CBPF-NF-077/95

Estimate of Coulomb energies in the non-linear theory of magnetic multilayers

W. Baltensperger and *J.S. Helman*

Centro Brasileiro de Pesquisas Físicas (CBPF),

Rua Dr. Xavier Sigaud 150, Rio de Janeiro, RJ 22290, Brazil

Abstract

A magnetic plane, exchange coupled to an electron gas, generates besides the spin polarization also a charge distribution. The corresponding electrostatic energy per unit surface is evaluated. For an electron gas at metallic densities this is negligible, while it must be taken into account in dilute degenerate semiconductors.

Key-words: Magnetic Multilayers; Coulomb Energy.

PACS: 75.30.Hx, 75.70.-i

In the Ruderman-Kittel theory [1] the spin polarization is linear in the coupling constant of the exchange interaction between magnetic ions and the spins of conduction electrons. The changes in the charge densities of the upspin electrons are then exactly compensated by those of the downspin electrons. In the non-linear theory [2,3], however, this compensation is incomplete. The theory is exact for a Hamiltonian which does not contain Coulomb energies. A more realistic model should include such terms. The present paper contains an estimate of the Coulomb energies.

Since charge densities already exist with one magnetic plane [3], let us consider this case. The charge density per unit surface is given by Eq. (16) of Ref. [3], which using Eqs. (8) and (12) of Ref. [3] results in

$$\begin{aligned} Q(z) = & \quad e\frac{k_F^2+l_0^{-2}}{4\pi l_0}\mathrm{e}^{-2|z|l_0^{-1}} \\ & - \frac{e}{2\pi^2}\int_0^{k_F} dk\ (k_F^2-k^2)\,\frac{\cos(2kz)}{1+k^2l_0^2}, \end{aligned} \tag{1}$$

where the first term is due to the localized band and the second due to conduction electron states. e is the charge of an electron, z the distance from the plane, k_F the Fermi wave number and $l_0 = \hbar^2/(\beta m)$ the range of the localized states, which is reciprocal to the exchange coupling constant β, m being the mass of an electron. Eq. (1) corresponds to a net charge per unit surface of

$$\int_{-\infty}^{\infty} Q(z)\,dz = \frac{e}{4\pi\, l_0^2} < 0. \tag{2}$$

This increase of the integrated electron density is made possible by the use of the grand canonical potential, which keeps the chemical potential fixed. Note that in vacuum an infinite plane with a net charge per unit surface produces an infinite electrostatic energy per unit surface, corresponding to the fact that the lines of force which are perpendicular to the surface extend to infinity. In a metal, however, the charges are screened [4]. The interaction between two charges separated by a distance r takes the form $e^2\,\mathrm{e}^{-k_c r}/r$, where k_c is the screening parameter. Since the charge density has planar symmetry and is an even function of the coordinate z, the interaction energy per unit surface becomes

$$E_c = \tfrac{1}{2}\int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz'\, 2\pi \int_0^{\infty} \rho\, d\rho\, Q(z)\, Q(z')\, \frac{\mathrm{e}^{-k_c\sqrt{\rho^2+(z-z')^2}}}{\sqrt{\rho^2+(z-z')^2}} \tag{3}$$

$$= \tfrac{\pi}{k_c}\int_0^{\infty} dz \int_0^{\infty} dt\, Q(z)\, Q(z+t)\, \mathrm{e}^{-k_c t}. \tag{4}$$

E_c is a positive quantity [5].

In this paper we evaluate E_c using the density of Eq. (1) obtained with a Hamiltonian without charge interactions. This corresponds to lowest order perturbation theory and indicates the range of exchange couplings for which charge effects can be neglected. Inserting $Q(z)$ of Eq. (1) into Eq. (4) gives three kinds of terms: bound charges interacting with bound charges, free-free couplings and cross terms. The corresponding integrals can be done analytically. The weak coupling expansion of each of these contributions contains terms of order l_0^{-1} and l_0^{-3}, which, however, cancel so that E_c is of order l_0^{-4}. This shows that the bound states have to be included even in the weak coupling limit, since otherwise terms of order l_0^{-1} would dominate the whole calculation. The closed result is

$$\begin{aligned} E_c = \quad & \tfrac{e^2}{32\pi^2 l_0^4 k_c (l_0^2k_c^2-4)^2}\{ -2l_0k_c(l_0^2k_F^2+1)^2(l_0^2k_c^2-12)\arctan(l_0k_F) \\ & + 2l_0^2k_F^2((k_c/k_F)^2+4)(l_0^2k_c^2-8-4l_0^2k_F^2)\arctan(2k_F/k_c) \\ & + (l_0^2k_F^2+1)\,(l_0k_c-2)\,[\pi\,(l_0^2k_F^2+1)\,(l_0k_c(l_0k_c+2)-8) - 2l_0^2k_ck_F(l_0k_c+2)]\}. \end{aligned} \tag{5}$$

In the weak coupling limit, $l_0k_F \to \infty$, this becomes

$$\begin{aligned} E_c \Rightarrow \tfrac{e^2k_F^4}{48\pi^2 l_0^4 k_c^5}\Big\{ & 3\left[(k_c/k_F)^4 - 16\right]\arctan\left(2k_F/k_c\right) \\ & + \quad 2\left[(k_c/k_F)^3 - 12\,(k_c/k_F) + 12\pi\right]\Big\}. \end{aligned} \tag{6}$$

This differs by about 1 % from Eq. (5) for $l_0k_F = 1.5$.

The Coulomb selfenergy E_c is to be compared with the magnitude of the grand potential of the magnetic plane per unit surface, $|\xi|$, Eq. (29) of Ref. [3]. Table I shows this ratio for several electron densities n and effective masses m^*, so that situations of metals and of degenerate semiconductors are covered. For the exchange coupling constant the value $\beta = 0.3$ eV $\mathring{A}$ was assumed. The screening parameter suggested by Pines [4], $k_c = 0.353\sqrt{r_s}k_F$, was adopted with $(4\pi/3)(r_sa_B)^3 = 1/n$, $a_B = \hbar^2/(e^2m^*)$ being the

Bohr radius. Table I also lists the values of ϵ_0/E_F, where $\epsilon_0 = \beta^2 m^*/\hbar^2 = -2E_0$ with E_0 the lowest energy of the localized band [3]. It is seen that the region where the electrostatic energy dominates, $E_c/|\xi| > 1$, is contained within the domain of strong coupling: $\epsilon_0/E_F > 1$. When $E_c > |\xi|$, however, our estimate of E_c which corresponds to a Born approximation is not reliable. At metallic densities the electrostatic energy is negligible. In multilayer configurations each plane carries a charge density of the same (negative) sign. Since there is no compensation, the domain where electrostatic energies can be neglected, should be similar to that of one plane.

TABLES

n	$m*/m$	$E_c/\|\xi\|$	ϵ_0/E_F
10^{15}	0.1	$1.6\ 10^{0}$	$3.2\ 10^{0}$
10^{15}	0.3	$5.5\ 10^{0}$	$2.9\ 10^{1}$
10^{15}	1.0	$1.4\ 10^{1}$	$3.2\ 10^{2}$
10^{17}	0.1	$8.3\ 10^{-2}$	$1.5\ 10^{-1}$
10^{17}	0.3	$7.7\ 10^{-1}$	$1.4\ 10^{0}$
10^{17}	1.0	$4.0\ 10^{0}$	$1.5\ 10^{1}$
10^{19}	0.1	$2.4\ 10^{-3}$	$7.0\ 10^{-3}$
10^{19}	0.3	$3.1\ 10^{-2}$	$6.3\ 10^{-2}$
10^{19}	1.0	$4.1\ 10^{-1}$	$7.0\ 10^{-1}$
10^{21}	0.1	$5.8\ 10^{-5}$	$3.2\ 10^{-4}$
10^{21}	0.3	$8.4\ 10^{-4}$	$2.9\ 10^{-3}$
10^{21}	1.0	$1.5\ 10^{-2}$	$3.2\ 10^{-2}$
10^{23}	0.1	$7.6\ 10^{-7}$	$1.5\ 10^{-5}$
10^{23}	0.3	$2.0\ 10^{-5}$	$1.4\ 10^{-4}$
10^{23}	1.0	$3.8\ 10^{-4}$	$1.5\ 10^{-3}$

TABLE I. Ratio of screened electrostatic energy E_c to the magnitude of the exchange interaction energy of a magnetic plane $|\xi|$ for various values of the electron density n and the effective mass m^*. The ratio of ϵ_0, half the binding energy of the bound state, to the Fermi energy E_F is a measure of the coupling strength.

REFERENCES

[1] C. Kittel, in *Solid State Physics*, edited by F.Seitz, D. Turnbull and H. Ehrenreich, (Academic, New York, 1968), Vol.22, p.11.

[2] P. Bruno, Europhys.Lett., **23**, 615 (1993), J. Magn. & Magn. Mater, **121**, 248 (1993) and Phys.Rev. B **52**, 411 (1995).

[3] J.S. Helman and W. Baltensperger, Phys.Rev. B, (to appear).

[4] David Pines, in *Solid State Physics*, edited by F.Seitz, D. Turnbull and H. Ehrenreich, (Academic, New York, 1968), Vol.1, p.367.

[5] J.D. Jackson, *Classical Electrodynamics*, John Wiley, N.Y., pg. 21, 1^{st} ed., (1967). This proof for the Coulomb interaction is easily adapted to the screened Coulomb coupling of Eq. (3) or the exponential coupling of Eq. (4).