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SPIN SUSCEPTIBILITY OF AN ELECTRON GAS IN A TIME DEPENDENT HOMOGENEOUS MAGNETIC FIELD

by

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ABSTRACT

In calculations of the Pauli susceptibility, χ_p, spin flip processes are ignored but for the implicit recognition that they must provide the angular momentum to populate states with different magnetizations. These processes are here taken into account within the linear response formalism using a model Hamiltonian. Corrections introduced into the dynamic and Lindhard's susceptibilities are also calculated.

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1 INTRODUCTION

In elementary textbooks on solid state physics [1], the Pauli susceptibility χ_P is derived from the Fermi distributions of the electrons with spin up and spin down, whose energies, in the presence of an external magnetic field B, are modified in the amounts $\mp \mu_B B$ respectively. It results

$$\chi_P = \frac{mk_F}{\pi^2} \mu_B^2 \qquad (1)$$

where k_F is the Fermi wavector, m is the free electron mass and μ_B is the Bohr magneton. It is not mentioned, however, how the new thermodynamical equilibrium is reached after the field is applied. That is, there is no reference to the spin flip mechanism which provides the necessary angular momentum to the electron system. [2]

In more advanced treatments [3], χ_P is obtained as the long wavelength limit ($q \to 0$) of the linear response $\chi(q)$ to a magnetic field which varies in space with wave vector q. It is not obvious, however, that such a limiting process must lead to the correct result. For $q \neq 0$, the average space magnetization is zero; regions of positive and negative magnetization are compensated. Thus, no spin flip process is necessary and the separation of spin up and spin down electrons can take place very fast, with velocities of the order of the Fermi velocity v_F as expressed by the Lindhard formula $\chi_L(q,\omega)$. [4]. Let us see this in more detail by using the Kubo formalism [5]; we have

$$\chi(q,\omega) = iF\langle[\vec{m}_{\vec{q}}(t) , m_{-\vec{q}}(0)]\rangle \quad . \tag{2}$$

Here F denotes de Fourier transform, <...> stands for thermodynamical average and

$$m_{\vec{q}}(t) = e^{iHt} m_{\vec{q}}(0) e^{-iHt} \tag{3}$$

where H is the Hamiltonian of the system, which for the free electron gas reads

$$H = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} a^{+}_{\vec{k},\sigma} a_{\vec{k},\sigma} \quad , \tag{4}$$

where $\varepsilon_{\vec{k}}$ is the free electron energy and $a^{+}_{\vec{k}\sigma}$ and $a_{\vec{k}\sigma}$ are the creation and destruction electron operators corresponding to momentum $\vec{k}$ and spin σ . Here,

$$m_{\vec{q}} = \sum_{\vec{k}} m_{\vec{k},\vec{q}} \tag{5}$$

with

$$m_{\vec{k},\vec{q}} = a^{+}_{\vec{k}+\vec{q}\uparrow} a_{\vec{k}\uparrow} - a^{+}_{\vec{k}+\vec{q}\downarrow} a_{\vec{k}\downarrow} \tag{6}$$

Using the commutation relations

$$[H, m_{\vec{k},\vec{q}}] = (\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}) m_{\vec{k},\vec{q}} \tag{7}$$

and

$$\left[m_{\vec{k}',\vec{q}}\ ,\ m_{\vec{k},-\vec{q}}\right] = 2\delta_{\vec{k}',\vec{k}-\vec{q}}\left[n_{\vec{k}',\vec{k}+\vec{q}} - n_{\vec{k}'}\right] \tag{8}$$

where $n_{\vec{k}} = a^{+}_{\vec{k}} a_{\vec{k}}$, we have

$$e^{iHt}\, m_{\vec{k},\vec{q}}\, e^{-iHt} = e^{i(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}})t} m_{\vec{k},\vec{q}} \tag{9}$$

and Eq. (2) leads to

$$\chi_L(q,\omega) = -2\sum_{\vec{k}} \frac{f(\vec{k}+\vec{q}) - f(\vec{k})}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} - \omega - i\eta} \tag{10}$$

where $f(\vec{k})$ is the Fermi distribution.

The fact that H does not commute with the $\vec{q}$ component of the magnetization for $\vec{q} \neq 0$, (Eq. (7)), means that the kinetic energy alone induces local fluctuations of the magnetization. On the other hand, it cannot produce fluctuations of the total magnetization since

$$\left[H, m_o\right] = 0 \tag{11}$$

rigurously. It is therefore a dubious procedure (which at least needs some justification) the obtention of χ_P from the limit of $\chi_L(q,0)$ for $q \to 0$, when we know that H alone can only lead to $\chi(0,0) = 0$. The point $q = 0$ must be a singularity.

In other words, a finite $\chi(q,\omega)$ for $q \neq 0$ is compatible with angular momentum conservation, while a finite $\chi(0,\omega)$ requires a source of angular momentum.

2 A MODEL FOR THE INTRODUCTION OF SPIN-FLIP PROCESSES

Let us assume the existence of some perturbation which induces spin-flips in the electron gas. For instance an exchange interaction with a system of diluted localized spins, S, of the form

$$H_{sf} = \sum_{i=1}^{K} \vec{S}_i . \vec{s}\, \lambda(\vec{r} - \vec{R}_i) \tag{12}$$

where $\vec{S}_i$ is the spin operator of the localized spin at site $\vec{R}_i$, $\vec{s}$ is the conduction electron spin operator and $\lambda(\vec{r} - \vec{R}_i)$ the exchange integral. The spin-flip terms (the only ones in which we are interested) in second quantized form read

$$H_{sf} = \frac{1}{2} \sum_{\vec{k}} \sum_{\vec{q}} \{\lambda_{\vec{q}} S^{+}_{\vec{q}} a^{\dagger}_{\vec{k}+\vec{q}\downarrow} a_{\vec{k}\uparrow} + \lambda_{-\vec{q}} S^{-}_{-\vec{q}} a^{\dagger}_{\vec{k}\downarrow} a_{\vec{k}+\vec{q}\uparrow}\} \tag{13}$$

where

$$S^{\mp}_{\vec{q}} = \sum_{i=1}^{K} S^{\pm}_i e^{-i\vec{q}.\vec{R}_i} \tag{14}$$

and

$$\lambda_q = \int d^3r \lambda(r) e^{-i\vec{q}.\vec{r}} \quad . \tag{15}$$

Eq. (13) can also be written in alternative, more familiar forms, however, the form used is more convenient for our purposes because each $\vec{q}$-term of the sum is manifestly hermitic.

In the problem we are dealing with, H_{sf} cannot be treated

as a small perturbation. For $H_{sf} = 0$ there is no susceptibility as expressed by Eq. (11), and an infinitesimal interaction H_{sf} is enough to induce a finite static susceptibility. On the other hand, the Hamiltonian $H + H_{sf}$ cannot be exactly diagonalized. We therefore introduce two simplifications: a) we limit ourselves to a single $\vec{q}$-term of H_{sf} to be specified later, and b) we diagonalize the remaining Hamiltonian in a reduced basis containing only two states of the localized spin system S. That is, we deal with the Hamiltonian

$$\mathcal{H} = \sum_{\vec{k}} \left\{ \varepsilon_{\vec{k}} a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma} + \frac{1}{2} \left[\lambda_{\vec{q}} S^{+}_{\vec{q}} a^{\dagger}_{\vec{k}+\vec{q}\downarrow} a_{\vec{k}\uparrow} + \lambda_{-\vec{q}} S^{-}_{-\vec{q}} a^{\dagger}_{\vec{k}\uparrow} a_{\vec{k}+\vec{q}\downarrow} \right] \right\} \equiv \sum_{\vec{k}} \mathcal{H}_{\vec{k}} \qquad (16)$$

and a basis of functions

$$|\vec{k}\uparrow, \phi_1\rangle \ , \ |\vec{k} + \vec{q}\downarrow, \phi_2\rangle \qquad (17)$$

where ϕ_1 and ϕ_2 are states (not necessarily eigenstates) of the system S. The system S may in principle be described by any reasonable Hamiltonian H_s which incorporates mechanisms for relaxing angular momentum to the lattice. Its details will not concern us and we will neglect the energies $E_\phi = \langle \phi | H_s | \phi \rangle$ in comparison to electron energies. A basis with electron spins opposite to that given by Eq. (17) leads to identical results.

The diagonalization of $\mathcal{H}_{\vec{k}}$ yields the eigenvalues

$$E^{\pm}_{\vec{k}} = \frac{1}{2} \left\{ \varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{q}} \pm \left[(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}})^2 + \lambda^2 \right]^{1/2} \right\} \qquad (18)$$

with

$$\lambda^2 = |\lambda_{\vec{q}}|^2 |\langle \phi_2 | S^{+}_{\vec{q}} | \phi_1 \rangle|^2 \qquad (19)$$

and the corresponding eigenfunctions

$$\psi^{\pm}_{\vec{k}} = \alpha^{\pm} |\vec{k}\uparrow, \phi_1\rangle + \beta^{\pm} |\vec{k} + \vec{q}\uparrow, \phi_2\rangle \qquad (20)$$

with

$$\alpha^{\pm} = -\frac{1}{2} \lambda_{-\vec{q}} \langle \phi_1 | S^{-}_{-\vec{q}} | \phi_2 \rangle \, C^{\pm} \qquad (21)$$

$$\beta^{\pm} = (\varepsilon_{\vec{k}} - E^{\pm}_{\vec{k}}) C^{\pm} \qquad (22)$$

where

$$(C^{\pm})^{-2} = (\varepsilon_{\vec{k}} - E^{\pm}_{\vec{k}})^2 + \frac{1}{4} \lambda^2 \quad . \qquad (23)$$

The matrix elements of the q = 0 component of the magnetition operator given by Eq. (5) in the basis (2) are

$$\sum_{\vec{k}'} \langle \psi^{\pm}_{\vec{k}} | m_{\vec{k}',0} | \psi^{\pm}_{\vec{k}} \rangle = |\alpha^{\pm}|^2 - |\beta^{\pm}|^2 \qquad (24)$$

$$\langle \psi^{+}_{k} | \sum_{\vec{k}'} m_{\vec{k}',0} | \psi^{-}_{k} \rangle = (\alpha^{+})^{*} \alpha^{-} - (\beta^{+})^{*} \beta^{-} \qquad (25)$$

$$= \frac{\lambda}{\left[(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}})^2 + \lambda^2\right]^{1/2}} \quad .$$

From Eq. (2) the spin susceptibility in a homogeneous field is

$$\chi(\omega) \equiv \chi(0,\omega) = i\int_0^\infty \langle [m_o(t), m_o(0)] \rangle = i\int_0^\infty \langle [e^{i\mathcal{H}t} m_o e^{-i\mathcal{H}t}, m_o] \rangle \qquad (26)$$

$$= i\int_0^\infty \langle e^{i\mathcal{H}t} m_o e^{-i\mathcal{H}t} m_o - m_o e^{i\mathcal{H}t} m_o e^{-i\mathcal{H}t} \rangle$$

We use

$$\langle \ldots \rangle = \mathrm{Tr}(f(\mathcal{H}) \ldots) \qquad (27)$$

where $f(E) = (e^{(E-\mu)/k_B T} + 1)^{-1}$ is the Fermi function and μ the chemical potential. Furthermore, we introduce the complete set of eigenfunctions (20) as intermediate states to obtain

$$\chi(\omega) = i\int_0^\infty \left\{ \sum_{\vec{k}} |\langle \psi^+_{\vec{k}} | m_o | \psi^-_{\vec{k}} \rangle|^2 (f(E^+_{\vec{k}}) - f(E^-_{\vec{k}})) \right.$$
$$\left. \left[e^{i(E^+_{\vec{k}} - E^-_{\vec{k}})t} - e^{-i(E^+_{\vec{k}} - E^-_{\vec{k}})t} \right] \right\} . \qquad (28)$$

Performing the Fourier transform we get

$$\chi(\omega) = -\sum_{\vec{k}} \frac{\lambda^2}{\Delta^2_{\vec{k}} + \lambda^2} \left\{ \frac{1}{(\Delta^2_{\vec{k}} + \lambda^2)^{1/2} - \omega - i\eta} + \right.$$
$$\left. + \frac{1}{(\Delta^2_{\vec{k}} + \lambda^2)^{1/2} + \omega + i\eta} \right\} (f(E^+_{\vec{k}}) - f(E^-_{\vec{k}})) \qquad (29)$$

where

$$\Delta_{\vec{k}} = \varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} \quad . \qquad (30)$$

The model is further simplified if, for every vector $\vec{k}$, we choose a momentum transfer $\vec{q}$ such that $\Delta_{\vec{k}} = 0$. That is, we restrict ourselves to the mixing of degenerate states, where the spin flip Hamiltonian has maximum effect. It is interesting to note that if the spin-flip Hamiltonian has the symmetry of the lattice, scattering is only possible if $\vec{q}$ equals a reciprocal lattice vector $\vec{G}$, and thus the condition $\Delta_{\vec{k}} = 0$ can only be realized at certain definite regions of the fermi surface of polyvalent metals [6].

For $\Delta_{\vec{k}} = 0$, Eq. (29) reduces to

$$\chi(\omega) = -\left\{\frac{1}{\lambda - \omega - i\varepsilon} + \frac{1}{\lambda + \omega + i\varepsilon}\right\} \sum_{\vec{k}} \left(f(E^{+}_{\vec{k}}) - f(E^{-}_{\vec{k}})\right) \qquad (31)$$

where

$$E^{\pm}_{\vec{k}} = \varepsilon_{\vec{k}} \pm \lambda/2 \quad . \qquad (32)$$

The chemical potential μ is obtained from the condition

$$\sum_{\vec{k}} \left(f(E^{+}_{\vec{k}}) + f(E^{-}_{\vec{k}})\right) = N \qquad (33)$$

where N is the total number of electrons. Up to terms of order $(\lambda/2\varepsilon_F)^2$ and for temperature T = 0, we get

$$\mu = \varepsilon_F \left[1 - (\lambda/2\varepsilon_F)^2/4\right] \quad , \qquad (34)$$

where $\varepsilon_F = (3\pi^2 N)^{2/3}/(2m)$ is the Fermi energy of the free electron gas. We then obtain

$$\sum_{\vec{k}} \left(f(E_{\vec{k}}^{+}) - f(E_{\vec{k}}^{-})\right) = -\chi_P/\lambda \left[1 - \frac{1}{6}\left(\frac{\lambda}{2\varepsilon_F}\right)^2\right] \qquad (35)$$

and finally

$$\mathrm{Re}\chi(\omega) = \chi_P \frac{\lambda^2}{\lambda^2 - \omega^2}\left[1 - \frac{1}{6}\left(\frac{\lambda}{2\varepsilon_F}\right)^2\right] \qquad (36)$$

and

$$\mathrm{Im}\chi(\omega) = \chi_P \pi\lambda^2 \delta(\omega^2 - \lambda^2)\left[1 - \frac{1}{6}\left(\frac{\lambda}{2\varepsilon_F}\right)^2\right] . \qquad (37)$$

DISCUSSION

In the static case, $\omega = 0$, we obtain the Pauli susceptibility with a very small correction of the order of $(\lambda/2\varepsilon_F)^2$ resulting from the spin flip scattering processes [7].

The divergent singularity of $\chi(\omega)$ at $\omega = \lambda$ essentially arises from the use of a single parameter λ independent of q. An average of $\chi(\omega)$ over a distribution $p(\lambda)$ would soften or even eliminate the singularity. For instance, Fig. 1 shows the real and imaginary parts of $\overline{\chi(\omega)}$ obtained by averaging (36) and (37) with a logarithmic distribution of λ:

$$p(\lambda) = \begin{cases} \frac{-1}{\lambda_0} \ell n(\lambda/\lambda_0) & \text{for } \lambda < \lambda_0 \\ 0 & \text{for } \lambda > \lambda_0 \end{cases} \qquad (38)$$

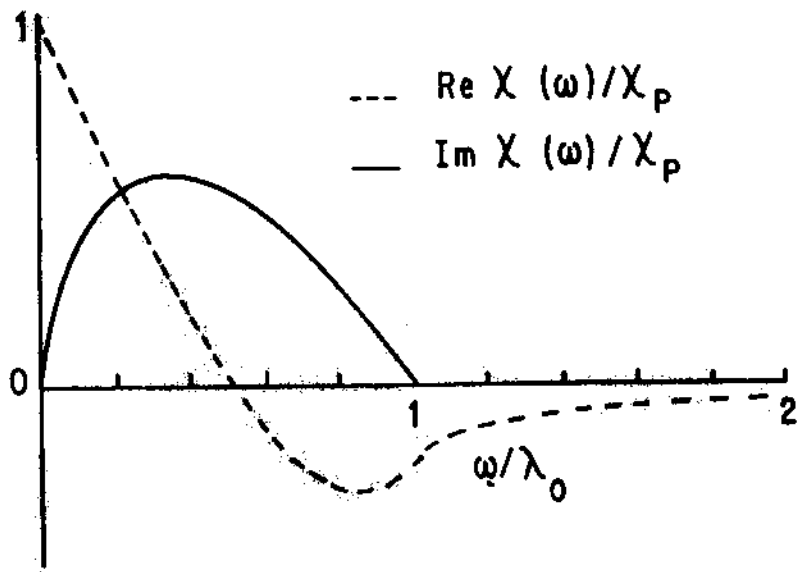
Corrections to the Lindhard's susceptibility due to spin-flip processes are only sizable in the region $\omega > qv_F$ where

$$\chi(q,\omega) \simeq - \chi_P \left[\frac{1}{3} \left(\frac{qv_F}{\omega} \right)^2 + \frac{\lambda^2}{\omega^2} \right] . \tag{39}$$

This region is not accessible to neutron scattering experiments.

FIGURE CAPTION

Fig. 1 - Averaged dynamic susceptibility (see text).


1
0
1
2
--- Re χ (ω)/χ_P
___ Im χ (ω) / χ_P
ω/λ_0

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[2] An analogous situation arises when the Maxwell-Boltzmann distribution of an ideal gas in derived: an infinitesimal intermolecular interaction is implicit. Or when the Planck distribution of the black-body radiation in a cavity with reflecting walls is considered; an infinitesimal "coal particle" is assumed to catalyze the transition towards thermal equilibrium.

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