Temperature-dependent RKKY interaction in one dimension

1994 J. Phys.: Condens. Matter 6 1037

(http://iopscience.iop.org/0953-8984/6/5/013)

J. Phys.: Condens. Matter 6 (1994) 1037–1046. Printed in the UK

Temperature-dependent RKKY interaction in one dimension

Eun Kyung Lee†, Eok Kyun Lee† and Soonchil Lee‡

† Department of Chemistry, Korea Advanced Institute of Science and Technology, 373-1 Gusongdong, Yusongku, Taejon, Korea

‡ Department of Physics, Korea Advanced Institute of Science and Technology, 373-1 Gusongdong, Yusongku, Taejon, Korea

Received 20 September 1993

Abstract. The temperature-dependent behaviour of the RKKY interaction in one dimension is investigated for the free electron gas model by both analytical and numerical methods. The present studies show that the range function has the form $\cos(2k_F r)e^{-\alpha(T)r}/r^{\beta(T)}$, where the exponents $\alpha(T)$ and $\beta(T)$ increase and decrease monotonically, respectively, with increasing temperature.

1. Introduction

The RKKY interaction is the indirect interaction between local spins mediated by itinerant electron spins. It is known that this interaction is oscillatory, and its envelope falls off as $1/r^d$ at zero temperature in the long-range limit in the d-dimensional free electron gas model [1–3]. This zero-temperature behaviour implies that the pure one-dimensional RKKY interaction has the potential to produce the phase transition to spin ordering, because a phase transition can take place at a finite temperature even in one dimension if the interaction falls off no more quickly than $1/r^2$ [4]. However, the coupling constant of this interaction is proportional to the itinerant electron susceptibility, which depends in general on temperature. Therefore, the interaction form at zero temperature does not supply enough information on whether a phase transition is possible or not at finite temperature.

The coupling constant J_{ij} of the RKKY interaction in spin Hamiltonian form

$$H = -\sum_{ij} J_{ij} S_i S_j \tag{1}$$

is proportional to the free electron susceptibility as

$$J_{ij} = \frac{V}{2}\left(\frac{J}{N\mu_B}\right)^2 \chi(r_{ij}) \tag{2}$$

where $\chi(r_{ij})$ is the free electron susceptibility. The indices i and j denote local spins, and J represents the exchange interaction between local spins and itinerant electron spins. The susceptibility $\chi(r)$ is obtained by the Fourier transform of the susceptibility in momentum space:

$$\chi(q) = \mu_B^2 \sum_k \frac{f_k - f_{k+q}}{\varepsilon_{k+q} - \varepsilon_k} = \mu_B^2 F(q) \tag{3}$$

0953-8984/94/051037+10$07.50

where f_k and ε_k are the Fermi distribution function and free electron energy at wavevector k, respectively.

In one dimension, $\chi(q)$ diverges at $q = \pm 2k_F$ at zero temperature. The susceptibility $\chi(r)$, which decays as $\cos(2k_F r)/r$ in the long-range limit, reflects this divergence in its period [1]. As temperature increases from zero this divergence disappears, which has been already noticed by Rice and Strässler [5, 6]. Their study has shown that $\chi(2k_F)$ diverges logarithmically with temperature. For the case $d = 3$, Darby has shown that, by use of a first-order perturbation method, the asymptotic form of the susceptibility is

$$\chi(r) = \frac{m\mu_B^2}{2\pi^3\hbar^2}\frac{1}{r^4}\left[\sin(2k_F r) - 2k_F r\cos(2k_F r)\right]\exp[-(\pi^2/6\eta^2)(k_F r)^2] \qquad (4)$$

in the low-temperature limit [7]. However, the method which he used cannot be generalized to the one-dimensional case. A direct application of his method with the one-dimensional free electron Green function, which has the form $(i/2k)e^{ikx}$, would lead to the same erroneous result which was derived in [3] for the case $T = 0$. This was first pointed out Nagamiya; more recently, a rigorous derivation was given by Yafet [1]. In the present study we choose the case of one itinerant electron per site, where the ground-state energy per spin is lowest and therefore the highest transition temperature is expected, if any exists.

In section 2 we discuss the analytic derivation of the temperature-dependent behaviour of the RKKY interaction by the use of a low-temperature expansion technique. As the lowest order of approximation, the derivative of the Fermi distribution function is approximated by the rectangular and triangular form for finite temperature. The range function in these cases shows an oscillatory decaying beat form, which is somewhat unrealistic. Cubic and quintic polynomial functions were utilized as the next stage of approximation, which leads to a qualitatively correct behaviour of $\chi(r)$. In section 3, the range functions evaluated by a numerical method are compared with those of the analytical method. The result shows that the RKKY interaction decays exponentially rather than algebraically at finite temperature, which manifests itself in the fact that the interaction has a short-range character at non-zero temperature.

2. Analytical approach

In one dimension, $F(q)$ defined in (3) can be rewritten as

$$F(q) = \frac{mL}{\pi\hbar^2 q}\int_{-\infty}^{\infty} dk f(k)\left(\frac{1}{2k+q} - \frac{1}{2k-q}\right) = \frac{mL}{2\pi\hbar^2 q}\int_{-\infty}^{\infty} dk\left(-\frac{\partial f(k)}{\partial k}\right)\ln\left|\frac{2k+q}{2k-q}\right| \qquad (5)$$

where the independent electron gas model was assumed. Since the integrand of equation (5) is singular at $q = \pm 2k$, a Sommerfeld type of expansion cannot reflect the correct behaviour of $F(q)$ near $q = \pm 2k_F$, and accordingly the long-range behaviour of the susceptibility $\chi(r)$ in one dimension, since it is heavily dependent on the form of $\chi(q)$ near $q = \pm 2k_F$. In this work, the low temperature expansion of $f'(\varepsilon)$ was used instead of the Sommerfeld method; $F(q)$ can then be obtained analytically for the following approximations of $f'(\varepsilon)$.

The simplest approximation of $f'(\varepsilon)$ will be the normalized rectangular function, which is defined as

$$f_r'(\varepsilon) = \begin{cases} -1/2\delta & \varepsilon_F - \delta < \varepsilon < \varepsilon_F + \delta \\ 0 & \text{otherwise.} \end{cases} \qquad (6)$$

The parameter δ is a measure of temperature because $f'(\varepsilon_F)$ is inversely proportional to temperature, i.e. $f'(\varepsilon_F) = 1/4k_BT$. In this approximation, $F(q)$ is derived to be

$$F(q) = \frac{L}{4\pi\delta}[-G_r(k_1, q) + G_r(k_2, q)] \tag{7}$$

where

$$G_r(k, q) = k + \frac{4k^2 - q^2}{4q} \ln\left|\frac{q + 2k}{q - 2k}\right| \tag{8}$$

and

$$k_{1,2} = \left(k_F^2 \mp \frac{2m\delta}{\hbar^2}\right)^{1/2}. \tag{9}$$

In the above calculation the chemical potential at finite temperature was approximated to the Fermi energy. This substitution does not affect the result, except for the fact that the characteristic wavenumbers remain unchanged with temperature. If the chemical potential were used instead of the Fermi energy, the oscillation wavelength of the range function increases slowly with increasing temperature and therefore the coupling constant of the RKKY interaction is expected to show a beat form though its envelope remains same.

The range function, which is proportional to $\chi(r)$, is defined as the Fourier transform of $F(q)$:

$$\varphi_r(r) = \int_{-\infty}^{\infty} dq e^{iqr} F(q) = \frac{L}{4\pi\delta} \int_{-\infty}^{\infty} dq e^{iqr}[-G_r(k_1, q) + G_r(k_2, q)]. \tag{10}$$

The integral

$$\int_{-\infty}^{\infty} dq e^{iqr} G_r(k, q) = \int_{-\infty}^{\infty} dq e^{iqr}\left(k + \frac{4k^2 - q^2}{4q} \ln\left|\frac{q + 2k}{q - 2k}\right|\right) \tag{11}$$

can be rewritten in the following form:

$$\int_{-\infty}^{\infty} dq e^{iqr}\left[k + \frac{4k^2 - q^2}{4q} \ln\left(\frac{q + 2k}{q - 2k}\right)\right] - \pi i \int_{-2k}^{2k} dq e^{iqr} \frac{4k^2 - q^2}{4q}. \tag{12}$$

Consider the first integral on the right-hand side for complex q along the closed contour, as depicted in figure 1. The path of integration from $q = -2k$ to $q = 2k$ goes infinitesimally above a cut along the real axis. The contribution of the infinite semicircle is then zero by Jordan's lemma, because the integrand goes to zero in the limit $|q| \to \infty$. Contributions from infinitesimal semicircles α and γ are also zero because $\lim_{\varepsilon \to 0} \varepsilon \ln \varepsilon = 0$; however, the contribution from β is $-k^2\pi^2$. The second part of the right-hand side of (12) becomes

$$-\frac{\pi}{2}\left(\frac{\sin 2kr}{r^2} - \frac{2k \cos 2kr}{r}\right) + \pi k^2 \int_{-2k}^{2k} dq \frac{\sin qr}{q} \tag{13}$$

by use of the Cauchy principal value theorem. Consequently, the range function in the rectangular approximation is

$$\varphi_r(r) = \frac{L}{4\pi\delta}\left[k_1^2\pi^2 + \frac{\pi}{2}\left(\frac{\sin 2k_1 r}{r^2} - \frac{2k_1 \cos 2k_1 r}{r}\right) - \pi k_1^2 \int_{-2k_1}^{2k_1} dq \frac{\sin qr}{q} - k_2^2\pi^2 \right.$$
$$\left. - \frac{\pi}{2}\left(\frac{\sin 2k_2 r}{r^2} - \frac{2k_2 \cos 2k_2 r}{r}\right) + \pi k_2^2 \int_{-2k_2}^{2k_2} dq \frac{\sin qr}{q}\right]. \tag{14}$$

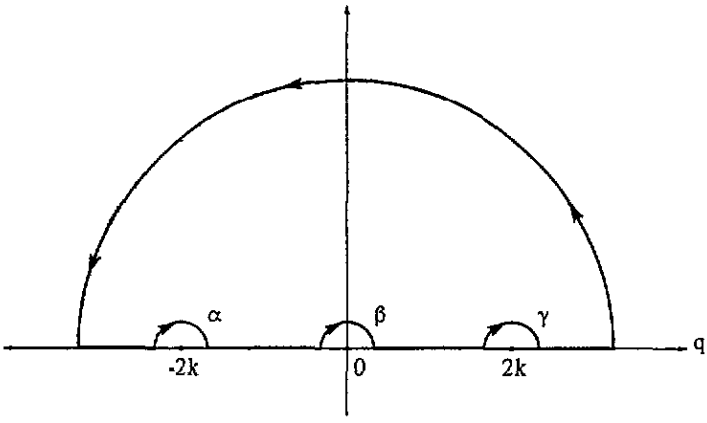

Figure 1. The path of integration in (1).

A straightforward, but somewhat tedious, calculation shows that the range function in the above equation reduces to the correct zero-temperature form as δ goes to zero:

$$\lim_{\delta \to 0} \varphi_r(r) = -\frac{mL}{2\hbar^2} \frac{\cos 2k_F r}{k_F r}. \tag{15}$$

At finite temperature, Rice and Strässler showed that $F(2k_F)$ can be approximated as $\frac{1}{2}N(0)\ln(1.14\varepsilon_B/k_B T)$ [5], where $N(0)$ is the density of states at the Fermi surface. This expression was obtained on the assumption that the energy near the Fermi surface is linear as $\varepsilon_k = \varepsilon_F + \hbar(|k| - k_F)\hbar k_F/m$ for $|\varepsilon_k - \varepsilon_F| < \varepsilon_B$. On the other hand, our rectangular approximation of $f'(\varepsilon)$ leads to $\frac{1}{2}N(0)[1 + \ln(2\varepsilon_F/k_B T)]$, using the fact that δ approaches $2k_B T$ for $\delta \ll 1$. Both of the expressions show that $F(2k_F)$ diverges logarithmically in the low-temperature limit. At a finite temperature the range function $\varphi_r(r)$ is an oscillatory decaying beat form for $k_F r \gg 1$ since there are two characteristic wavenumbers, k_1 and k_2. This unrealistic property implies that the rectangular approximation is too crude to reflect the correct long-range behaviour of the range function even in a qualitative sense.

The second approximation, named the triangular approximation, is expressed as

$$f_t'(\varepsilon) = \begin{cases} -(\varepsilon - \varepsilon_F + \delta)/\delta^2 & \varepsilon_F - \delta < \varepsilon < \varepsilon_F \\ (\varepsilon - \varepsilon_F - \delta)/\delta^2 & \varepsilon_F < \varepsilon < \varepsilon_F + \delta \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

Then $F(q)$ for the one-dimensional free electron gas model becomes

$$F(q) = -\frac{\hbar^2 L}{2\pi m q \delta^2}[G_t(k_1, q) + G_t(k_2, q) - 2G_t(k_F, q)] \tag{17}$$

where

$$G_t(k, q) = \tfrac{1}{16}q^3 k - \tfrac{5}{12}qk^3 - \tfrac{1}{4}(k^2 - \tfrac{1}{4}q^2)^2 \ln\left|\frac{q + 2k}{q - 2k}\right|. \tag{18}$$

The range function can be derived by a similar method used for the rectangular case once the terms are grouped properly to be Fourier transformed. Omitting the detailed calculation, the range function is

$$\varphi_t(r) = -\frac{\hbar^2 L}{2\pi m \delta^2}[\phi(k_1, r) + \phi(k_2, r) - 2\phi(k_F, r)] \tag{19}$$

where

$$\phi(k,r) = \frac{\pi^2 k^4}{4} - \frac{\pi^2 k^4}{4}\int_{-2k}^{2k} \mathrm{d}q \frac{\sin qr}{q} \tag{20}$$

$$-\frac{\pi}{4}\left(\frac{k^2}{2r^2} - \frac{3}{4r^4}\right)\sin 2kr - \frac{\pi}{4}\left(\frac{k^3}{r} + \frac{3k}{2r^3}\right)\cos 2kr. \tag{21}$$

The range function $\varphi_t(r)$ in the triangular approximation is also an oscillatory decaying beat form, because of three characteristic wavenumbers k_1, k_2 and k_F. These unrealistic beat forms in the rectangular and triangular approximations originate from the discontinuities of $f_r'(\varepsilon)$ and $f_t'(\varepsilon)$.

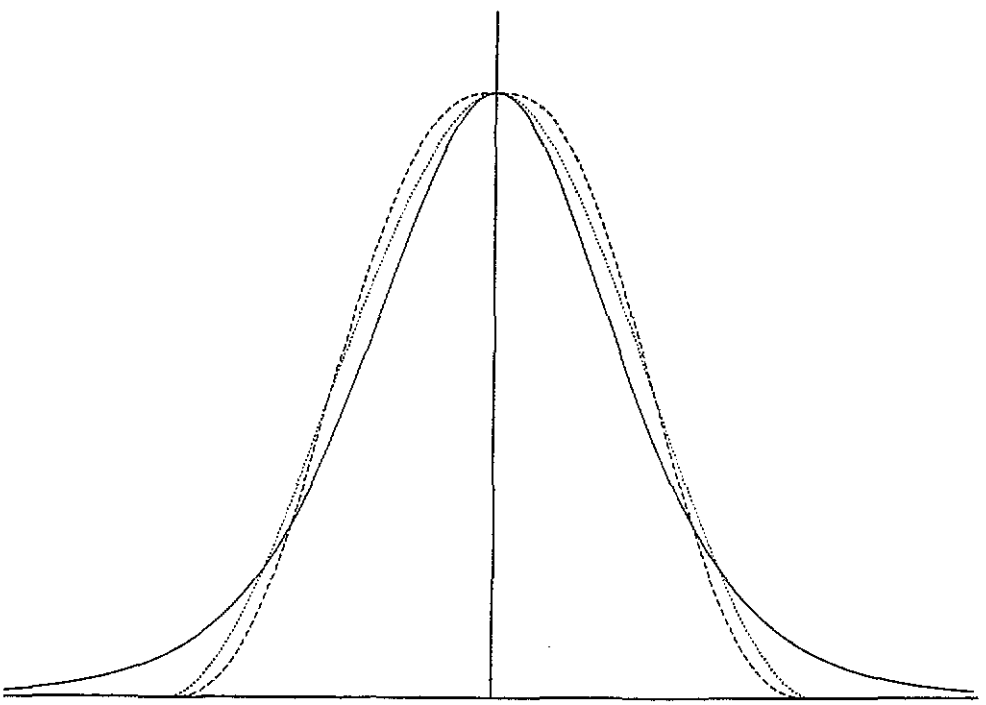

Figure 2. The cubic and quintic approximations compared with the real $f'(\varepsilon)$. The full curve represents $f'(\varepsilon)$, and the dotted and broken curves represent the cubic and quintic approximations, respectively.

The lowest-order differentiable approximation is the cubic approximation (figure 2), defined as

$$f_c'(\varepsilon) = \begin{cases} (\varepsilon - \varepsilon_F + \delta)^2[2(\varepsilon - \varepsilon_F) - \delta]/\delta^4 & \varepsilon_F - \delta < \varepsilon < \varepsilon_F \\ -(\varepsilon - \varepsilon_F - \delta)^2[2(\varepsilon - \varepsilon_F) + \delta]/\delta^4 & \varepsilon_F < \varepsilon < \varepsilon_F + \delta \\ 0 & \text{otherwise.} \end{cases} \tag{22}$$

The analytical expression of $F(q)$ can also be derived in this approximation. However, $F(q)$ consists of too many terms and it is non-trivial to group these terms so that it can

be Fourier transformed. We therefore adopted numerical methods, rather than spending too much time to get analytical solution. The sample plot of the range functions in this approximation is shown in figure 3 for two different δ. As can be seen in the figure, the envelope of the range function decays monotonically, and no beat form is observed. At $\delta/\varepsilon_F = 10^{-4}$, the range function is very close to the sine integral function, which is expected at zero temperature. The sine integral function $\mathrm{si}(x)$ differs from $\cos x/x$ by only 3% even at $x = 3.0$, and the long-range limit approximation $\cos(2k_F r)/r$ is exact to within 1% error after the first period. The figure shows that the amplitude of the oscillation at $\delta/\varepsilon_F = 0.05$ decays much faster than that at 10^{-4}. It is the general tendency that the amplitude of the oscillation decays faster with increasing δ. Since the range function is proportional to the free electron charge (or spin) density near an external point charge (or magnetic field), this means that free electrons are attracted more loosely to screen the point charge (or magnetic) field at finite temperature.

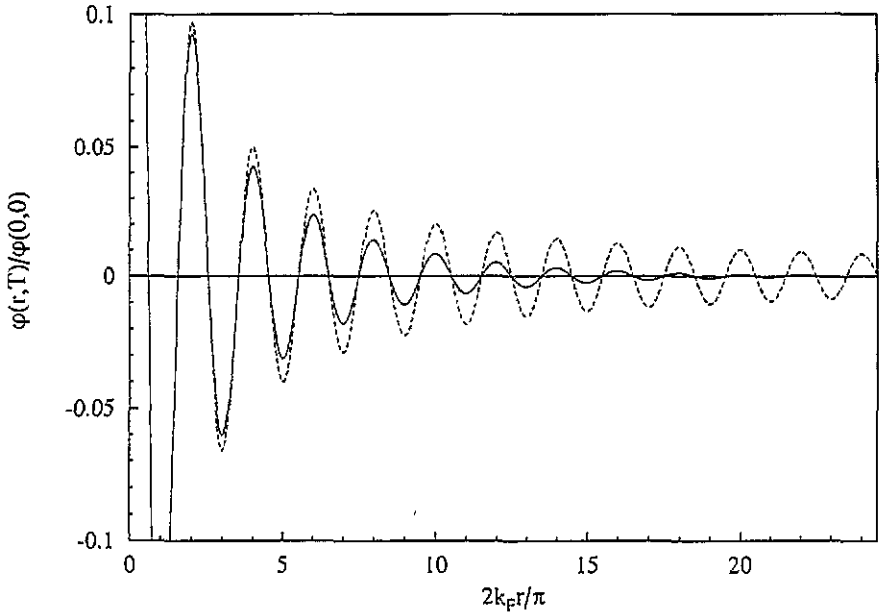

Figure 3. The range functions for $\delta/k_B T = 10^{-4}$ (broken curve) and 0.05 (full curve).

The strongest interaction between local spins occurs when the number of itinerant electrons per site is one, since local spins locate at every local extreme point. In this case, the envelope of the oscillation itself represents the coupling constant of the RKKY interaction. By carefully studying the decay pattern of the envelope as explained in the next section, we found that the envelope includes the exponentially decaying factor at finite temperature. The envelope fits well to the form $e^{-\alpha r}/r^{\beta}$ where the exponents α and β increase and decrease monotonically with increasing δ, respectively.

The approximations, of which the order is higher than cubic, also produce exponentially decaying range functions with no beat symptoms. For example, the envelope of the range function in the quintic approximation (figure 2) defined as

$$f'_q(\varepsilon) = \begin{cases} -(\varepsilon - \varepsilon_F + \delta)^3[6(\varepsilon - \varepsilon_F)^2 - 3\delta(\varepsilon - \varepsilon_F) + \delta^2]/\delta^6 & \varepsilon_F - \delta < \varepsilon < \varepsilon_F \\ (\varepsilon - \varepsilon_F - \delta)^3[6(\varepsilon - \varepsilon_F)^2 + 3\delta(\varepsilon - \varepsilon_F) + \delta^2]/\delta^6 & \varepsilon_F < \varepsilon < \varepsilon_F + \delta \\ 0 & \text{otherwise} \end{cases} \tag{23}$$

fits to the same form even though the temperature dependences of the exponents are slightly different from those of the cubic approximation. It is worth noting that the higher-order approximations of $f'(\varepsilon)$ do not guarantee a more precise result because they do not necessarily resemble $f'(\varepsilon)$ better than the lower ones. In figure 2, for example, we can see that the quintic approximation fits worse than the cubic one to the real $f'(\varepsilon)$. For this reason, we calculated $F(q)$ and the range function $\varphi(r)$ numerically to find the accurate temperature dependence of the exponents.

3. Numerical simulation

For the summation in (3) the IMSL integration routine for the integrand, which has a finite number of non-analytic points, was used. Since $F(q)$ is symmetric with respect to q, the cosine transform routine in IMSL was used to get $\varphi(r)$. The limits of the summation in (3) were set so that the value of $f'(\varepsilon)$ is less than e^{-100} outside the integration range. The interval of the integration was the integration range divided by $128k$. Finer intervals than this did not produce a noticeable change. All the calculations were performed in convex C1 in double precision.

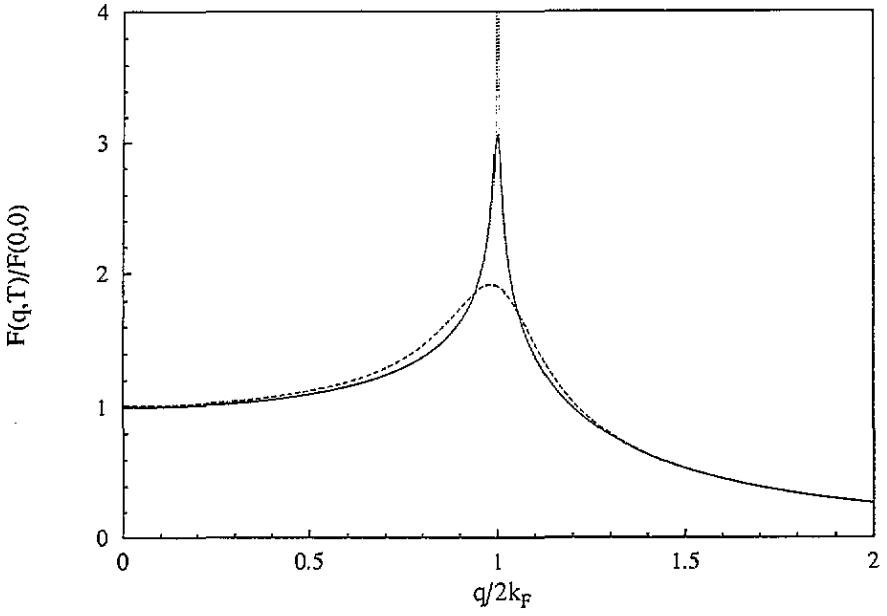

Figure 4. $F(q, T)$ against wavenumber q. $F(q, T)$ is normalized by the value at $q = 0$ and $T = 0$. The broken, full and long-dash broken curves correspond to $T = 10^{-4}$, $T = 0.01$, and $T = 0.1$, respectively, where T is the temperature normalized with respect to the Fermi energy.

Figure 4 shows the sample plot of $F(q)$ for three different temperatures normalized with respect to the Fermi energy. At finite temperature, the divergence of $\chi(q)$ at $q = 2k_F$ disappears, and the peak value decreases with increasing temperature. The range function obtained by Fourier transformation of $F(q)$ shows a monotonically decaying oscillation, similar to the graph in figure 3. The period of the oscillation does not change from the value at zero temperature even at $T = 0.05$, which is well above room temperature in most cases. At this temperature, the result of the numerical simulation did not show any noticeable symptom of period change up to the 50th period.

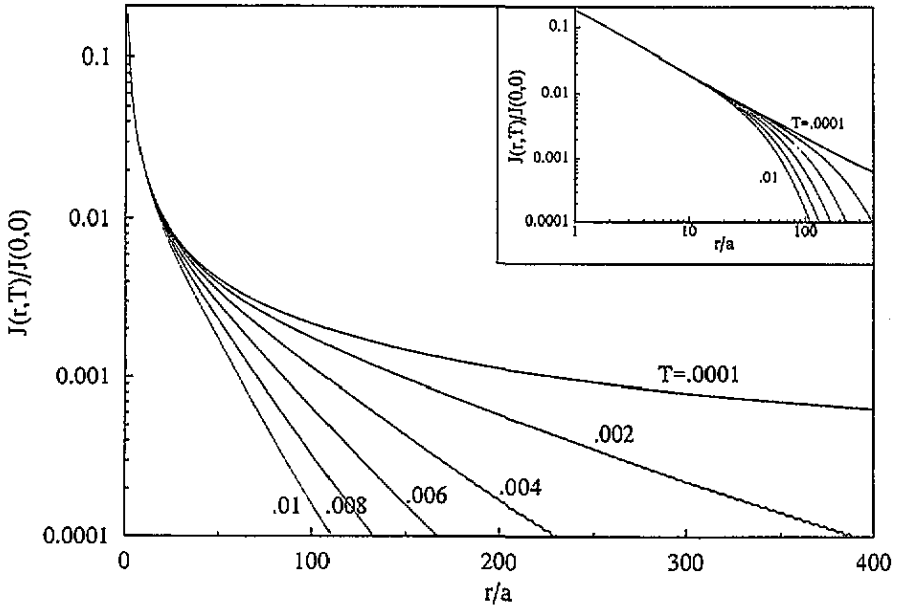

Figure 5. Semilog plot of the range function for the case of an antiferromagnetic ground state. The temperatures are 0.0001, 0.002, 0.004, 0.006, 0.008, 0.01 respectively, from right to left. Inset: log–log plot of the same data.

The inset in figure 5 is a log–log plot of the envelopes of these oscillations in a larger range for various temperatures. The curve at $T = 0.0001$ is very close to a straight line with slope one, i.e. the envelope decays almost as $1/r$, as expected at zero temperature. The envelopes decay faster with increasing temperature. The semilog plot in figure 5 clearly shows that these envelopes include an exponentially decaying factor. We found that these curves fit well not to a form $e^{-\alpha r}/r$, but to $e^{-\alpha r}/r^{\beta}$, where both the exponents α and β have a temperature dependence. Figures 6 and 7 show the temperature-dependent behaviour of exponents α and β obtained by least-squares fitting. The exponent factor α is very close to a straight line of slope 0.03, except at very low temperatures, at least up to $T = 0.015$. The exponent factor $\beta(T)$ decreases quickly at low temperatures; after that its the rate of decrease slows with increasing temperature.

4. Conclusion

The free electron susceptibility $\chi(r)$ has the form $\cos(2k_F r)e^{-\alpha(T)r}/r^{\beta(T)}$ where the exponent

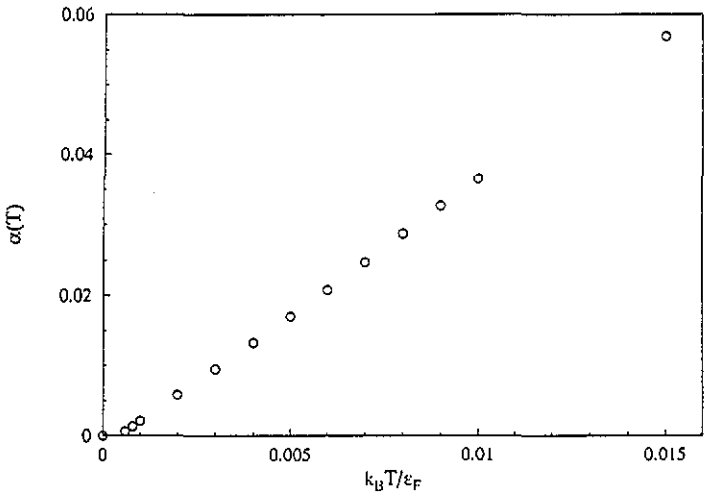

Figure 6. The exponent factor α against temperature.

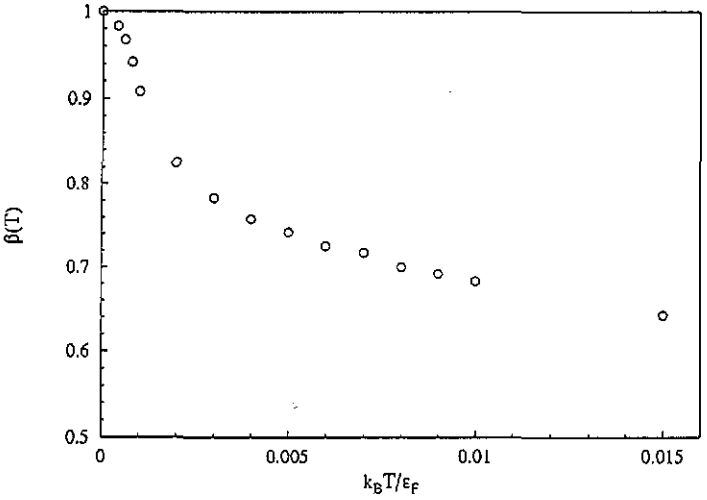

Figure 7. The exponent factor β against temperature.

factors $\alpha(T)$ and $\beta(T)$ monotonically increase and decrease, respectively. The low-temperature approximations of $f'(\varepsilon)$, such as the rectangular and triangular forms which have discontinuous points, are inadequate to analyse the envelope shape of the range function because of its beat form. The higher-order approximations, which are differentiable, produce a qualitatively correct form for $\chi(r)$.

The faster decay of the range function at finite temperature means that the number of electrons gathering to screen the perturbation decreases with increasing temperature. The exponentially decaying factor in the coupling constant of the RKKY interaction implies that the ferromagnetic or antiferromagnetic phase transition due to this interaction is not possible at a finite temperature in one dimension.

It was reported that a phase transition was observed in copper phthalocyanine iodine (Cu(pc)I) [8]. Cu(pc)I is the molecular metal which is a highly one-dimensional system having a dense array of local moments embedded in itinerant electrons of which the number per site is 5/3. The d electron spins localized at the Cu sites interact with each other via the

π electrons conducting along the chain. In Cu(pc)I, the direct dipole–dipole interaction is too weak to invoke the phase transition at the observed temperature 8 K, and therefore this phase transition is believed to be due to the indirect exchange interaction. This situation seems to make it reasonable to use the RKKY interaction as the model Hamiltonian for the description of this indirect interaction in this system. However, our analysis shows that the phase transition observed in Cu(pc)I is not due to a pure one-dimensional RKKY-type indirect interaction, because if the number of itinerant electrons is other than one the indirect interaction becomes weaker, as explained above.

Acknowledgments

The authors acknowledge that this research was supported by Korea Science and Engineering Foundation and one of the authors (Eok Kyun Lee) by the Center for Thermal and Statistical Physics.

References

[1] Yafet Y 1987 *Phys. Rev.* B **36** 3948
[2] Béal-Monod M T 1987 *Phys. Rev.* B **36** 8835
[3] Kittel C 1968 *Solid State Physics* **22** ed F Seitz *et al* (New York: Academic) p 1
[4] Dyson F J 1969 *Commun. Math. Phys.* **12** 91
[5] Rice M J 1975 *Low-dimensional Cooperative Phenomena (Nato Advanced Study Institutes Series 7)* ed H J Keller (New York: Plenum) p 23
[6] Rice M J and Strässler S 1973 *Solid State Commun.* **13** 125
[7] Darby M I 1969 *Am. J. Phys.* **37** 354
[8] Ogawa M Y 1986 *Phys. Rev. Lett.* **57** 1177