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DECAY OF THE ELECTRONIC SPIN POLARIZATION OUTSIDE A SURFACE OF A FERROMAGNETIC METAL

by

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Abstract

It is shown that the spin polarization of the electron cloud in thermal equilibrium with a ferromagnetic surface decays within a few Angstroms from the surface. This explains the vanishing spin polarization found in thermoemission from Ni and Fe by Vaterlaus et al [*Phys. Rev. Letters* **65**, 3041 (1990)].

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A. Vaterlaus et al[1] have discovered that the spin polarization of electrons thermoemitted from cesiated surfaces of Ni and Fe vanishes. This is contrary to expectation, if one considers that inside ferromagnetic materials the densities of states for spin up and spin down electrons differ even at the vacuum level. This letter calls attention to the fact that thermoemitted electrons are extracted from the electron cloud outside the surface, which is depolarized in agreement with experiment.

The electrons outside the surface are trapped by the long range image potential. The question arises: what is the spin polarization of an electron gas outside a homogeneously magnetized ferromagnet? If the outside gas were homogeneous and degenerate with the same density as in the inside, the answer would be obtained from the Ruderman-Kittel[2] susceptibility. In that case an integration over a homogeneous exchange coupling inside the ferromagnetic half space produces an oscillating and decaying polarization $P(L)$ at a distance L outside[3]:

$$\begin{aligned} P(L) &= (JN\chi_P/2)\,F(2k_F L) \\ F(x) &= [x\,\mathrm{si}(x) + \sin(x)/x + \cos(x)]/2 \end{aligned} \tag{1}$$

with $\mathrm{si}(x) = -\int_x^\infty dt\,\sin(t)/t$. Here $P(L)$ is the net electron spin per unit volume, and k_F the Fermi vector. χ_P is the Pauli susceptibility which gives the spin density per exchange field, $\chi_P = D_F/2$ where $D_F = mk_F/2\pi^2\hbar^2$ is the density of states at the Fermi level per spin. J is the exchange coupling constant with dimension erg cm^3, N the density of ion spins in the ferromagnet, and m the electron mass. A similar theory applied to a Boltzmann gas gives a positive susceptibility[4]. It has a Gaussian space dependence with a range $k_T^{-1} = \hbar(2mk_BT)^{-1/2}$. Here k_T equals the wave number of an electron with thermal kinetic energy k_BT; it is independent of the density of electrons.

If the Boltzmann gas, with density n_B , would fill the whole space, the polarization outside the ferromagnet would be given by

$$P_B(L) = (JN\chi_B/2)\,G(k_BL)$$
$$G(x) = e^{-x^2} - \sqrt{\pi}x[1-\Phi(x)], \qquad \Phi(x) = (2/\sqrt{\pi})\int_0^x dt\ e^{-t^2}. \tag{2}$$

$\chi_B = n_B/(4k_BT)$ is the analog to χ_P for the Boltzmann gas. $F(x)$ and $G(x)$ are shown in Fig.1.

Within the ferromagnet the polarization of the electron gas shows also a space dependence. In a model in which the electron gas inside the ferromagnet is subject to an exchange field, the polarization as a linear response is that of the field in the whole space plus that of a compensating field outside. Thus, inside, the polarization is obtained by replacing $F(x)/2$ by $1 - F(|x|)/2$.

It is important to realize that these space dependencies of the polarization result from the perturbation of the exchange interaction on the spin-up and spin-down wave functions, which lead to inhomogeneous densities in space. In particular the vanishing polarization in the outer regions has nothing to do with spin flips or mean free paths. It is a simple consequence of this model that the polarization decreases to zero in the outer region. Note that a similar one-dimensional model would lead to spin polarizations at unlimited distances[5].

Outside an actual surface the electron cloud is not homogeneous. If it is degenerate close to the surface, then its density and the corresponding value k_F vary rapidly with distance. In this area a functional density theory may be appropriate[6]. In the outer part, the Fermi-Dirac distribution is used at its high energy end, where it is a

Boltzmann distribution. In this case the range k_T^{-1} is space independent and determines the decay.

For the temperature $T = 450$ K of the experiment[1] , $k_T^{-1} = 10$ Å. The potential of the image force and an extracting field E, $V(L) = -e^2/(4L) - EeL$ has a maximum at $L = (1/2)(e/E)^{1/2}$. For a field $E = 1$ statVolt/cm this amounts to $L = 1000$Å, which is much larger than k_T^{-1}. The electron cloud in that area is not polarized. Furthermore, the current of thermally emitted electrons will not appreciably modify this equilibrium distribution. Since the thermally emitted electrons emerge from this area they are not polarized. Only experiments which probe the electron cloud at a few Angstroms from the surface such as Electron Capture Spectroscopy (ECS)[7] or Scanning Tunneling Microscopy (STM)[8] could detect its spin polarization.

In photo-emission the excitation of an electron from an occupied state into an empty state above the vacuum level takes place in the bulk. The dipole operator of the matrix element of this transition is spin independent. Therefore the excited states, which are only weakly perturbed by the exchange forces, are selected to match the spin polarization of the initial states. Hence this polarization is carried into the vacuum.

It is noteworthy that the absence of spin polarization of the thermally emitted electrons stems directly from the subtle questions which gave rise to the papers of Yosida[9] and Van Vleck[10] on the methods of calculation of the Ruderman–Kittel polarization. We mention this because often erroneously the Pauli spin susceptibility alone is considered in this problem. The analysis of Yosida shows that this contribution is exactly equal to that arising from the term $\mathbf{k}' = \mathbf{k}$ in the perturbation expansion of the one particle state $\phi_{\mathbf{k}}$. This term must be left out in Yosida's treatment. In view of this, the Pauli term is incorporated into the sum, resulting in an integration with principal parts over all $\mathbf{k}'$. This then coincides with the method of Ruderman and Kittel, in which the Fermi spheres for up and down spins are equal, but where the integration is done with principal parts. This treatment actually implies perturbed wave functions whose admixture is not orthogonal to the unperturbed state, so that they are not normalized to linear order in the perturbation[11]. The result of the two treatments is the same: around each point at which an exchange field acts there is a local polarization cloud, and there is no background of long range polarization in regions without an exchange field, as one would expect considering only unequal Fermi spheres.

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Figure Captions

Dimensionless functions which describe the decay of the polarization of a degenerate, $F(x)$,and non-degenerate (Boltzmann), $G(x)$, electron gas outside a ferromagnetic half space, where the dimensionless variable x stands for $2k_F L$ or $k_T L$, respectively.

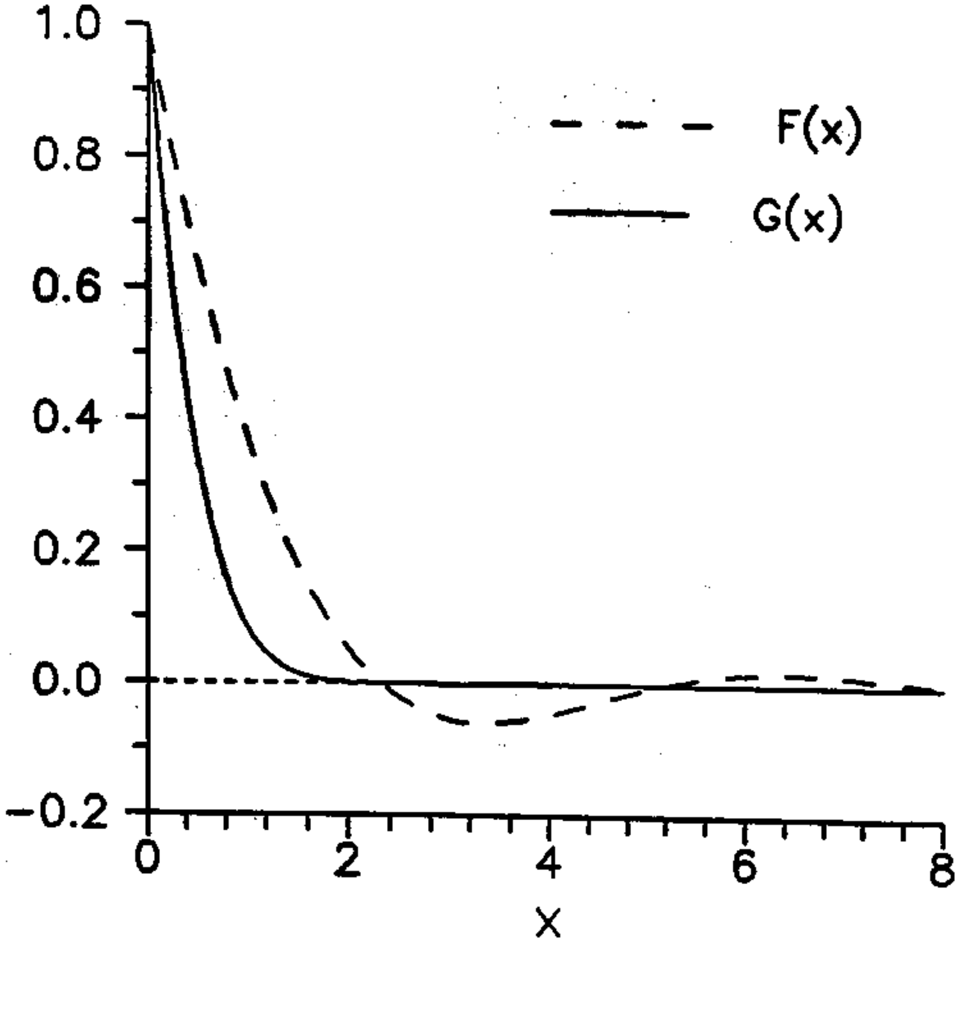

Fig. 1

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