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Effective-Mass Splitting in a Magnetized Metal

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The (density-of-states) effective masses at the two Fermi surfaces of a magnetized, free-electron metal are calculated as a function of fractional spin polarization P. Coulomb interactions cause the minority-spin mass to exceed the majority-spin mass. The effective-mass splitting is linear in P, for small P, and approaches 20% at $P=1$. It is concluded that the smallness of exchange and correlation corrections to m^* for an ideal metal is accidental. For real band structures they may be of greater significance.

I. INTRODUCTION AND CONCLUSION

For many years it has been known that many-body corrections (arising from Coulomb interactions) to the energy spectrum $E(k)$ of a free-electron metal are very small. The density-of-states effective mass m^*, at the Fermi surface, deviates from m by only a few percent.[1] A recent study[2] has shown in detail how this small effect results from the cancellation of two large contributions. $E(k)$ is the sum of three terms:

$$E(k)=\hbar^2k^2/2m+E_x(k)+E_c(k) \ . \qquad (1)$$

$E_x(k)$ arises from exchange, is *kinematic* in origin, and contributes a positive, (logarithmically) infinite term to dE/dk at the Fermi surface. $E_c(k)$ arises from correlation, is *dynamic* in origin, and contributes a negative, (logarithmically) infinite term to dE/dk. That the singularities in these two terms should cancel has long been appreciated,[3] and results from screening of the long-range part of the Coulomb interaction.

It is possible, however, that the *near-perfect* cancellation of dE_x/dk and dE_c/dk at the Fermi surface of a free-electron metal is fortuitous. The differing physical origins of exchange and correlation, emphasized above, suggest that under more general conditions, contributions from exchange and correlation to m^* may be quantitatively significant. This question is of considerable importance when mathematically accurate band calculations (employing well-chosen crystalline potentials) are compared with experimentally determined band parameters. Perhaps good agreement should not be expected in all cases.

It is easy to perceive how the balance between dE_x/dk and dE_c/dk can be upset. $E_x(k)$ may be regarded as an attraction *in* $\vec{k}$ *space* of the electron in state $\vec{k}$ to the filled states $\{\vec{k}'\}$ with a strength $4\pi e^2/|\vec{k}'-\vec{k}|^2$. Similarly, for small $|\vec{k}'-\vec{k}|$, $E_c(k)$ may be regarded as a repulsion from filled states together with an attraction to empty states, each of half-strength, $2\pi e^2/|\vec{k}'-\vec{k}|^2$. For larger $|\vec{k}'-\vec{k}|$, however, the recoil energy $E(k')-E(k)$ of the electron (as it suffers a virtual excitation from $\vec{k}$ to $\vec{k}'$) becomes important and modifies each contribution to $E_c(k)$.[2] Obviously $E_c(k)$ depends on $E(k)$, whereas $E_x(k)$ does not. This difference alone indicates that changes in $E(\vec{k})$ caused by band structure will upset the balance between exchange and correlation.

It must be remembered that the k dependences of $E_x(k)$ and $E_c(k)$ individually are quite large. For a typical metal they exceed the first term of Eq. (1). Consequently significant fractional changes in $E_c(k)$, for example, will cause proportionate changes in the total (quasiparticle) energy $E(k)$.

The foregoing speculations can be easily tested by computing the effective mass at the two Fermi surfaces of a magnetized, free-electron metal. Such an inquiry has the advantage that Bloch functions need not be substituted for plane waves and energy gaps need not be incorporated in $E(k)$. The plasmon model[2] for computing $E_c(k)$ can be employed after a relatively minor generalization to include change of the electron-gas dielectric function with fractional spin polarization P. Details are given in Secs. II and III.

The radius k^+ of the Fermi sphere for spin-up electrons is

$$k^+=k_F(1+P)^{1/3} \ , \qquad (2)$$

where k_F is the Fermi radius of the unpolarized metal. The spin-up energy spectrum is

$$E^+(k)=\hbar^2k^2/2m+E_x^+(k)+E_c^+(k) \ . \qquad (3)$$

The effective mass for spin-up electrons is found from the reciprocal of dE^+/dk, computed at $k=k^+$. Equivalent expressions apply for spin-down electrons.

The variation of the majority-spin and minority-spin effective mass with polarization P is shown in Fig. 1. The splitting is linear in P (for small P) and approaches 20% at $P=1$. The total electron density was taken to be that of the conduction electrons in sodium metal. These results show that significant changes in effective mass can be caused by a minor change in electronic configuration.

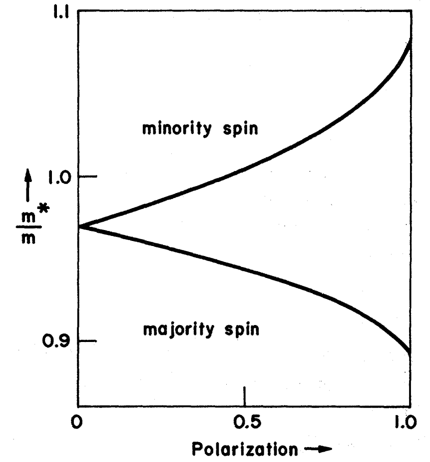

FIG. 1. Effective mass at the two Fermi surfaces of a magnetized, free-electron metal. Total electron density is that of the conduction band in sodium, $r_s = 3.93$ Bohr radii.

The energy-band problem for the case studied here—an empty lattice—is exactly solvable: $E^{\pm}(k) = \hbar^2 k^2/2m$. $m^*/m = 1$ for both spin states, independent of P. Therefore an accurate band calculation (without detailed many-body corrections) cannot be expected to yield reliable $E(k)$.[4]

We conclude that the smallness of many-body contributions to m^* in an ideal metal is fortuitous. In a real metal such contributions may occasionally be much larger. They will depend critically on the over-all band structure, Fermi-surface topology, proximity of energy gaps, etc. It seems worthwhile to emphasize these inherent limitations of band-structure theory in view of the great accuracy of modern techniques for measuring Fermi-surface properties.

II. DIELECTRIC FUNCTION OF MAGNETIZED METAL

The correlation energy $E_c(k)$ depends[2] on the plasmon frequency spectrum ω_q, which, in turn, is related to the electron-gas dielectric function ϵ_q ($\vec{q}$ is the wave vector in a Fourier decomposition),

$$\epsilon_q = 1 + \frac{Q(x)}{1 - G(x)Q(x)} \quad . \tag{4}$$

$Q(x)$ is the response function of an electron gas:

$$Q(x) = Cf(x)/x^2 \ , \tag{5}$$

where $x \equiv q/2k_F$, $C \equiv me^2/\pi\hbar^2 k_F$, and

$$f(x) \equiv \frac{1}{2} + \frac{1 - x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| \quad . \tag{6}$$

$G(x)$ relates the Fourier coefficient V_{xc} of the exchange and correlation potential to the amplitude Δn of an electron-density deviation,

$$V_{xc} = -(e^2 k_F/3\pi n x^2) G(x) \Delta n \ . \tag{7}$$

We seek a generalization of these relations, applicable to a polarized metal. We shall generalized the derivation given in Sec. IV of Ref. 2.

The Fourier amplitude of the spin-up and spin-down density deviations, caused by self-consistent potentials $V^{\pm}$, are

$$\begin{aligned} \Delta n^+ &= -(3n/4E_F) u V^+ f(x/u) \ , \\ \Delta n^- &= -(3n/4E_F) v V^- f(x/v) \ , \end{aligned} \tag{8}$$

where $u \equiv (1+P)^{1/3}$, $v \equiv (1-P)^{1/3}$, $E_F = \hbar^2 k_F^2/2m$, and $P \equiv (n^+ - n^-)/n$. The Fourier coefficient of the electrostatic potential is

$$\varphi = (4\pi/q^2)(\mu - e\Delta n^+ - e\Delta n^-) \ , \tag{9}$$

where μ is the Fourier amplitude of an imposed charge distribution. The Fourier amplitudes of the self-consistent potentials are

$$V^{\pm} = -e\varphi + V_{xc}^{\pm} \ , \tag{10}$$

where $V_{xc}^{\pm}$ are the exchange and correlation potentials caused by $\Delta n^{\pm}$. The generalization of Eq. (7) is

$$\begin{aligned} V_{xc}^+ &= -(e^2 k_F/3\pi n x^2)(G_1 \Delta n^+ + G_2 \Delta n^-) \ , \\ V_{xc}^- &= -(e^2 k_F/3\pi n x^2)(G_3 \Delta n^+ + G_4 \Delta n^-) \ , \end{aligned} \tag{11}$$

where $\{G_i\}$ are functions of x and P. These four functions, which describe the exchange and correlation potentials caused by spin-up and spin-down density deviations, are not well known. The seven equations (8)–(11) relating the eight variables $\Delta n^{\pm}$, $V^{\pm}$, $V_{xc}^{\pm}$, φ, and μ can be solved to yield a linear relation $\varphi = 4\pi\mu/q^2\epsilon_q$ which defines the dielectric function ϵ_q.

Rather than speculate about the precise behavior of $\{G_i\}$, we shall approximate, $G_i = G(x)$. The dielectric function then reduces to Eq. (4), but with $Q(x)$ given by

$$Q(x) = \tfrac{1}{2} C x^{-2} [uf(x/u) + vf(x/v)] \tag{12}$$

instead of by (5). The exchange and correlation function $G(x)$ will be taken to be the one employed previously,[2]

$$G(x) = 1.1x^2/(1 + 10x^2 + 1.5x^4)^{1/2} \ . \tag{13}$$

The splitting shown in Fig. 1 is not very sensitive to the details of $G(x)$.

III. SPIN-DEPENDENT ENERGY SPECTRUM

The exchange energy $E_x^+(k)$ for spin-up electrons is given by

$$E_x^+(k) = -(2e^2 k_F/\pi) u f(y/u) \ , \tag{14}$$

where $y \equiv k/k_F$ and f is the function defined by Eq. (6). The spin-down energy is obtained by substituting v for u in (14).

The correlation energy for spin-up electrons is easily obtained.[5] We quote the final result. With $s \equiv q/2k^+$, $t \equiv k/k^+$,

$$E_c^+(k) = -\frac{me^4}{3\pi^2\hbar^2u^3}\left(\int_0^{|1+t|/2}(1-G)^2\,\frac{Hds}{st}\right.$$
$$\times \ln\left|\frac{1-Hst-Hs^2}{1+Hst-Hs^2}\right| + \int_{|1+t|/2}^{|1+t|/2}(1-G)^2\,\frac{Hds}{st}$$
$$\times \ln\left|\frac{(1+Hst+Hs^2)(4-H+Hs^2)}{(1+Hst-Hs^2)(4+H-Hs^2)}\right|$$
$$\left. + \int_{|1+t|/2}^{\infty}(1-G)^2\,\frac{Hds}{st}\ln\left|\frac{1+Hst+Hs^2}{1-Hst+Hs^2}\right|\right) . \tag{15}$$

This expression is valid for $t \leq 1$. For $t > 1$, the argument in the logarithm of the first term (only) must be replaced by the argument appearing in the third term. The function H is

$$H = \{3u^2F/[s^2 + Cu^{-2}(1-G)F]\}^{1/2} , \tag{16}$$

where $G = G(us)$ in (15) and (16), and

$$F = \tfrac{1}{2}\,uf(s) + \tfrac{1}{2}\,vf(su/v) . \tag{17}$$

Equation (15) gives the majority-spin spectrum for $P > 0$ and the minority-spin spectrum for $P < 0$.

In computing the slope of $E(k)$ at the Fermi surface one should be aware of the anomalous behavior of $E_x(k) + E_c(k)$ (see Fig. 4 of Ref. 2). The m^* values shown in Fig. 1 were obtained by evaluating Eq. (15) at $t = 0.99$ and 1.01.

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[1] L. Hedin and S. Lundqvist, Solid State Phys. 23, 1 (1969); see p. 103.

[2] A. W. Overhauser, Phys. Rev. B 3, 1888 (1971). The theoretical method used in this study is similar to one proposed earlier by B. I. Lundqvist, Phys. Kondensierten Materie 6, 206 (1967).

[3] E. P. Wohlfarth, Phil. Mag. 41, 534 (1950); D. Pines, Phys. Rev. 92, 626 (1953).

[4] We omit here any consideration of electron-phonon interactions, which are known to cause further changes in $E(k)$ within $k_B\Theta_D$ of the Fermi surface.

[5] Reference 2, Sec. VI.