0)/k$, and (3) the contribution from the infinitesimal semicircle at origin is zero. The calculation of $\chi^{(1)}(r)$ is straightforword and also give the same result as the second line in Eq. (12). The Fourier transform of $\chi^{(2)}(q)$ has to be done with care, since its singular points turn out to be second order. The result is again the same with the third line in Eq. (12) which is obtained by the direct application of the general formula to $\chi(r)$.

Finally we point out that if, in Eq. (9), the order of integration is changed and integration over q is done first as was shown in Kittel *et al.*,[1] $\chi(r)$ becomes

$$\frac{mL\mu_B^2 T' k_F^2}{\hbar^2}\sum\left(\frac{e^{2ik_m^+ r}}{k_m^{+2}}+\frac{e^{2ik_m^- r}}{k_m^{-2}}\right)-\frac{mL\mu_B^2}{\hbar^2}f(0). \quad (14)$$

It differs with the correct one by $-(mL\mu_B^2/\hbar^2)f(0)$ [see Eq. (11)]. It can be easily shown that at $T=0$, Eq. (14) is reduced to $(2mL\mu_B^2/\pi\hbar^2)[\int_{2k_F}^{\infty}\sin(kr)/kdk-(\pi/2)]$. Therefore, the difference from the interchange of order of integration becomes $-(\pi/2)$ as shown in Yafet *et al.*[13] This difference is originated from the contribution of the pole at $k=0$ which would not have been counted in the proper order of integration.

The susceptibility at finite temperature cannot be expressed as a simple product of temperature dependent damping factor and zero temperature susceptibility like $F(T,r)\chi(T=0,r)$, but in the low temperature limit, an exponential form of damping factor can be factored out in the first term of Eq. (12) as follows:

$$-e^{-2\eta_0 r\sin\varphi_0}\left[\frac{\sin(2\eta_0 r\cos\varphi_0)}{2\eta_0 r\sin\varphi_0}+\frac{2\eta_0 r\cos\varphi_0\cos(2\eta_0 r\cos\varphi_0)-\sin(2\eta_0 r\cos\varphi_0)}{(2\eta_0 r\sin\varphi_0)^2}+\cdots\right]. \quad (15)$$

Then all the terms in the series expansion have the common exponential damping factor $\exp(-2\eta_0 r\sin\varphi_0)$ which becomes $e^{-\pi k_F r T'}$ in the low temperature limit. The damping factor is the same as the one in three dimensions. Kohn and Vosco[12] remarked that if the width of the Fermi distribution function in k space near the Fermi surface is Δk, the amplitude of the oscillation decays by an extra factor $e^{-\Delta kr}$ for large r. The diffuseness of the Fermi surface Δk at finite temperature may be defined as $f'(k_F)\Delta k\sim 1$. Since $f'(k_F)=\beta\hbar^2 k_F/4m$ in the free-electron gas, $\Delta kr=2T'k_F r$, which is qualitatively consistent with the exponent in our derivation. The faster decay of range function at finite temperature implies that the number of electrons gathering to screen a perturbation decreases with increasing temperature. The exponentially decaying factor in the coupling constant of the RKKY interaction suppresses the ferromagnetic or antiferromagnetic phase transition in one dimension at finite temperature.

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