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Field-induced magnetization of a free-electron gas in thin films

T. BALCERZAK[1*]

[1]Department of Solid State Physics, University of Łódź, Pomorska 149/153, 90-236 Łódź, Poland

A free-electron model in thin film embeded in an external magnetic field is considered. Based on the paramagnetic susceptibility, a formula for magnetization of the electron gas in the uniform magnetic field is derived. Selected results are presented for the films with the thickness of several atomic planes, and with the electron density corresponding to copper.

Key words: *thin film; free-electron gas; paramagnetic susceptibility; magnetization*

1. Introduction

Studies of combined electronic and magnetic properties of thin films are important from the point of view of modern technology [1]. As far as the theoretical description is concerned, the model of free electrons placed in a quantum well turned out to be very useful for the discussion of various physical properties of thin films [1, 2]. In the present paper, this model will be further analyzed in order to study the magnetization of the electronic gas in thin films when the magnetization is induced by the external field.

Thin film is understood here as a set of n monoatomic layers perpendicular to the z-axis, with each layer having its own thickness d. As a result, the total thickness of the film is given by $L_z = nd$, and the total volume is $V = L_z S$, where S is the film surface area $(\sqrt{S} >> L_z)$. Apart from the thickness, the important parameter is a dimensionless electron density ρ, defined by the formula: $\rho = (N_e/V)d^3$, where N_e is the total number of electrons in the sample, and the volume is expressed in d^3 units.

The considerations of single-particle electronic states in such a model system lead to the discretization of the Fermi surface, as discussed in detail in [3]. In particular, the formulas for the Fermi wave vector k_F in thin film and the parameter τ_F have been

*Corresponding author, e-mail: t_balcerzak@uni.lodz.pl

derived, where τ_F is the highest number of the standing-wave mode in the ground state. In order to avoid a redundant repetition of the formalism, for the method of determination of k_F and τ_F adopted in this paper the reader is referred to Ref. [3].

2. Theory

The magnetization of the electron gas (i.e., the magnetic moment per unit volume) induced by the external field at a point $(z,\vec{r})$ of the thin film is given by the expression:

$$\sigma(z,\vec{r}) = \frac{1}{V}\sum_{p}\sum_{\vec{q}} \chi_{p,\vec{q}} H_{p,\vec{q}} \exp\left[-i\left(\frac{2\pi}{L_z}\right)pz\right]\exp[-i\vec{q}\vec{r}] \tag{1}$$

where $\vec{r}$ denotes the position of a given point in the film plane, whereas z denotes the coordinate perpendicular to the film ($0 \le z \le L_z$). $H_{p,\vec{q}}$ is the Fourier component of the external field and $\chi_{p,\vec{q}}$ stands for the paramagnetic susceptibility. In Eq. (1), a quasi-continuous summation over $\vec{q}$ is performed in the film plane, and the discrete summation over p ($p = 0, \pm1, \pm2, ...$) concerns the perpendicular modes.

The paramagnetic electronic susceptibility in a thin film is given by the formula [4]:

$$\chi_{p,\vec{q}} = \frac{m}{\hbar^2} g_e \mu_B \frac{1}{2}\sum_{\tau=1}^{\tau_F}\left[f_{\tau,|\tau+2p|}(q) + f_{\tau,|\tau-2p|}(q)\right] \tag{2}$$

where $f_{\tau,\tau'}(q)$ is a generalized Lindhard function:

$$f_{\tau,\tau'}(q) = \frac{S}{4\pi}\left(1+\frac{a_{\tau,\tau'}}{q^2}\right)\left[1-\sqrt{1-b_{\tau,\tau'}(q)}\,\theta\left(1-b_{\tau,\tau'}(q)\right)\right] \tag{3}$$

where

$$a_{\tau,\tau'} = \left(\frac{\pi}{L_z}\right)^2\left(\tau'^2-\tau^2\right) \tag{4}$$

$$b_{\tau,\tau'}(q) = \left(\frac{2k_{F\tau}}{q}\frac{1}{1+\frac{a_{\tau,\tau'}}{q^2}}\right)^2 \tag{5}$$

and

$$k_{F\tau}^2 = k_F^2 - \frac{\pi^2\tau^2}{L_z^2} \tag{6}$$

It has been shown in Ref. [4] that Eq. (3) presents a generalization of the ordinary Lindhard function as being discussed in [5] for a two-dimensional system.

Assuming in Eq. (1) that the external field is spatially uniform, we have:

$$H_{p,\vec{q}} = H\delta_{p,0}\delta_{\vec{q},0} \tag{7}$$

With the help of Eqs. (7) and (2)–(6) we can then obtain from Eq. (1) the magnetization induced by this field in the form:

$$\sigma(z,\vec{r}) = \frac{1}{V}\chi_{0,0}H = \frac{1}{4\pi}\frac{m}{\hbar^2} g_e^2 \mu_B^2 \frac{\tau_F}{L_z} H \equiv \sigma \tag{8}$$

For such a case it is seen from Eq. (8) that the magnetization of electron gas in the film is also uniform (we denote it by σ).

As a system with the reference magnetization, we shall assume the bulk material in which the magnetization of the electron gas induced by the same external field is given by the formula:

$$\sigma_0 = \frac{1}{V}\chi_P^b H = \frac{1}{4\pi^2}\frac{m}{\hbar^2} g_e^2 \mu_B^2 k_F^b H \tag{9}$$

In Eq. (9) χ_P^b is the Pauli paramagnetic susceptibility [6] and k_F^b is the Fermi wave vector of the bulk material. By dividing Eqs. (8) and (9) by sides, we finally obtain the relative field-induced magnetization in the form:

$$\frac{\sigma}{\sigma_0} = \pi\frac{\tau_F}{n}\frac{1}{dk_F^b} \tag{10}$$

The above magnetization depends on the film thickness L_z and the electron density ρ (via dependence of τ_F and k_F^b upon ρ). In the limiting case (when $n \to \infty$) we have $\pi\tau_F/nd \to k_F^b$ (see [3]) and thus $\sigma \to \sigma_0$.

3. Numerical results and discussion

The numerical results are obtained based on Eq. (10). The value of $d = 1.805$ Å is assumed to correspond to the interplanar distance of the (100) planes in copper. In Fig. 1, the relative magnetization σ/σ_0 is shown for several film thicknesses n, when the dimensionless density ρ is freely changed from 0 to 1. The value of $\rho = 0.5$ corresponds exactly to copper. It can be seen that for the monolayer (with $n = 1$), magnetization is a monotonously decreasing function of ρ (whereas $\sigma > \sigma_0$). It is connected with the fact that for $n = 1$ we have the only value $\tau_F = 1$ in this range of ρ. However, for $n = 2$ and $n = 3$ the curves are no longer monotonic. For instance, for $n = 2$, a jump of magnetization can be observed at $\rho = 0.589$, which is connected with the change from $\tau_F = 1$ to $\tau_F = 2$, whereas ρ increases. In the same way, two jumps are apparent for $n = 2$; the first at $\rho = 0.175$ is connected with the change from $\tau_F = 1$ to $\tau_F = 2$, and the second at $\rho = 0.756$ is the change from $\tau_F = 2$ to $\tau_F = 3$. In particular, it can be seen in Fig. 1 that for $\rho = 0.5$ the magnetization of the trilayer system (with $n = 3$) is between those of $n = 1$ and $n = 2$.

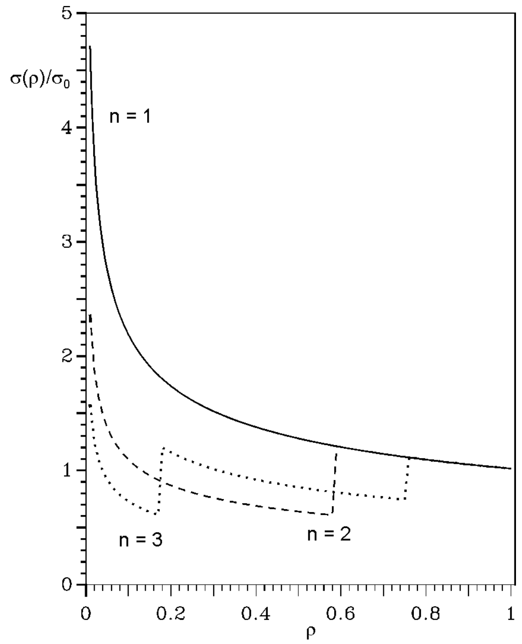

Fig. 1. Dependence of the field-induced relative magnetization σ/σ_0 of the electron gas upon the dimensionless density ρ. The three curves labelled by $n = 1$ (solid), $n = 2$ (dashed) and $n = 3$ (dotted) correspond to various film thicknesses

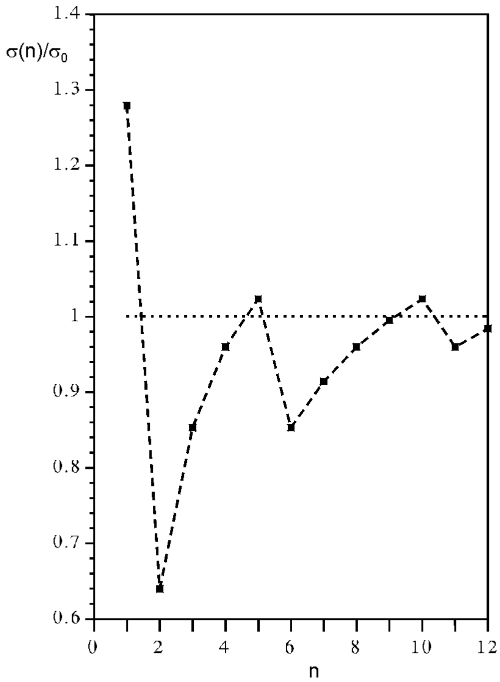

Fig. 2. Dependence of the field-induced relative magnetization σ/σ_0 of the electron gas upon the film thickness n, when $\rho = 0.5$. The interplanar distance is $d = 1.805$Å (the same as in Fig. 1), which corresponds to the (100) film of copper

Figure 2 corresponds to the case when $\rho = 0.5$ is constant but the thickness n changes. One can see that the magnetization is an oscillating, saw-toothed function of the film thickness. The amplitude of the oscillations decreases as n increases. A detailed analysis shows that this behaviour is the same as the oscillations of the density of states at the Fermi surface, as found for this model in [3]. It is worth noting that the oscillating behaviour of the density of states has been found experimentally ([2] and references therein). Thus, we see that the behaviour of the field-induced magnetization in thin films is directly correlated with the density of states at the Fermi level. Such a correlation could be expected to some extent because an analogous relationship is well established in bulk materials. However, in the bulk material there are no size-dependent oscillations. The final conclusion which can be drawn from the paper is of a general character: despite of the relatively simple model considered here, the predicted results seem to be interesting and non-trivial.

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