

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 study² has shown in detail how this small effect results from the cancellation of two large contributions. $E(k)$ is the sum of three terms:

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

$E_x(k)$ 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 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 $E(\vec{k}') - E(\vec{k})$

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 model² 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

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

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

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

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.

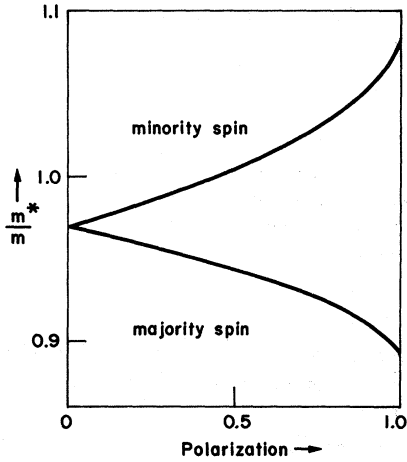


FIG. 1. Effective mass at the two Fermi surfaces of a magnetized, free-electron metal. Total electron density is that of the conduction band in sodium, $r_s = 3.93$ Bohr radii.

The energy-band problem for the case studied here—an empty lattice—is exactly solvable: $E^*(k) = \hbar^2 k^2 / 2m$. $m^*/m = 1$ 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 $E_c(k)$ depends² 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),

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

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

$$Q(x) = Cf(x)/x^2, \quad (5)$$

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

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

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

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

We seek a generalization of these relations, applicable to a polarized metal. We shall generalize 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

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

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

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

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

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

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

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

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 Δn^\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

$$Q(x) = \frac{1}{2} C x^{-2} [u f(x/u) + v f(x/v)] \quad (12)$$

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

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

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

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

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 $s \equiv q/2k^*$, $t \equiv k/k^*$,

$$\begin{aligned}
 E_c^+(k) = & -\frac{me^4}{3\pi^2\bar{n}^2u^3} \left(\int_0^{11+t/2} (1-G)^2 \frac{Hds}{st} \right. \\
 & \times \ln \left| \frac{1-Hst-Hs^2}{1+Hst-Hs^2} \right| + \int_{11+t/2}^{11+t/2} (1-G)^2 \frac{Hds}{st} \\
 & \times \ln \left| \frac{(1+Hst+Hs^2)(4-H+Hs^2)}{(1+Hst-Hs^2)(4+H-Hs^2)} \right| \\
 & \left. + \int_{11+t/2}^{\infty} (1-G)^2 \frac{Hds}{st} \ln \left| \frac{1+Hst+Hs^2}{1-Hst+Hs^2} \right| \right). \quad (15)
 \end{aligned}$$

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

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

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

$$F = \frac{1}{2}uf(s) + \frac{1}{2}vf(su/v). \quad (17)$$

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 .

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

²A. 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).

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

⁴We 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.

⁵Reference 2, Sec. VI.