The Rôle of Bound States of Magnetic Layers in the Theory of Multilayer Interaction

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ABSTRACT

Using planar Dirac delta-functions to describe the coupling of magnetic layers to an electron gas, the interaction between the layers is calculated. Both the bound and free states give contributions which are shaped by the range of the bound states. Due to a remarkable cancellation of terms the combined result does not show this shape. In fact, it differs appreciably from the weak coupling limit only when the binding energy of the bound states is comparable or larger than the Fermi energy.

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1 Introduction

It is well known that a potential represented by a three dimensional Dirac delta-function, $\delta(\mathbf{x})$, has no bound states while a one dimensional $\delta(z)$ has one bound state. The first is often used to describe point interactions of spins to conduction electrons and the latter to simulate a planar distribution of spins. A planar lattice of spins in an electron gas leads to a bound band. So far treatments of magnetic multilayers[1]-[6] have not introduced these bound states explicitely. This is consistent with the use of lowest order perturbation theory[1]. Nevertheless, typical exchange couplings and spin densities in layers produce bound states that extend over distances that are relevant for multilayer physics. This paper discusses the contributions of occupied bound and free states to the coupling between magnetic layers.

2 Bound states

In one dimension the Hamiltonian for an electron coupled to a point field is

$$H_1 = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} - \beta\,\delta(z)\,\sigma_z, \tag{1}$$

where σ_z is a Pauli matrix. Let $\beta > 0$. Then a spin up electron has one bound state with orbital wave function and energy

$$\varphi_+(z) = (1/\sqrt{l_0})\,\mathrm{e}^{-|z|/l_0}, \quad E_0 = -\epsilon_0/2 \tag{2}$$

where

$$l_0 = \hbar^2/(\beta m), \quad \epsilon_0 = \beta^2 m/\hbar^2. \tag{3}$$

The quantities l_0 and ϵ_0 are natural units of length and energy in this problem. As an example, with $\beta = 0.3$ eV Å, $l_0 = 24$ Å and $\epsilon_0 = 69$ K k_B, where k_B is the Boltzmann constant.

In three dimensions a potential of the form $-\gamma\,\delta(\mathbf{x}-\mathbf{R})$ has no bound state. This potential is used to describe a point interaction of an electron to an ion spin located at position $\mathbf{R}$, where γ includes a coupling constant times a scalar product of spins. A corresponding interaction with a planar ferromagnetic lattice of spins is obtained by summing over the lattice positions $\mathbf{R}_j$. It is essential for the following discussion to realize that even such a discrete lattice has a bound state localized near the plane. This is evident from a variational argument using $\psi_+(x,y,z) = \varphi_+(z)$ with φ_+ from Eq. (2) as a trial function. Here z is the distance from the lattice plane. ψ is normalized to unit area. The corresponding energy is given by E_0 of Eq. (2) with $\beta = \gamma n$, where n is the density of lattice points. The true ground state energy can only be lower. The approximation which uses a continuous planar distribution of spins corresponds to the limit in which the lattice constant vanishes while β remains constant.

The Hamiltonian Eq. (1) with the kinetic energy for three dimensions is

$$H_1 = -\frac{\hbar^2}{2m}\Delta - \beta\,\delta(z)\,\sigma_z. \tag{4}$$

The localized orbital wave functions and corresponding energies become

$$\psi_{+,k_x,k_y}(x,y,z) = \varphi_+(z)\,e^{i(k_x x+k_y y)} \qquad (5)$$
$$E_0(k_x,k_y) = E_0 + \tfrac{\hbar^2}{2m}\left(k_x^2+k_y^2\right) \qquad (6)$$

3 Polarization due to a magnetic plane

The density of spin up electrons has a contribution from the occupied bound states Eq. (5):

$$\rho_{+,b}(z) = \tfrac{1}{(2\pi)^2}\int_{E_0(k_x,k_y)<E_F} dk_x\,dk_y\,|\varphi_+(z)|^2 \qquad (7)$$
$$= \tfrac{k_F^2+1/l_0^2}{4\pi l_0}e^{-2|z|/l_0}, \qquad (8)$$

where $E_F = \hbar^2 k_F^2/(2m)$ is the chemical potential. The free states for spin $\sigma_z = \pm 1$ with the apropriate boundary conditions at $z = 0$ are plain waves $e^{i(k_x x+k_y y)}$ multiplied by a function $\varphi_{\pm,k_z}(z)$ chosen to be either even, $\varphi_{\pm,k_z,e}$, or odd , $\varphi_{\pm,k_z,o}$

$$\varphi_{\pm,k_z,e} = \sqrt{2}\,\cos\{k_z|z| \pm \arctan(1/(k_z l_0))\} \qquad (9)$$
$$\varphi_{\pm,k_z,o} = \sqrt{2}\,\sin(k_z z). \qquad (10)$$

The orbital states with $k_z = 0$ do not exist, since they vanish identically.

The contribution to the electron density from the free states becomes for the two spin orientations

$$\rho_{\pm,f}(z) = \tfrac{1}{(2\pi)^3}\int_{(\hbar^2/2m)(k_x^2+k_y^2+k_z^2)<E_F} dk_x\,dk_y\,dk_z\left\{|\varphi_{\pm,k_z,e}(z)|^2+|\varphi_{\pm,k_z,o}(z)|^2\right\} \qquad (11)$$
$$= \tfrac{1}{2(2\pi)^2}\int_0^{k_F} dk_z\,(k_F^2-k_z^2)2\left[1-\tfrac{\cos(2k_z z)\pm k_z l_0\sin(2k_z|z|)}{1+k_z^2 l_0^2}\right]. \qquad (12)$$

The spin polarization is

$$P(z) = (\rho_{+,b}+\rho_{+,f}-\rho_{-,f})/2. \qquad (13)$$

The contribution of the free states is

$$P_f(z) = \frac{1}{(2\pi)^2}\,\mathrm{Im}\int_0^{k_F} dk_z\,\left(k_F^2-k_z^2\right)\frac{k_z l_0\,e^{2ik_z|z|}}{1+k_z^2 l_0^2}. \qquad (14)$$

Since the contribution of the bound state, Eq. (8), can be obtained by an integration around the pole at $k_z = i/l_0$, the whole spin polarization is given by the integral

$$P(z) = \frac{-1}{(2\pi)^2}\,\mathrm{Im}\int_{k_F}^{k_F+i\infty} dk_z\,\left(k_F^2-k_z^2\right)\frac{k_z l_0\,e^{2ik_z|z|}}{1+k_z^2 l_0^2}. \qquad (15)$$

In a jellium model the homogeneous positive charge background is $-ek_F^3/(3\pi^2)$, where e is the charge of an electron. Then the charge density is

$$Q(z) = e[\rho_{+,b}+\rho_{+,f}+\rho_{-,f}-k_F^3/(3\pi^2)]. \qquad (16)$$

When $Q(z)$ differs from zero, a Hamiltonian which includes Coulomb couplings will lead to further effects.

For small coupling constant β, $Q(z)$ is of order $1/l_0^2 = (\beta m/\hbar^2)^2$. The dominant terms in $P(z)$ are of order $1/l_0$:

$$P(z) \Rightarrow \frac{k_F^2}{8\pi l_0} - \frac{1}{4\pi^2 l_0}\int_0^{k_F} dk_z\,(k_F^2 - k_z^2)\frac{\sin(2k_z|z|)}{k_z} \tag{17}$$

$$= \frac{k_F^2}{4\pi^2 l_0}\left\{\frac{\pi}{2} - \mathrm{Si}(2k_F|z|) + \frac{\sin(2k_F|z|)-2k_F|z|\cos(2k_F|z|)}{(2k_F|z|)^2}\right\}. \tag{18}$$

Note that the constant $\pi/2$ in the curly bracket arises from the bound state as $\mathrm{e}^{-2|z|/l_0} \Rightarrow 1$. Thus this result cannot follow from finite perturbation theory. Historically, this polarization was first discussed by C. Kittel[1] in the one dimensional case. Kittel did not consider the bound state and used perturbation theory for plane waves. Thus he did not get the constant $\pi/2$ and concluded that in one dimension the polarization had long range. Yafet[2] challenged this conclusion and, still within perturbation theory, proposed a modification in the integration over a singularity which produced this constant $\pi/2$.

For later use, let us calculate the magnetic part of the grand potential of a single layer per unit surface at zero temperature, which is the work necessary to introduce a unit surface of the layer into the electron gas with fixed chemical potential. It is noteworthy that the free states give a contribution only through the change of the density of particles $\Delta N(k_z)$, since the energies of the levels remain $\hbar^2k^2/2m$. From Eq. (12) the change in density due to the states with wave number k_z becomes

$$\Delta\rho_{\pm,k_z,f}(z) = -2\frac{\cos(2k_z z) \pm k_z l_0 \sin(2k_z|z|)}{1+k_z^2 l_0^2}. \tag{19}$$

Then

$$\Delta N_{\pm,f}(k_z) = \int_{-\infty}^{\infty} dz\,\Delta\rho_{\pm,k_z,f}(z) = -2\pi\,\delta(k_z) \mp \frac{2l_0}{1+k_z^2 l_0^2}. \tag{20}$$

The δ-function arises from the fact that in the presence of the potential the orbital states with $k_z = 0$ do not exist. Note that

$$\frac{1}{2\pi}\int_0^{\infty} dk_z\,\Delta N_{\pm,f}(k_z) = \begin{cases} -1 & \text{for spin up } (+) \\ 0 & \text{for spin down } (-), \end{cases} \tag{21}$$

which just confirms the completeness of the free and bound states. The appendix offers a more visual approach. From that point of view Eq. (21) is reminiscent of Levinson's theorem[7]. In the weak coupling limit $l_0 \to \infty$, $\Delta N_{-,f}(k_z) \to 0$, while $\Delta N_{+,f}(k_z) \to -4\pi\delta(k_z)$.

The contribution of the free states to the grand potential becomes with $\Delta N_f = \Delta N_{+,f} + \Delta N_{-,f}$

$$\xi_f = \frac{1}{(2\pi)^3}\int_{|k|<k_F} d^3k\,\frac{\hbar^2}{2m}(k^2 - k_F^2)\Delta N_f(k_z) \tag{22}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{(2\pi)^2}\frac{1}{4}\int_0^{k_F} dk_z\,(k_F^2 - k_z^2)^2\,\Delta N_f(k_z) \tag{23}$$

$$= \frac{\hbar^2}{2m}\frac{1}{4\pi}k_F^4\int_0^{k_F} dk_z\,\delta(k_z) \tag{24}$$

$$= \frac{\hbar^2 k_F^4}{2m\,4\pi}\frac{1}{2} = \frac{E_F k_F^2}{8\pi} = C. \tag{25}$$

C is the kinetic energy of a two dimensional band filled from zero up to the level E_F. This term which is independent of the coupling constant will be compensated later.

The contribution of the bound state to the grand potential is

$$\begin{aligned} \xi_b = & \frac{1}{4\pi^2} \int \int_{E_0(k_x,k_y)\leq E_F} dk_x\, dk_y\, [E_0(k_x,k_y) - E_F] & (26) \\ = & -(1 - E_0/E_F)^2\, C. & (27) \end{aligned}$$

The total potential is

$$\begin{aligned} \xi = & \quad \xi_b + \xi_f & (28) \\ = & \quad C(2 - E_0/E_F)(E_0/E_F) & (29) \\ \Rightarrow & \quad -\frac{E_F}{\pi^2 l_0^2}\frac{\pi}{4} \qquad \text{for } k_F l_0 \gg 1 & (30) \end{aligned}$$

4 Bound states of two delta functions

Some features of the interaction between two magnetic planes are contained in a one dimensional model for the indirect interaction of two ion spins coupled to one electron[10]. Here, let us consider the Hamiltonian

$$H_2 = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} - \beta\left[\delta\left(z - \frac{L}{2}\right) \pm \delta\left(z + \frac{L}{2}\right)\right]\sigma_z, \tag{31}$$

where $\beta > 0$ and the plus or minus sign refers to situations with parallel or antiparallel magnetizations respectively. The localized orbital wave functions have the form

$$\varphi(z) = \begin{cases} A\,e^{qz} & \text{for } z < L/2 \\ B\,e^{qz} + F\,e^{-qz} & \text{for } |z| < L/2 \\ D\,e^{-qz} & \text{for } z > L/2 \end{cases} \tag{32}$$

with the energy eigenvalue $E = -\hbar^2 q^2/(2m)$. The wave function is continuous with discontinuous slopes at $\pm L/2$. This determines the coefficients

$$B = A/K, \;\; F = A(ql_0 - 1)e^{qL}/K, \;\; D = Aql_0 e^{qL}/K \tag{33}$$

with $K = 1 + (ql_0 - 1)e^{2qL}$, and where A is a normalization constant. In the parallel case [+ sign in Eq. (31)] the equations for the energy E_1 of the (symmetric) ground state and the energy E_2 of the (antisymmetric) excited state are obtained from

$$\begin{aligned} e^{-q_1 L} + 1 - q_1 l_0 = & \; 0 & (34) \\ e^{-q_2 L} - 1 + q_2 l_0 = & \; 0. & (35) \end{aligned}$$

For $L < l_0$ only the symmetric solution exists. In the antiparallel case ($-$ sign in Eq. (31)) there is one bound state for each spin direction with an energy E_3 given by

$$e^{-q_3 L} - \sqrt{1 - q_3^2 l_0^2} = 0. \tag{36}$$

Figure 1 shows these energies as functions of the distance L.

5 Bound states for two ferromagnetic layers

In a metal with two parallel ferromagnetic plates the planar translational invariance allows a generalization of the results of the previous section to three dimensions. The wave functions and energies are given by Eqs. (5), (6) now with a band index $j \in \{1, 2, 3\}$:

$$E_j(k_x, k_y) = E_j + \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right) \tag{37}$$

To discuss the stability of the parallel versus the antiparallel configuration, the thermodynamic potential has to be evaluated. In the parallel case the grand canonical potential per unit area (at zero temperature) has the contribution of the localized states

$$\begin{aligned}\Xi_{b,p} = \;& \tfrac{1}{4\pi^2}\int\int_{E_1(k_x,k_y)\leq E_F} dk_x\, dk_y \left[E_1(k_x, k_y) - E_F\right] \\ &+ \tfrac{1}{4\pi^2}\int\int_{E_2(k_x,k_y)\leq E_F} dk_x\, dk_y \left[E_2(k_x, k_y) - E_F\Theta(L - l_0)\right],\end{aligned} \tag{38}$$

where $\Theta(z)$ is the step function. Similarly, in the antiparallel case

$$\Xi_{b,a} = \frac{2}{4\pi^2}\int\int_{E_3(k_x,k_y)\leq E_F} dk_x\, dk_y \left[E_3(k_x, k_y) - E_F\right]. \tag{39}$$

The integrations of Eqs. (38) and (39) yield

$$\begin{aligned}\Xi_{b,p} = \;& \left[(2 - E_1/E_F)E_1/E_F + (2 - E_2/E_F)E_2/E_F\right] C \\ & - \left[1 + \Theta(L - l_0)\right] C\end{aligned} \tag{40}$$

$$\Xi_{b,a} = 2C(2 - E_3/E_F)E_3/E_F - 2C. \tag{41}$$

6 Free states in the presence of two magnetic layers

6.1 Parallel magnetizations

When the contribution of bound states to the energy is considered, it is necessary to use free waves which are orthogonal to the bound states. This is automatically fulfilled by the eigenfunctions of the Hamiltonian. Thus, in the presence of bound states the contribution of the running waves is not given by the Ruderman-Kittel function.

The wave functions factor into plane waves for the x and y directions and a z dependent function $\phi_{k_z}(z)$. For the case of two layers with parallel magnetizations we use a set of even or odd eigenfunctions

$$\phi_{k_z,p,e}(z) = \begin{cases} a\cos(k_z z) & \text{for } |z| < L/2 \\ \sqrt{2}\cos(k_z|z| + b) & \text{for } |z| > L/2 \end{cases} \tag{42}$$

$$\phi_{k_z,p,o}(z) = \begin{cases} A\sin(k_z z) & \text{for } |z| < L/2 \\ \sqrt{2}\sin(k_z|z| + B)\,\text{sign}(z) & \text{for } |z| > L/2 \end{cases} \tag{43}$$

where for spin up

$$a^2 = \frac{2}{1+2\sin(k_zL)/(k_zl_0)+4\cos^2(k_zL/2)/(k_zl_0)^2} \tag{44}$$

$$b = -k_zL/2 + \arctan\{\tan(k_zL/2) + 2/(k_zl_0)\} \tag{45}$$

$$A^2 = \frac{2}{1-2\sin(k_zL)/(k_zl_0)+4\sin^2(k_zL/2)/(k_zl_0)^2} \tag{46}$$

$$B = -k_zL/2 + \arctan\left[\frac{1}{\mathrm{ctg}(k_zL/2)-2/(k_zl_0)}\right]. \tag{47}$$

For spin down l_0 is to be replaced by $-l_0$.

The integrated excess probability density of the spin up states over the unperturbed value is

$$\Delta N_{p,e,\uparrow}(k_z) = \frac{a^2}{2}\left[L - \frac{4}{l_0k_z^2}\cos^2\left(\frac{k_zL}{2}\right)\right] - L - 2\pi\,\delta(k_z) \tag{48}$$

$$\Delta N_{p,o,\uparrow}(k_z) = \frac{A^2}{2}\left[L - \frac{4}{l_0k_z^2}\sin^2\left(\frac{k_zL}{2}\right)\right] - L. \tag{49}$$

Again the substitution $l_0 \to -l_0$ yields the spin down results. The total excess probability for k_z is

$$\Delta N_p(k_z) = \Delta N_{p,e,\uparrow}(k_z) + \Delta N_{p,e,\downarrow}(k_z) + \Delta N_{p,o,\uparrow}(k_z) + \Delta N_{p,o,\downarrow}(k_z). \tag{50}$$

The contribution of the free states to the grand potential becomes

$$\Xi_{f,p} = -\frac{\hbar^2}{2m}\frac{1}{(2\pi)^2}\frac{1}{4}\int_0^{k_F} dk_z\,(k_F^2 - k_z^2)^2\,\Delta N_p(k_z). \tag{51}$$

In view of the singular properties of $\Delta N_p(k_z)$ at $k_z = 0$, the integral over k_z is written as

$$\int_0^{k_F} dk_z\,\ldots = \lim_{\alpha\to+0}\left[\int_\alpha^{k_F} dk_z\,\ldots + \int_0^\alpha dk_z\,\ldots\right]. \tag{52}$$

In order to make a connection with the work of Bruno[4], we introduce $\Omega_{f,p}(k_z)$ such that

$$d\Omega_{f,p}(k_z)/dk_z = \Delta N_p(k_z) \quad \text{for } k_z > 0. \tag{53}$$

Thus

$$\Omega_{f,p}(k_z) = -2\,\mathrm{Im}\,\ln\left\{\frac{e^{ik_zL}+1+ik_zl_0}{1+ik_zl_0}\,\frac{e^{ik_zL}+1-ik_zl_0}{1-ik_zl_0}\,\frac{e^{ik_zL}-1-ik_zl_0}{-1-ik_zl_0}\,\frac{e^{ik_zL}-1+ik_zl_0}{-1+ik_zl_0}\right\} \tag{54}$$

$$= -2\arctan\left\{\frac{\sin(4k_zL)-2\sin(2k_zL)(1-k_z^2l_0^2)}{\cos(4k_zL)-2\cos(2k_zL)(1-k_z^2l_0^2)+(1+k_z^2l_0^2)^2}\right\} + 4\,\mathrm{Im}\,\ln\left[1+(k_zl_0)^2\right]. \tag{55}$$

The numerators of the four factors of the logarithm in Eq. (54) correspond, for $k_z > 0$, to the four terms of Eq. (50) in the same order. The product of the denominators is positive and therefore of no effect. Individually they produce, for $k_z > 0$, self-terms as given by Eq. (29) multiplied by ± 1. On the positive imaginary axis, $k_z = i\,q$, the first and third factors of the numerator vanish for the values $q_{1,2}$ of Eqs. (34) and (35), respectively.

The branches of arctan in Eq. (55) have to be chosen in such a way that $\Omega_{f,p}(k_z)$ is a continuous function of k_z. $\Xi_{f,p}$, Eq. (51), can be expressed through $\Omega_{f,p}(k_z)$ by a partial integration

$$\begin{aligned}\Xi_{f,p} = & -\tfrac{\hbar^2}{2m}\tfrac{1}{(2\pi)^2}\tfrac{1}{4}\lim_{\alpha\to 0}\Big\{ -(k_F^2-\alpha^2)^2\Omega_{f,p}(\alpha) \\ & + 4\int_\alpha^{k_F} dk_z\,(k_F^2-k_z^2)k_z\Omega_{f,p}(k_z) + \int_0^\alpha dk_z\,(k_F^2-k_z^2)^2\,\Delta N_p(k_z)\Big\}. \end{aligned} \tag{56}$$

The first term does not vanish because of the singular behaviour of $\Omega_{f,p}(k_z)$ at the lower limit:

$$\lim_{\alpha\to +0}\Omega_{f,p}(\alpha) = 2\pi\,\Theta(L-l_0). \tag{57}$$

In the second term of Eq. (56), the lower limit of the integral can be put equal to zero. The third term has a contribution according to Eq. (48). Thus $\Xi_{f,p}$ consists of three terms:

$$\Xi_{f,p} = -\frac{\hbar^2}{2m}\frac{1}{(2\pi)^2}\int_0^{k_F} dk_z\,(k_F^2-k_z^2)k_z\,\Omega_{f,p}(k_z) + [\Theta(L-l_0)+1]\,C. \tag{58}$$

The first term of Eq. (58) coincides with Eq. (1) of ref. [4] applied to our case: $\cos\theta = 1$, $r_A^{\pm} = r_B^{\pm} = 1/(1\pm ik_z l_0)$, $T=0$, $q_z = 2k_z$.

In the weak coupling limit, $k_F l_0 \gg 1$, Eq. (58) reduces to

$$\Xi_{f,p} \Rightarrow -\frac{E_F}{\pi^2 l_0^2}\left\{-\mathrm{Si}(2k_F L) + \frac{\sin(2k_F L) - 2k_F L\,\cos(2k_F L)}{(2k_F L)^2}\right\} + C. \tag{59}$$

with C given by Eq. (25). The expression in the curly bracket differs from that of Eq. (18) by the absence of the term $\frac{\pi}{2}$, which in Eq. (18) was contributed by the bound state. Apart from this and the constant C, $-2\beta P(L)$ of Eq. (18) agrees with Eq. (59).

The complete change of the grand potential due to the magnetic layers includes the contribution of the bound states, Eq. (40):

$$\Xi_p = \Xi_{f,p} + \Xi_{b,p}. \tag{60}$$

In this equation the last terms of Eq. (40) cancel with the corresponding terms of Eq. (58). Therefore

$$\begin{aligned}\Xi_p = & E_F k_F^2\Big\{ -\tfrac{1}{(2\pi)^2}\tfrac{1}{4}\lim_{\alpha\to 0}\int_\alpha^1 dy\,(1-y^2)^2\Delta N_p(yk_F) \\ & + \tfrac{1}{8\pi}\Big[\Big(2-\tfrac{E_1}{E_F}\Big)\tfrac{E_1}{E_F} + \Big(2-\tfrac{E_2}{E_F}\Big)\tfrac{E_2}{E_F} - \Theta(L-l_0)\Big]\Big\} \end{aligned} \tag{61}$$

where the integration over $\Delta N_p(k_z)$ excludes the contribution at $k_z = 0$. Alternatively,

$$\begin{aligned}\Xi_p = & E_F k_F^2\Big\{\tfrac{1}{(2\pi)^2}\int_0^1 dy\,(1-y^2)y\,\Omega_{f,p}(yk_F) \\ & + \tfrac{1}{8\pi}\Big[\Big(2-\tfrac{E_1}{E_F}\Big)\tfrac{E_1}{E_F} + \Big(2-\tfrac{E_2}{E_F}\Big)\tfrac{E_2}{E_F}\Big]\Big\} \end{aligned} \tag{62}$$

with the definition of arctan mentioned above.

For $k_F L > k_F l_0 \gg 1$, Ξ_p becomes

$$\Xi_p \Rightarrow -\frac{E_F}{\pi^2 l_0^2}\,\pi. \tag{63}$$

Thus the bound states have contributed the missing term $\frac{\pi}{2}$ in the curly bracket of Eq. (59) making it a coupling of finite range, plus the self-terms, Eq. (30), of two single layers.

The full result, Eq. (62) minus the self-terms of two separate layers, can be obtained from the first line alone, however, with a different integration path in the complex plane, in analogy to Eq. (15). Since the integrand vanishes for $y \to i\infty$, we have (with $k_z = y k_F$)

$$-\operatorname{Im}\int_{k_F}^{k_F+i\infty} dk_z \ldots = -\operatorname{Im}\int_0^{i\infty} dk_z \ldots + \operatorname{Im}\int_0^{k_F} dk_z \ldots . \tag{64}$$

The last integral is that of the first line of Eq. (62). We shall show that the integral along the imaginary axis yields the contribution of the bound states (second line of Eq. (62) minus the self-terms). Let us consider the first factor in Eq. (54).

$$f(k_z) = \left(\mathrm{e}^{ik_zL} + 1 + ik_z l_0\right)/(1 + ik_z l_0)\,. \tag{65}$$

For Im $k_z > 0$ and $L \to \infty$ this goes to 1, showing that the denominator subtracts the self-terms. The numerator vanishes for $k_z = iq_1$ as seen from Eq. (35), and the denominator for $k_z = i/l_0$. Im ln (z) is zero if z is positive and $+\pi$ if z is negative. On the imaginary axis $f(k_z)$ is negative from $k_z = il_0$ to $k_z = iq_1$. Then

$$\begin{aligned} &-\tfrac{\hbar^2}{2m}\tfrac{2}{(2\pi)^2}\operatorname{Im}\textstyle\int_0^{i\infty} dk_z\, k_z(k_F^2 - k_z^2)\,\ln(f(k_z)) \\ =\quad & E_F k_F^2 \tfrac{1}{8\pi}\Big[\left(2 - \tfrac{E_1}{E_F}\right)\tfrac{E_1}{E_F} - \left(2 - \tfrac{E_0}{E_F}\right)\tfrac{E_0}{E_F}\Big] \end{aligned} \tag{66}$$

with an analogous result for the third factor in Eq. (54), while the others do not contribute. Therefore the integration path of the left hand side of Eq. (64) yields the full interaction of the magnetic layers without the self-terms. If this integration path is used in the integral of Eq. (1) of ref.[4], then the contribution of the bound states is incorporated. Similarly, Eq. (6) of ref.[5] takes the poles on the positive imaginary axis into account.

In fig. 2 the contributions from free and bound states are shown separately. Both are shaped by the exponential decay of the bound states with a length l_0. The sum of the two terms, however, hides this length. The shape remains close to the result of Yafet[2] which becomes rigorous for $k_F l_0 \gg 1$. The amplitude is, of course, proportional to $1/l_0^2$ in this limit. The remarkable cancellation shown in fig. 2 is reminiscent of the theorem of Bruno, Eq. (6) of ref.[5], which states that the characteristic length $\sqrt{2mV}/\hbar^2$ of a potential well of depth V is not apparent in the coupling between two magnetic layers.

6.2 Antiparallel magnetizations

In the antiparallel case the Hamiltonian Eq. (31) is invariant with the transformation which simultaneously inverts the z-axis and the spin direction. Thus, the z and spin dependent part of the wave function can be written as

$$\varphi_{\uparrow,k_z,a}(z) = \begin{cases} \sqrt{2}\,\cos(k_z z - c) & \text{for } z < -L/2 \\ a\cos(k_z z) + b\sin(k_z z) & \text{for } -L/2 < z < L/2 \\ \sqrt{2}\,\cos(k_z z + C) & \text{for } z > L/2 \end{cases} \tag{67}$$

for spin up and

$$\varphi_{\downarrow,k_z,a}(z) = \begin{cases} \sqrt{2}\,\cos(k_z z - C) & \text{for } z < -L/2 \\ a\cos(k_z z) - b\sin(k_z z) & \text{for } -L/2 < z < L/2 \\ \sqrt{2}\,\cos(k_z z + c) & \text{for } z > L/2 \end{cases} \tag{68}$$

for spin down. The boundary conditions yield two solutions:

$$b/a = (1/k_z l_0)\left(1 \pm \sqrt{1 + k_z^2 l_0^2}\right). \tag{69}$$

$$a^2 = k_z^2 l_0^2 / \left\{(b/a)^2 + (b/a)k_z l_0 + 1 + k_z^2 l_0^2 - \left[(b/a)^2 - 1 + 2(b/a)k_z l_0\right]\cos(k_z L)\right\}, \tag{70}$$

$$c = \; -\tfrac{k_z L}{2} + \arccos\left[\tfrac{a}{\sqrt{2}}\cos\left(\tfrac{k_z L}{2}\right) - \tfrac{b}{\sqrt{2}}\sin\left(\tfrac{k_z L}{2}\right)\right] \tag{71}$$

$$C = \; -\tfrac{k_z L}{2} + \arccos\left[\tfrac{a}{\sqrt{2}}\cos\left(\tfrac{k_z L}{2}\right) + \tfrac{b}{\sqrt{2}}\sin\left(\tfrac{k_z L}{2}\right)\right]. \tag{72}$$

The excess probability for one solution and spin becomes

$$\Delta N_{a,\pm,\uparrow}(k_z) = \Delta N_{a,\pm,\downarrow}(k_z) = \frac{a^2}{2k_z}\left\{-\frac{4}{k_z l_0}\frac{b}{a}\sin(k_z L) + \left[1 + \left(\frac{b}{a}\right)^2\right]k_z L\right\} - L - \pi\delta(k_z). \tag{73}$$

Summed over the two states and the spin directions

$$\Delta N_a(k_z) = 8\frac{\cos(2k_z L)(1 + k_z^2 l_0^2)L - \sin(2k_z L)k_z l_0^2 - L}{2 - 2\cos(2k_z L)(1 + k_z^2 l_0^2) + 2k_z^2 l_0^2 + k_z^4 l_0^4} - 4\pi\delta(k_z), \tag{74}$$

so that

$$\Xi_{f,a} = -\frac{\hbar^2}{2m}\frac{1}{(2\pi)^2}\frac{1}{4}\int_0^{k_F} dk_z\,(k_F^2 - k_z^2)^2\,\Delta N_a(k_z). \tag{75}$$

With

$$d\Omega_{f,a}(k_z)/dk_z = \Delta N_a(k_z) \quad \text{for } k_z > 0, \tag{76}$$

$$\Omega_{f,a}(k_z) = \; -4\;\mathrm{Im}\;\ln\left[\frac{\mathrm{e}^{ik_z L} - \sqrt{1+k_z^2 l_0^2}}{-\sqrt{1+k_z^2 l_0^2}}\,\frac{\mathrm{e}^{ik_z L} + \sqrt{1+k_z^2 l_0^2}}{\sqrt{1+k_z^2 l_0^2}}\right] \tag{77}$$

$$= \; -2\arctan\left[\frac{\sin(4k_z L) - 2\sin(2k_z L)(1+k_z^2 l_0^2)}{\cos(4k_z L) - 2\cos(2k_z L)(1+k_z^2 l_0^2) + (1+k_z^2 l_0^2)^2}\right] + 4\,\mathrm{Im}\;\ln(1 + k_z^2 l_0^2), \tag{78}$$

$$\lim_{\alpha\to 0}\Omega_{f,a}(\alpha) = 2\pi, \tag{79}$$

the contribution to the grand potential from the free states becomes

$$\Xi_{f,a} = -\frac{\hbar^2}{2m}\frac{1}{(2\pi)^2}\int_0^{k_F} dk_z\,(k_F^2 - k_z^2)k_z\,\Omega_{f,a}(k_z) + 2C. \tag{80}$$

As with Eq. (58), the first term agrees with Eq. (1) of ref.[4] with $\cos\theta = -1$. In the weak coupling limit it leads to minus the result of Eq. (59). The full change of the grand potential is

$$\Xi_a = \Xi_{f,a} + \Xi_{b,a} \tag{81}$$

with $\Xi_{b,a}$ from Eq. (41). Thus

$$\begin{aligned}\Xi_a = \; & E_F k_F^2 \Big\{ -\tfrac{1}{(2\pi)^2}\tfrac{1}{4}\lim_{\alpha\to 0}\textstyle\int_\alpha^1 dy\,(1-y^2)^2 \Delta N_a(yk_F) \\ & + \tfrac{1}{4\pi}\Big[\Big(2 - \tfrac{E_3}{E_F}\Big)\tfrac{E_3}{E_F} - 1\Big]\Big\}\end{aligned} \tag{82}$$

or alternatively

$$\begin{aligned}\Xi_a = \; & E_F k_F^2 \Big\{ -\tfrac{1}{(2\pi)^2}\textstyle\int_0^1 dy\,(1-y^2)y\,\Omega_{f,a}(yk_F) \\ & + \tfrac{1}{4\pi}\Big(2 - \tfrac{E_3}{E_F}\Big)\tfrac{E_3}{E_F}\Big\}.\end{aligned} \tag{83}$$

This can also be represented by a single integration as in Eqs. (15) or (64).

In the weak coupling limit E_3 vanishes as l_0^{-4} and Ξ_a tends to minus Eq. (59) without the term C. For $L = 0$ this vanishes as it should, since the two magnetizations cancel. At large distance, $L \to \infty$, it tends to the self energies of two layers, 2ξ of Eq. (30).

7 stability of relative magnetizations of the two layers

To compare the stability of the two configurations, we introduce the quantity

$$\Delta\Xi = \Xi_p - \Xi_a \tag{84}$$

which is negative when the parallel arrangement is favoured. $\Delta\Xi$ is plotted in Fig. 3 as a function of L for four values of l_0.

For figures 2 and 3 the Eqs. (62) and (83) were used. The results agree with those obtained from Eqs. (61) and (82), exept for a narrow region around $L = l_0$, where a step function is compensated numerically. The method of integration parallel to the imaginary axis, Eq. (64), was also tested numerically using a rather complicated real integrand generated by computer algebra.

8 conclusions

The δ-functions used to describe the exchange coupling of magnetic layers to the spin of conduction electrons produce bound states. These have not been discussed so far in treatments of the indirect interactions of the magnetic layers. The standard perturbative treatment of the one dimensional case by Kittel[1] leads to a coupling of unlimited range. This was corrected by Yafet[2] who proposed an ad hoc way to integrate over a singularity. Here it is shown that the bound states are responsible for the finite range of the interaction in the weak coupling limit in one dimensional geometries. Bound states require non perturbative methods. Bruno[4] introduced a treatment, which goes beyond perturbation theory. Explicitely it deals with the free states only. His result, Eq. (1) of ref.[4] agrees with the expressions for the free states. Since the energies of the bound states are poles of his Green's functions in ref. [12], a particular integration prescription in the complex k_z plane exists which gives the complete result.

The range of the bound states defines a length l_0, which, however, does not appear in the shape of the interaction. The question whether distances connected with bound states show up in the indirect interactions of magnetic layers is of current interest[8][9][5]. The present problem is a particular case, which can be treated analytically.

In conclusion, this paper presents a consistent theory of the indirect interaction between two magnetic layers described by planar δ-functions coupled to a degenerate electron gas. Closed formulas valid for any coupling strength are given. The general result follows closely the weak coupling limit until the binding energy becomes larger than the Fermi energy.

Appendix A

A heuristic argument is applied to the simple system with one magnetic layer, whereby formulas which appear throughout this paper can be visualized. Using the boundary condition of an incoming plane wave, $e^{ik_z z}|\pm\rangle$, the transmission coefficient $t_\pm$ and the reflection coefficient $r_\pm$ are obtained as

$$t_\pm = \frac{\pm i k_z l_0}{\pm i k_z l_0 + 1} = 1 - r_\pm. \tag{A.1}$$

The transmitted and reflected waves suffer a phase change

$$t_\pm = |t_\pm|\, e^{i\phi_{t,\pm}}, \qquad r_\pm = |r_\pm|\, e^{i\phi_{r,\pm}}. \tag{A.2}$$

The derivatives of the phase shifts with respect to the energy $\epsilon = \hbar^2 k_z^2/2m$ are time delays[13]

$$\tau_\pm = \hbar\frac{\partial\phi_{t,\pm}}{\partial\epsilon} = \hbar\frac{\partial\phi_{r,\pm}}{\partial\epsilon}. \tag{A.3}$$

The change of the number of particles is the product of time delays and outgoing fluxes:

$$\begin{aligned}
\Delta N_\pm(k_z) = &\quad 2\tfrac{\hbar k_z}{m}\left(|t_\pm|^2 + |r_\pm|^2\right)\tau_\pm = 2\tfrac{\partial\phi_{t,\pm}}{\partial k_z} && \text{(A.4)}\\
= &\quad 2\tfrac{\partial}{\partial k_z}\,\mathrm{Im}\,\ln(t_\pm) = \pm 2\tfrac{\partial}{\partial k_z}\arctan\left(\tfrac{1}{k_z l_0}\right) && \text{(A.5)}\\
= &\quad \tfrac{\mp 2 l_0}{1 + k_z^2 l_0^2} && \text{(A.6)}
\end{aligned}$$

where the factor 2 accounts for the two fluxes with $\pm k_z$. The last expression coincides with Eq. (20) for $k_z > 0$.

Figure Captions

Figure 1 - Energies of the bound states of two δ-functions a distance L apart. E_1 and E_2 belong to the localized symmetric and antisymmetric states of the parallel spin configuration, and E_3 to the two degenerate states of the antiparallel spin configuration. Distance in units of l_0 and energies in units of ϵ_0.

Figure 2 - Interaction energy per unit area between two magnetic layers in the parallel spin configuration for $l_0 = 8$. $\Xi_{b,p}$ and $\Xi_{f,p}$ are the contributions from the bound and free states, respectively. Their sum Ξ_p shows a remarkable cancellation. Distance L in units of k_F^{-1}, and Ξ in units of $E_F k_F^2$.

Figure 3 - Energy difference per unit area $\Delta\Xi$ between the parallel and antiparallel configurations of two magnetic layers as a function of their separation L for various values of the coupling constant. $\Delta\Xi$ in units of $E_F/(\pi^2 l_0^2)$, and L in units of k_F^{-1}. For vanishing coupling constant (full line) $\Delta\Xi = -\pi$ for $L = 0$ in these units. Long dashes show a case of weak coupling: $k_F l_0 = 8$ so that $E_F/\epsilon_0 = 32$. Intermediate dashes belong to intermediate coupling: $k_F l_0 = \sqrt{2}$ i.e. $E_F/\epsilon_0 = 1$. Strong coupling (short dashes) with $k_F l_0 = 0.5$, $E_F/\epsilon_0 = 0.125$ leads to a rapidly damped interaction.

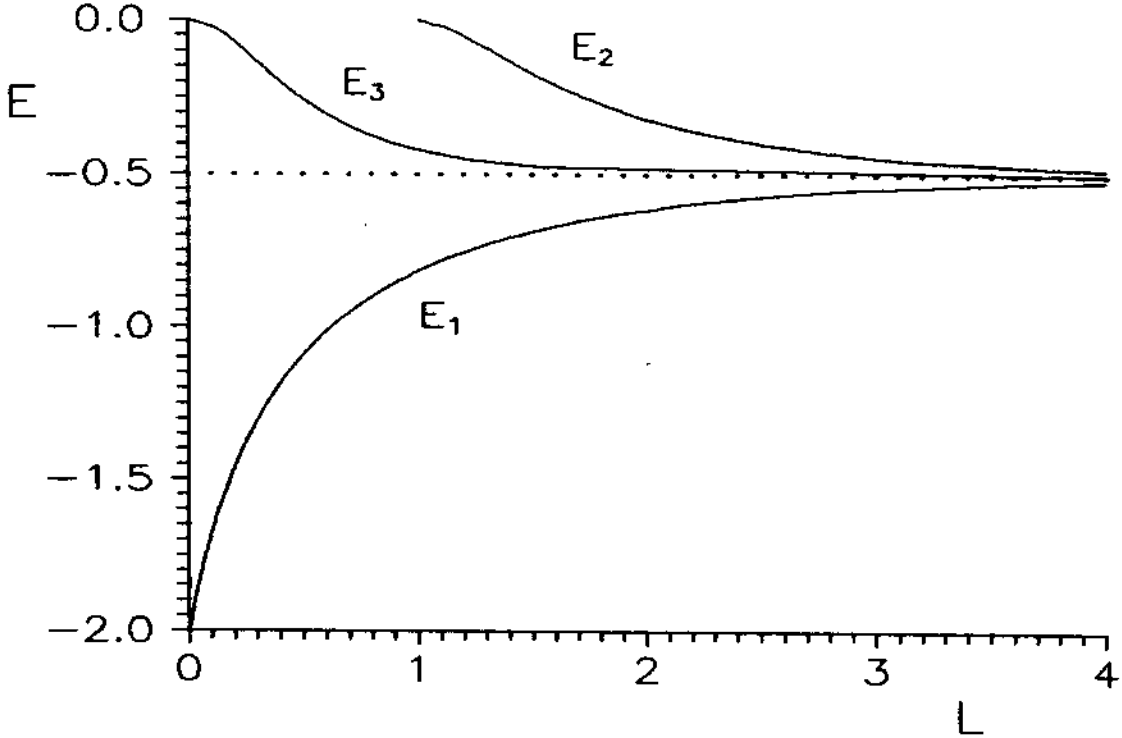

Fig. 1

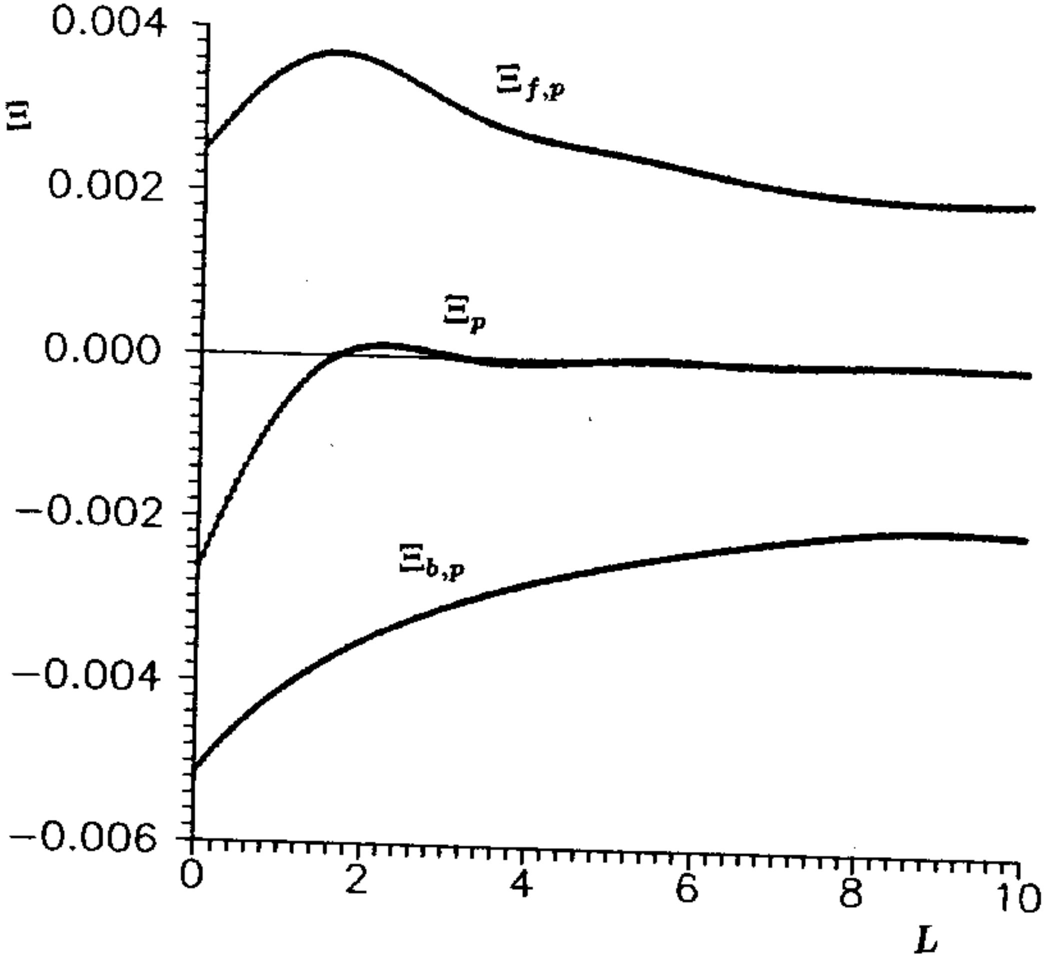

Fig. 2

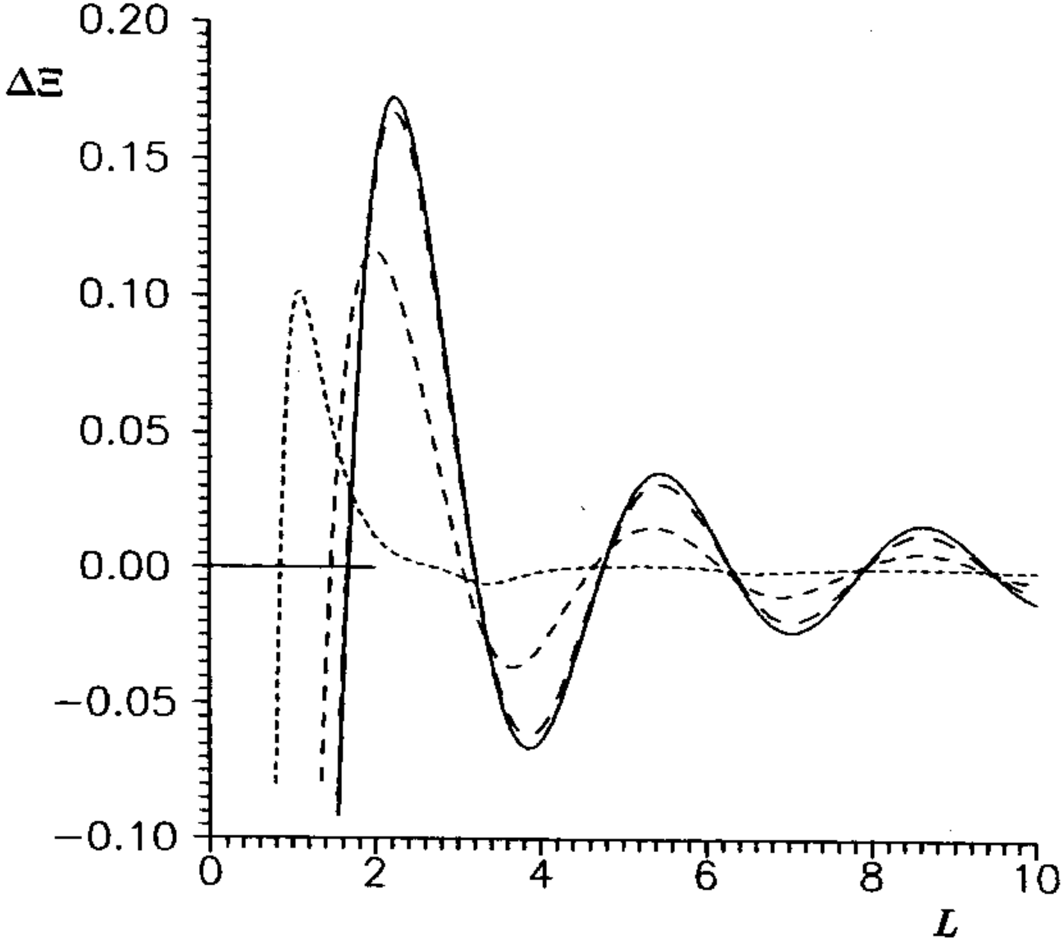

Fig. 3

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