Ruderman-Kittel-Kasuya-Yosida range function of a one-dimensional free-electron gas

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The dependence of the calculated Ruderman-Kittel-Kasuya-Yosida range function of a one-dimensional free-electron metal on the order of the integrations over the occupied states, and over the Fourier components of the perturbation is discussed and clarified. The correct result is derived. The range function of a magnetized layer (e.g., a magnetic layer in a multilayer material) is also calculated and compared with the range functions of point sources in the one-dimensional and in the three-dimensional cases.

In connection with recent experiments[1] on ferromagnetic metallic superlattices which, as far as the interaction between layers is concerned, may be viewed as one-dimensional (1D) systems, I was led to consider the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in 1D systems. In a review article[2] Kittel derives the RKKY range function in three-, two-, and one-dimensional free-electron systems. In a subsequent erratum,[2] he states that his derived result is incorrect for the 1D case, due to his having interchanged the order of integrations in momentum space: k and q being, respectively, the wave vector of a state of the Fermi sea and the momentum transfer due to the perturbation, the integrations in Ref. 2 were done first over q and then over k, while the allegedly correct result is obtained by integrating first over k and then over q. There seems to be no discussion in print of the reason for the difference between the two results, or of what determines the correct choice between them, or of the actual calculation of the final answer. It is the purpose of this paper to address these points and clarify the situation in the 1D case. In addition, I will calculate the range function of a single ferromagnetic layer (e.g., of a superlattice) in 3D space. It will be seen that if x is the direction of the normal to the layer, the range function of this pseudo-1D system falls off asymptotically as $\sin(2k_Fx)/x^2$, while for a true 1D system the range function falls off as $\cos(2k_Fx)/x$.

Following Ref. 2, consider the function

$$F(q)=\mathrm{P}\frac{2}{L}\sum_k \frac{n_k-n_{k+q}}{E_{k+q}-E_k} \tag{1}$$

for a 1D free-electron system. Here L is the length of the specimen, the factor 2 includes the summation over spin, and n_k and E_k are, respectively, the occupation factor and energy of state k. If magnetic moments β_0 and β_1 are at positions x_0 and x_1 and they interact with the free-electron spins according to

$$H_{\mathrm{int}}=A\beta_n\sum_i \sigma_i\delta(x_i-x_n) ,$$

where σ_i is twice the spin of electron i and $n=0$ or 1, then the RKKY interaction between β_0 and β_1 is given by

$$H=-A^2\beta_0\beta_1\Phi(x_1-x_0) ,$$

where the range function $\Phi(x)$ is given by the Fourier transform of $F(q)$,

$$\Phi(x)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}F(q)e^{iqx}dq . \tag{2}$$

To evaluate (2) at 0 K one may evaluate (1) and substitute it in (2). The result for (1) is

$$F(q)=\frac{1}{\pi}\frac{2m}{\hbar^2}\int_{-k_F}^{+k_F}\left[\frac{1}{2kq+q^2}-\frac{1}{2kq-q^2}\right]dk \tag{3a}$$

$$=\frac{2m}{\pi\hbar^2}\frac{1}{q}\ln\left|\frac{2k_F+q}{2k_F-q}\right| , \tag{3b}$$

where k_F is the Fermi wave vector. The integration of (2) with $F(q)$ given by (3b) appears complicated. Kittel substituted instead (3a) into (2) and changed the order of integration. Integrating over q first, he obtained

$$\Phi(x)=-\frac{2m}{\pi\hbar^2}\mathrm{Si}(2k_Fx) , \tag{4}$$

where Si is the sine integral function. The correct result quoted in the erratum is obtained by changing $\mathrm{Si}(2k_Fx)$ in (4) into $\mathrm{Si}(2k_Fx)-\pi/2$, thus

$$\Phi(x)=\frac{2m}{\pi\hbar^2}\left[\frac{\pi}{2}-\mathrm{Si}(2k_Fx)\right] . \tag{5}$$

One may ask which feature of the integrand in (3a) is responsible for the dependence of the double integral on the order of integration. One is led to suspect that it is the strong singularity at the point $q=0,k=0$. To verify this, consider the integrand of (3a) and define

$$I_q(\epsilon,\eta)=\int_{-\epsilon}^{+\epsilon}dk\int_{-\eta}^{+\eta}\frac{dq}{q}\left[\frac{1}{q+2k}+\frac{1}{q-2k}\right] , \tag{6}$$

where ϵ and η are two positive numbers. The subscript q on I means that the integration over q is done first. We find at once that

$$I_q=-\int_{-\epsilon}^{+\epsilon}\frac{dk}{k}\ln\left|\frac{k+2\eta}{k-2\eta}\right| ,$$

and integrating over k, we obtain

$$I_q(\epsilon,\eta)=-2[L_2(2\epsilon/\eta)-L_2(-2\epsilon/\eta)] , \tag{7}$$

where L_2 is the dilogarithm function.[3] Similarly, if the

order of integration in (6) is changed, we find

$$I_k(\epsilon,\eta)=2[L_2(\eta/2\epsilon)-L_2(-\eta/2\epsilon)] \ . \tag{8}$$

Subtracting (7) from (8), and making use of relations (4.2) and (4.3) in a paper by Mitchell[4] we find

$$I_k(\epsilon,\eta)-I_q(\epsilon,\eta)=\pi^2 \ , \tag{9}$$

which does show that the singularity at $q=0$ and $k=0$ contributes differently, depending on the order of the integration. It can similarly be seen that the lines of singularities $q=\pm 2k$, $q\neq 0$ give no contribution to the difference so that the whole effect of interchanging the order of integration is given by (9). Comparing (4) and (5) it is seen that the difference is in fact given by (9).

The inference is then that the physically correct way to obtain $\Phi(x)$ is to integrate over k first. The justification for this can be seen by going back to (1) and noticing that, at finite k, but $|k|<k_F$, the Pauli principle rules out any contribution from small q. The order of the integrations must hence be such that if we take $(\eta/\epsilon)\ll 1$, the value of the integral over the singularity must vanish. Since $L_2(x)$ vanishes in the limit $x=0$, it follows that (8) vanishes in this limit, which shows that to obtain the physically correct result one must integrate over k first.

An alternative and direct way to obtain (5) is to make use of an ingenious observation due to Van Vleck:[5] He noticed that in the 3D case the analytic form of $F_3(\mathbf{q})$ is such that in the evaluation of the range function the integral over q is not changed if the contour of integration is deformed to go infinitesimally above a cut along the real q axis from $-2k_F$ to $2k_F$. In the present 1D case the form of $F(q)$ is such that this device can also be used. The result is that, to within the factor $m/\pi^2\hbar^2$, the range function is given by

$$\Phi(x)\sim i\pi\int_{-2k_F}^{+2k_F}\frac{dq}{q+i\delta}e^{iqx} \ , \tag{10}$$

where the factor $i\pi$ is the difference

$$\ln\left|\frac{2k_F+q}{2k_F-q}\right|-\ln\left(\frac{2k_F+q}{2k_F-q}\right) \ ,$$

and q is in the interval $-2k_F$ to $2k_F$. Note the infinitesimal $i\delta$ in the denominator of (10), which arises from the deformation of the contour. The integration of (10) is immediate and gives the result (5), the term $i\delta$ contributing the constant term $\pi/2$ in (5).

Having discussed the one-dimensional case we now consider a three-dimensional free-electron system in which an atomic plane (e.g., the $y=0$, $z=0$ plane in a simple cubic lattice) is populated with ferromagnetically ordered magnetic moments. We may refer to this system as pseudo 1D, since in the continuum limit of the moment distribution the range function $\Phi_s(\mathbf{r})$ becomes independent of y and z. If the x axis is chosen to go through the observation point $\mathbf{r}$ then the range function $\Phi_s(x)$ is given by the following integral over the source points of the 3D range function:[2]

$$\Phi_s(x)\sim\int_x^\infty (rdr/r^4)[\sin(2k_Fr)-2k_Fr\cos(2k_Fr)] \ , \tag{11}$$

where $rdr=\rho d\rho$ is the element of area in the $y=0,z=0$ plane at constant x. Equation (11) can be integrated by parts. Defining $X=2k_Fx$, the result is

$$\Phi_s(x)\sim\frac{1}{2}\left[\left(\frac{\pi}{2}-\mathrm{Si}(X)\right)-\frac{\cos X}{X}+\frac{\sin X}{X^2}\right] \ . \tag{12}$$

This range function differs from that of the true 1D case in its last two terms. At large X, the asymptotic value of $(\pi/2-\mathrm{Si}(X)$ is $\cos X/X+\sin X/X^2$ so that $\Phi_s(X)$ behaves asymptotically as $\sin X/X^2$. In contrast, the asymptotic behavior in the 1D case is $\Phi(X)\sim\cos X/X$. Thus, the range function of the pseudo 1D case *falls off more rapidly* than that of the 1D case.

There is a simple reason for this difference: In general, the stronger the singularity of $F(q)$ at $q=2k_F$, the slower the fall-off rate of $\Phi(x)$ with increasing x. In the 1D case, the singularity of $F(q)$ is logarithmic. In the pseudo 1D case, which is three-dimensional as far as the electron gas is concerned, the susceptibility function is the three-dimensional susceptibility $F_3(q)$. The ferromagnetic layer in the plane $y=z=0$ produces a response at the point $\mathbf{r}$ which is proportional to

$$\Phi_s(x)\sim\sum_{\mathbf{r}'}\sum_{\mathbf{q}}\exp[i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')]F_3(\mathbf{q}) \ , \tag{13}$$

where $\mathbf{r}'$ is a source point in the yz plane. If $\mathbf{q}$ has a nonvanishing component in that plane the sum over $\mathbf{r}'$ vanishes, while if $\mathbf{q}$ is normal to it the sum is independent of $\mathbf{r}'$ and proportional to

$$\Phi_s(x)\sim\int F_3(q)e^{iqx}dq \ .$$

The singularity of $F_3(q)$ is only in its derivative, not in the function itself, and so it is weaker than that of $F(q)$. Hence $\Phi_s(x)$ falls off more rapidly than $\Phi(x)$. Finally, $\Phi_s(x)$ falls off less rapidly than $\Phi_3(r)$ of the 3D case because (13) has no contributions from the $\mathbf{q}$'s that are not normal to the yz plane, and so there is less destructive interference among the different q contributions than in the 3D case.

[1]C. F. Majkrzak, J. W. Cable, J. Kwo, M. Hong, D. B. McWhan, Y. Yafet, J. V. Waszczak, and C. Vettier, Phys. Rev. Lett. **56**, 2700 (1986). This paper gives references to other current work on the subject.

[2]C. Kittel, in *Solid State Physics,* edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1968), Vol. 22, p. 1. The following is the text of an erratum to this reference: In Appendix A (p. 295) the order of integration may not be interchanged as was done in going from (A1) to (A2). The term $-\frac{1}{2}\pi$ should be dropped from Eq. (A5), so that now the range function in one dimension does approach zero at large distances. This property of the correct range function was first pointed out to me by Professor T. Nagamiya and it was confirmed by calculation by Robert Cahn.

[3]W. Gröbner and N. Hofreiter, *Integraltafel* (Springer-Verlag, New York, 1957), Vol. 1, p 323.

[4]K. Mitchell, Philos. Mag. **40**, 351 (1949).

[5]J. H. Van Vleck, Rev. Mod. Phys. **34**, 681 (1962).