Journal of Magnetism and Magnetic Materials 441 (2017) 387–391

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Research articles

On calculation of RKKY range function in one dimension

Tomasz M. Rusin [a,*], Wlodek Zawadzki [b]

[a] Orange Poland sp. z o. o., Al. Jerozolimskie 160, 02-326 Warsaw, Poland
[b] Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-688 Warsaw, Poland

ARTICLE INFO

Article history:
Received 1 March 2017
Received in revised form 25 May 2017
Accepted 2 June 2017
Available online 3 June 2017

Keywords:
RKKY interaction
1D systems
Strong singularity

ABSTRACT

The effect of strong singularity in the calculation of range function for the RKKY interaction in 1D electron gas is discussed. The method of handling this singularity is presented. A possible way of avoiding the singularity in the Ruderman–Kittel perturbation theory in 1D is described.

1. Introduction

Some years after the discovery of Ruderman–Kittel–Kasuya–Yoshida (RKKY) interaction between localized magnetic moments in three dimensions [1], Kittel considered an extension of this interaction to lower dimensional system [2]. In the late 1980's and beginning of the 1990's the RKKY interaction was recognized as one of the mechanisms of coupling between magnetic layers in metallic superlattices [3], and the energy of RKKY interaction in quasi 1D systems was determined experimentally by Parkin and Mauri [4]. A review of these efforts is summarized in Ref. [5]. Later, the RKKY interaction in 1D or quasi-1D systems was investigated in many other works, see e.g. [6], and this subject is of actuality until present days, see e.g. [7]. For this reason, all subtleties of this problem should be clarified.

In his work, Kittel calculated the energy of RKKY interaction in one dimension between two localized magnetic moments embedded in a free electron gas [2]. He calculated first the magnetic susceptibility $\chi(q)$ of the electron gas in the presence of magnetic moments and then the range function was obtained as the Fourier transform of $\chi(q)$. In the appearing integral Kittel changed the order of integration which lead to erroneous results predicting a finite interaction energy at infinite distance between localized moments. This error was corrected in the Erratum to Ref. [2], and the correct result was obtained with a reverse order of integration. Some time later Yafet [8] showed that the problem reported by Kittel is caused by the presence of a strong singularity of the double integral at $k = q = 0$ and, because of the singularity, it is not allowed to change the order of integration over k and q variables. To show this, Yafet calculated twice the range function taking different orders of integrations and obtained different results. Then he determined the correct order of integrations. Further subtleties of this problem were discussed by Guliani et al. [9]. Litvinov and Dugaev [10] showed that an application of Green's function formalism allows one to avoid singularities at $k = q = 0$.

There exists an alternative method to calculate the RKKY interaction proposed in the original approach of Ruderman and Kittel (RK) to the 3D case [1]. This method is based on a direct calculation of the second order correction to the energy of free electron gas in the presence of two localized magnetic moments. In 3D one obtains a double integral over $|k'| > k_F$ and $|k| \leqslant k_F$ domain, which does not contain the strong singularity. This integral is then replaced by a difference of two integrals. Applying this procedure to 1D gas one finds that, surprisingly, each of the two integrals contains a strong singularity at $k = k' = 0$. This singularity does not exists in 2D or 3D cases. But in the 1D case there appears a singularity which is analogous to that appearing in the calculation of the range function in one dimension with the use of susceptibility $\chi(q)$ discussed by Yafet [8].

In the present note we analyze the effect of strong singularity at $k = k' = 0$ on the range function of the RKKY interaction in 1D calculated with the use of RK approach. Our results extend previous analyzes of singularities appearing in the calculations of the range function with use of susceptibility $\chi(q)$ in 1D, as described in Refs [2,8,9]. Then we show the effect of the order of integration over the singular part of the integral in the 1D case and determine the correct order of integration. Finally we propose another way to calcu-

* Corresponding author.
E-mail addresses: tmr@vp.pl (T.M. Rusin), zawad@ifpan.edu.pl (W. Zawadzki).

http://dx.doi.org/10.1016/j.jmmm.2017.06.007
0304-8853/

late the range function using a domain that is free of strong singularities.

2. Theory

Let us consider a one-dimensional free electron gas. Let the two spins $\hat{\boldsymbol{S}}_i$ be located at $\boldsymbol{R}_i$, where $i = 1, 2$. A coupling between the conduction electrons and the localized spins is assumed in the form of s-d interaction

$$\hat{H}_{sd} = \frac{J_{sd}}{N_{1D}} \sum_{i=1,2} \delta(\boldsymbol{R} - \boldsymbol{R}_i)\hat{\boldsymbol{S}}_i \hat{\boldsymbol{\sigma}}, \tag{1}$$

where $\hat{\boldsymbol{\sigma}}$ is electron spin operator, J_{sd} is the energy of s-d coupling, and N_{1D} is the one-dimensional density of magnetic atoms. Note that J_{sd}/N_{1D} has the dimensionality of [energy] $\times$ [length]. Following Ruderman and Kittel, the second order correction to the energy of electron gas perturbed by localized spins is [1]

$$\Delta E^{(2)} = \frac{J_{sd}^2}{(2\pi)^2 N_{1D}^2} \frac{2m^*}{\hbar^2} \hat{\boldsymbol{S}}_i \hat{\boldsymbol{S}}_j F_{1D}(r) \tag{2}$$

where

$$F_{1D}(r) = \int_{-k_F}^{k_F} dk \left[\left(\int_{-\infty}^{-k_F} + \int_{k_F}^{\infty} \right) \frac{\cos(kr)\cos(k'r)}{k'^2 - k^2} dk' \right], \tag{3}$$

in which m^* is the electron effective mass, k_F is the Fermi vector, $r = R_i - R_j$, and $F_{1D}(r)$ is the so-called range function. The order of integration in Eq. (3) follows from the method of calculation of $\Delta E^{(2)}$: first one selects the wave vector k, calculates the second order correction $\Delta E_k^{(2)}$ to the electron's energy E_k [square bracket in Eq. (3)], and then sums $\Delta E_k^{(2)}$ over k within the 1D Fermi sphere. Considering Eq. (3) one concludes that, since the k vectors are inside the 1D Fermi sphere and the k' vectors are outside the sphere, the denominators in Eq. (3) are always nonzero and no singularity occurs.

The difficulty in Eq. (3) is that the integral over dk' can not be calculated analytically. To overcome this problem RK [1] proposed to replace the integral in Eq. (3) over the domain

$$\mathcal{D}^{RK} : (k, k') \in [-k_F, k_F] \times \mathbb{R} \setminus [-k_F, k_F], \tag{4}$$

by the difference of two integrals over domains

$$\mathcal{D}^a : (k, k') \in [-k_F, k_F] \times \mathbb{R}, \tag{5}$$

$$\mathcal{D}^b : (k, k') \in [-k_F, k_F] \times [-k_F, k_F], \tag{6}$$

see Fig. 1. In the above expressions we used the notation of the set theory. As an example, if k is a member of set $\mathcal{A}$, the notation $k \in \mathcal{A}$ is used. Similarly, $\times$ denotes the cartesian product of two sets, $\mathcal{A} \setminus \mathcal{B}$ denotes difference between the two sets, and $\mathcal{A} \cup \mathcal{B}$ means the union of the two sets. For more detailed description of set notion see Ref. [11].

From (4)–(6) we have

$$F_{1D}(r) = \int \mathcal{D}^{RK} = \int \mathcal{D}^a - \int \mathcal{D}^b, \tag{7}$$

in which we use the notation

$$\int \mathcal{D}^a = \int \int_{(k,k') \in \mathcal{D}^a} \left(\frac{\cos(kr)\cos(k'r)}{k'^2 - k^2} dk' \right) dk, \tag{8}$$

and similarly for $\mathcal{D}^b$ and $\mathcal{D}^{RK}$. This method works correctly for 3D. However, doing so for 1D requires caution due to the presence of strong singularity at $k = k' = 0$ in Eq. (8) for the domains $\mathcal{D}^a$ and $\mathcal{D}^b$. We show below that this method may not be directly applied to the 1D case since the singularity at $k = k' = 0$ gives a nonzero contribution to the integrals.

Consider first $\int \mathcal{D}^a$, as given in Eqs. (5) and (8). The integral over k' is obtained with the use of formula 3.723.9 in [12]

$$\int_{-\infty}^{\infty} \frac{\cos(rk')}{k^2 - k'^2} dk' = \frac{\pi}{k} \sin(rk), \tag{9}$$

which is valid for $|r|, |k| > 0$. Then

$$\int \mathcal{D}^a = -\pi \int_{-k_F}^{k_F} \frac{\cos(kr)\sin(kr)}{k} dk = -\pi \mathrm{Si}(2k_F r), \tag{10}$$

where $\mathrm{Si}(x) = \int_0^x (\sin(t)/t) dt$ is the sine-integral in the standard notation, see [12].

The subtle point in the derivation of Eq. (10) is that the integral on the left hand side of Eq. (9) does not exist at $k = 0$, since for $k = 0$ and $|k'| \to 0$ the integrand diverges as $1/k'^2$. Therefore Eq. (9) in valid for all $\mathcal{D}^a$ except in the small domain

$$\mathcal{D}^\epsilon : (k, k') \in [-\epsilon, \epsilon] \times [-\epsilon, \epsilon], \tag{11}$$

with $\epsilon \to 0$, for which the identity (9) can not be used. To overcome this problem we isolate the domain $\mathcal{D}^\epsilon$ out of the integration domain: $\int \mathcal{D}^a = \int \mathcal{D}^{a\epsilon} + \int \mathcal{D}^\epsilon$, in which: $\mathcal{D}^{a\epsilon} = \mathcal{D}^a \setminus \mathcal{D}^\epsilon$. The contribution to the range function coming from $\mathcal{D}^\epsilon$ has to be calculated separately.

Turning to $\int \mathcal{D}^b$ we note that there is a similar problem with the singularity at $k = k' = 0$, so that we again isolate $\mathcal{D}^\epsilon$ out of the integration domain: $\int \mathcal{D}^b = \int \mathcal{D}^{b\epsilon} + \int \mathcal{D}^\epsilon$ in which: $\mathcal{D}^{b\epsilon} = \mathcal{D}^b \setminus \mathcal{D}^\epsilon$. Let us assume that the integral $\mathcal{D}^\epsilon$ is finite, which is crucial for the calculations. Then from Eq. (7) we have (see Fig. 2)

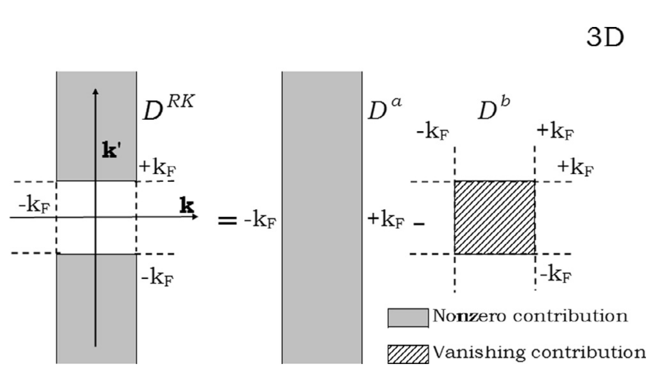

Fig. 1. Schematic visualization of integration domain defined in (4)–(6). Left side of equation: domain of integration in Eq. (3) (grey), right side: two domains of integration proposed in Ref. [1], gray and dotted. Grey areas give nonzero contribution to the range function while integral over dotted areas vanishes due to symmetry.

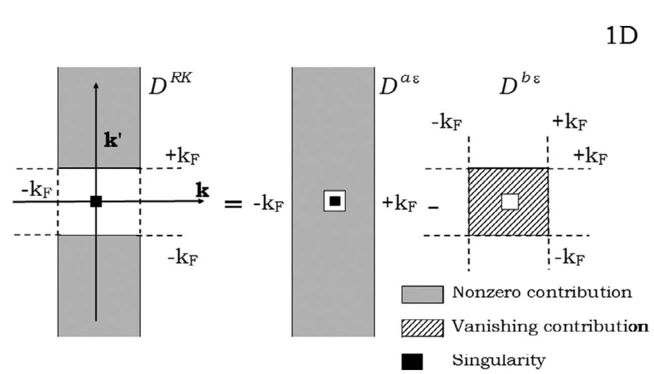

Fig. 2. Schematic visualization of difference of the two domains shown in Eq. (12). Grey and dotted areas have the same meaning as in Fig. 1. Black squares: strong singularity at $k = k' = 0$. Note that the two domains on the rhs still do not include strong singularity.