PHYSICAL REVIEW B VOLUME 2, NUMBER 6 15 SEPTEMBER 1970

Influence of Electron-Phonon Interactions on the de Haas-van Alphen Effect*

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(Received 2 March 1970)

The thermodynamic potential and magnetization are calculated for a system of electrons interacting with phonons in the presence of a magnetic field. The results are used for a numerical evaluation of the de Haas–van Alphen amplitude of the oscillations of the magnetization as a function of temperature in mercury. The calculated results show that although we are dealing with a strong-coupling system, the experimental observations of the de Haas–van Alphen effect should be very similar to that expected for free particles. We also apply the techniques used in the derivation to the case of nearly ferromagnetic electron systems and calculate the enhancement of the argument of the spin-splitting factor. The analysis for nearly ferromagnetic systems leads to the prediction that the cyclotron frequency which enters the amplitude of the oscillations is reduced by the same mass-enhancement factor as that which enters the specific heat.

I. INTRODUCTION

In this work we consider the influence of electron-phonon interactions on the de Haas–van Alphen (DHVA) effect (the oscillatory magnetic properties of a metal as a function of applied field). There have been a number of works on the effect of electron-electron and electron-phonon interactions[1–3] on DHVA oscillations in electron systems which conclude that at sufficiently low temperatures a quasiparticle picture should be applicable. However, as the temperature is raised, the temperature dependence of the effective mass (determined by the real part of the self-energy) and the temperature dependence of the damping of electrons (determined by the imaginary part of the self-energy) should enter to break down the quasiparticle picture.[4] It has been conjectured[5] that these deviations from quasiparticle behavior would be observable in the DHVA effect.

For mercury, with its strong-coupling and low-lying (~ 21 °K) phonon mode,[6] one might expect rather large departures from free-particle behavior for temperatures greater than about 4 °K. In experiments by Palin,[7] the behavior of mercury was found to be quasiparticlelike (with no deviations from free-particle behavior) over considerable temperature and field variations. The Dingle temperature, which ordinarily is interpreted as a measure of the scattering rate of electrons on the Fermi surface, was found to be essentially temperature independent. In this work we show that the results of Palin[7] are in agreement with predictions based on the theory of electron-phonon interactions.

In Sec. II we start with a general expression for the thermodynamic potential of the interacting electron-phonon system. Arguments similar to those made by Luttinger[1] are used to obtain the leading oscillatory term of the thermodynamic potential, neglecting terms of order $(\omega_c/\mu)^{1/2}$ smaller than the leading term. (ω_c is the cyclotron frequency, μ is the Fermi energy, and we use units where $\hbar = 1$.) It is shown that the effect of electron-phonon interactions can be incorporated in the oscillatory part of the thermodynamic potential by replacing, at a certain stage, the noninteracting single-particle electron energies by the noninteracting energy plus the full self-energy. The lack of observable deviations of the DHVA amplitude from the free-particle result is a consequence of a theorem which was first given in limited form by Fowler and Prange.[2] The limited theorem states that the analytic continuation of the full self-energy onto the first pole of the Fermi function on the imaginary axis has only a linear temperature dependence. The constant coefficient of the temperature is directly related to the zero-temperature effective mass. For $k_B T/\omega_c > 1$, only this first pole contributes significantly to the DHVA effect, hence, the observed quasiparticle behavior. The general form of the theorem gives the analytic continuation of the full self-energy onto all the poles along the imaginary axis. These results are used in conjunction with electron-tunneling data[6] for mercury to show that the experimental results[7] may be explained by the theory of electron-phonon interactions. Our results show that[3] since it does not incorporate the effects of electron-phonon scattering, the Dingle temperature is not a true measure of the full scattering rate of electrons on the Fermi surface. This conclusion is not in contradiction with the statement that the Dingle temperature measures the scattering rate from impurities.[8]

We present calculations of the DHVA amplitude for mercury as a function of temperature under

the optimal present-day experimental conditions, which indicate that maximum deviations of 15% from free-particle behavior are expected. If one were to use the calculated results of Grimvall[4,5] and Allen and Cohen[5] in the free-particle formula with $m^*(T)$ replacing m^* in the cyclotron frequency and the inverse lifetime $1/\tau(T)$ replacing the constant Dingle temperature, one would expect deviations by several orders of magnitude.

We also indicate briefly how, for nearly ferromagnetic electron systems,[9] Luttinger's[1] assumptions break down; we give the results expected in this case. The use of the theory of nearly ferromagnetic systems leads to an enhancement of the spin-splitting factor equal to that of the electronic spin susceptibility.

In the Appendix the shift in the thermodynamic potential to second order in the electron-phonon coupling is calculated in a model for which the integrals may be evaluated analytically. It is shown that the results for the oscillatory part of the thermodynamic potential are in agreement with the general formulation presented in Sec. II.

II. FORMULATION

In this section we outline a derivation of the formula which we use to calculate the DHVA amplitude.

Our analysis will follow that given by Luttinger[1] for the case of electron-electron interactions. However, since we will be concerned with the electron-phonon interactions and the temperature dependence of the DHVA amplitude, we will include the temperature dependence of the electron self-energy. Luttinger's arguments [Eqs. (6) and (8) of Ref. 1] for neglecting the temperature dependence of the self-energy are not valid, since we now have a new energy, that of the phonons, which sets a scale other than the Fermi energy μ for temperature variations. This may be seen explicitly in the calculations of, e.g., Grimvall.[4] Actually, even in the case of electron-electron interactions, Luttinger's arguments are not valid for nearly ferromagnetic electron systems.[9] In this case the new energy scale for temperature variations of the self-energy is the Fermi energy divided by the enhancement of the spin susceptibility. We will return to this point at a later stage.

The thermodynamic potential Ω may be obtained following the arguments of Abrikosov, Gorkov, and Dzyaloshinskii,[10] where, in their notation,

$$\Omega = -(1/\beta)\sum_n \mathrm{tr}\{\ln[-G^{-1}(\omega_n)] + \Sigma(\omega_n)G(\omega_n)\} + (1/2\beta)\sum_n \mathrm{tr}\{\ln[-D^{-1}(\omega_n)] + \Pi(\omega_n)D(\omega_n)\} + \Omega'\{G, D\}. \quad (2.1)$$

The phonon contribution to the oscillatory part of the thermodynamic potential may be neglected, because of the weakness of the coupling between density fluctuations and a magnetic field (in most models this coupling is taken to be zero[11]). The electronic contribution to the thermodynamic potential may be written[12]

$$\Omega_{el} = -(1/\beta)\sum_n \mathrm{tr}\{\ln[-G^{-1}(\omega_n)] + \Sigma(\omega_n)G(\omega_n)\} + \Omega'\{G\}. \quad (2.2)$$

The argument which Luttinger uses to neglect the oscillatory part of the self-energy applies also to electron-phonon interactions. It is based on neglecting terms of order $(\omega_c/\mu)^{1/2}$ smaller than the leading contribution. We will show this explicitly in a second-order perturbation calculation in the Appendix. We may also use Luttinger's approach to obtain an expression similar to his Eq. (14) for the oscillatory part of the thermodynamic potential:

$$\Omega_{\text{osc part}} = \left(-(1/\beta)\sum_n \mathrm{tr}\{\ln[\epsilon_{p,\sigma} + \Sigma_0(\omega_n)] - i\omega_n\}\right)_{\text{osc part}}, \quad (2.3)$$

where $\Sigma_0(\omega_n)$ is the nonoscillatory part of the electron self-energy which in our case has rather strongly temperature-dependent real and imaginary parts when evaluated at the Fermi energy. The noninteracting single-particle spectrum is chosen to be described within a Hartree-Fock effective-mass approximation

$$\epsilon_{p_z,l,\sigma} = p_z^2/2m + (l+\tfrac{1}{2})\omega_c + \tfrac{1}{2}\sigma g\mu_B H - \mu. \quad (2.4)$$

The magnetic field $\vec{H}$ is chosen to define the z direction, $\sigma = \pm 1$ indicates the spin orientation of the electron, μ_B is the Bohr magneton $e/2m_0c$, where m_0 is the bare-electron mass, and g is the band g factor.

The band structure of at least some metals can be approximated by an effective mass m in the region of the Fermi surface. The band mass m that enters ω_c in (2.4) is thus not quite the mass which enters the experimentally observed cyclotron resonance frequency $\omega_c^* = eH/m^*c$. The electron-phonon interaction enhances m by a factor which is estimated to be as large as 2.6 for mercury.[13]

It is well known that the electron-phonon interaction does not influence the spin susceptibility.[14] This is reflected in the fact that the spin factor in (2.4) will not be renormalized. However, within almost all models which include electron-electron interactions the spin factor is enhanced. We will return to this point later in treating the short-range model for electron-electron interactions.

We continue in the standard way by transforming the sum over complex frequencies $i\omega_n = i(2n+1)\pi/\beta$

into a contour circling the real axis, which may be rewritten as

$$\Omega_{\rm osc}=\mathrm{tr}\int_{-\infty}^{\infty}(dx/\pi)\,(e^{\beta x}+1)^{-1}\times\tan^{-1}\{\Gamma_0(x)/[x-\epsilon_{p_z,l,\sigma}-\Sigma_0(x)]\},\quad(2.5)$$

using $\Sigma_0(x\pm i\delta)=\Sigma_0(x)\mp i\Gamma_0(x)$. In taking the trace, we sum over the spin σ, the component of momentum parallel to the field p_z, and the Landau levels l. The number of states associated with each Landau level is $(m\omega_c/2\pi)\,L_xL_y$, where L_xL_y is the area of the system perpendicular to the magnetic field. Thus the thermodynamic potential (2.5) may be rewritten

$$\Omega_{\rm osc}=\frac{m\omega_c}{2\pi}L_xL_y\sum_{p_z,\sigma,l}\int_{-\infty}^{\infty}\frac{dx}{\pi}\,(e^{\beta x}+1)^{-1}\times\tan^{-1}\{\Gamma_0(x)/[x-\epsilon_{p_z,l,\sigma}-\Sigma_0(x)]\}.\quad(2.6)$$

We now go through a sequence of steps that reintroduces the single-particle spectrum $p^2/2m$ and eliminates the Landau levels from the single-particle spectrum. Firstly, we make use of the Poisson sum formula[15]:

$$\sum_{l=0}^{\infty}F(l)=\int_0^{\infty}dy\,F(y)\,[1+2\sum_{k=1}^{\infty}(-1)^k\cos(2\pi ky)],$$

which, when $F(y)$ is real, may be rewritten as

$$\sum_{l=0}^{\infty}F(l)=\mathrm{Re}\int_0^{\infty}dy\,F(y)\,[1+2\sum_{k=1}^{\infty}(-1)^k e^{2\pi iky}].\quad(2.7)$$

We then introduce the variable $p_\perp^2$, which plays the role of the momentum squared perpendicular to the magnetic field $p_\perp^2=2m\omega_c y$. The result for the oscillating part of the thermodynamic potential is

$$\frac{\Omega_{\rm osc}}{V}=\frac{1}{(2\pi)^2}\,\mathrm{Re}\sum_{\sigma}\int_{-\infty}^{\infty}dp_z\int_0^{\infty}dp_\perp^2\int\frac{dx}{\pi}(e^{\beta x}+1)^{-1}\times\tan^{-1}\frac{\Gamma_0(x)}{x-\epsilon_{p_z,p_\perp^2,\sigma}-\Sigma_0(x)}\sum_{k=1}^{\infty}(-1)^k\times\exp\left(\frac{2\pi ikp_\perp^2}{2m\omega_c}\right)\quad(2.8)$$

where V is the volume of the system.

We convert the integrals over momenta to an integral over energy by defining

$$\epsilon=p_z^2/2m+p_\perp^2/2m-\mu\quad(2.9)$$

and $\cos^2\theta=p_z^2/(p_z^2+p_\perp^2)$,

giving

$$\frac{\Omega_{\rm osc}}{V}=\frac{(2m)^{3/2}}{(2\pi)^2}\,\mathrm{Re}\sum_{\sigma}\int_{-\mu}^{\infty}d\epsilon\int_{-1}^{1}d(\cos\theta)(\epsilon+\mu)^{1/2}\times\int\frac{dx}{\pi}(e^{\beta x}+1)^{-1}\tan^{-1}\left(\frac{\Gamma_0(x)}{x-\epsilon-\frac{1}{2}\sigma g\mu_BH-\Sigma_0(x)}\right)\times\sum_{k=1}^{\infty}(-1)^k\exp\left(\frac{2\pi ik}{\omega_c}(\epsilon+\mu)(1-\cos^2\theta)\right).\quad(2.10)$$

We perform the integral over $\cos\theta$ by the method of stationary phase. This technique is applicable since ϵ will be limited to values close to zero by the Fermi function and arctangent which appear in the integrand, thus leaving the large coefficient $2\pi k\mu/\omega_c$ as a prefactor to $\cos^2\theta$ in the exponent. We obtain

$$\int_{-1}^{1}d(\cos\theta)\exp[-(2\pi ik/\omega_c)\,(\epsilon+\mu)\cos^2\theta]=e^{-\pi i/4}\left(\frac{\omega_c}{2k(\epsilon+\mu)}\right)^{1/2}+O\left(\frac{\omega_c}{\mu}\right).$$

Substitution of this result into (2.10) yields

$$\frac{\Omega_{\rm osc}}{V}=\frac{2m^{3/2}\omega_c^{1/2}}{(2\pi)^2}\,\mathrm{Re}\sum_{\sigma}\sum_{k=1}^{\infty}\frac{(-1)^k}{(k)^{1/2}}\exp\left(\frac{2\pi ik\mu}{\omega_c}-\frac{\pi i}{4}\right)\times\int_{-\infty}^{\infty}\frac{dx}{\pi}(e^{\beta x}+1)^{-1}\int_{-\mu}^{\infty}d\epsilon\,e^{2\pi ik\epsilon/\omega_c}\times\tan^{-1}\left(\frac{\Gamma_0(x)}{x-\epsilon-\frac{1}{2}\sigma g\mu_BH-\Sigma_0(x)}\right).\quad(2.11)$$

Here we integrate by parts on ϵ, neglecting the end-point contribution of the integrated term, which leads to

$$\frac{\Omega_{\rm osc}}{V}=-\frac{(m\omega_c)^{3/2}}{2\pi^2}\,\mathrm{Re}\sum_{\sigma}\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{3/2}}\exp\left(\frac{2\pi ik\mu}{\omega_c}-\frac{\pi i}{4}\right)\times\int_{-\infty}^{\infty}\frac{dx}{2\pi i}(e^{\beta x}+1)^{-1}\int_{-\mu}^{\infty}\frac{d\epsilon}{\pi}\,e^{2\pi ik\epsilon/\omega_c}\times\frac{\Gamma_0(x)}{[x-\epsilon-\frac{1}{2}\sigma g\mu_BH-\Sigma_0(x)]^2+\Gamma_0^2(x)}.\quad(2.12)$$

Since the region $\epsilon<-\mu$ will give a negligibly small contribution to $\Omega_{\rm osc}$, we extend the ϵ integration to $-\infty$ and perform the integral

$$\frac{\Omega_{\rm osc}}{V}=-\frac{(m\omega_c)^{3/2}}{2\pi^2}\,\mathrm{Re}\sum_{\sigma}\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{3/2}}\times\exp\left(\frac{2\pi ik\mu}{\omega_c}-\frac{\pi i}{4}-\frac{i\pi k\sigma g}{2}\,\frac{m}{m_0}\right)\times\int_{-\infty}^{\infty}\frac{dx}{2\pi i}(e^{\beta x}+1)^{-1}\times\exp\{(2\pi ik/\omega_c)\,[x-\Sigma_0(x)+i\Gamma_0(x)]\},\quad(2.13)$$

where we have used the fact that $\mu_B=e/2m_0c$. This result is identical with that which would be obtained for noninteracting particles except for the replacement of the noninteracting energy spectrum x by the fully interacting spectrum $x-\Sigma_0(x)+i\Gamma_0(x)$ in the oscillatory exponent. Here we may take the sum over spin σ, observing that the self-energy for the electron-phonon interaction is inde-

pendent of spin. Then we obtain

$$\frac{\Omega_{\rm osc}}{V} = -\frac{(m\omega_c)^{3/2}}{\pi^2}\,\mathrm{Re}\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{3/2}}\exp\left(\frac{2\pi i k\mu}{\omega_o}-\frac{\pi i}{4}\right)\times\cos\left(\frac{\pi k g}{2}\frac{m}{m_0}\right)\int_{-\infty}^{\infty}\frac{dx}{2\pi i}(e^{\beta x}+1)^{-1}\times\exp\{(2\pi i k/\omega_c)\,[x-\Sigma_0(x)+i\Gamma_0(x)]\}\,. \quad (2.14)$$

We see that the "spin splitting factor," $\cos(\frac{1}{2}\pi k g \times m/m_0)$ does *not* contain the mass-enhancement factor due to the electron-phonon interactions.

A major aim of this work is understanding the predicted temperature dependence of the amplitude. If we were to use rather naive arguments, we might consider the integral in (2.14) and treat it in the usual Sommerfeld-Watson way; i.e., integrate by parts giving the derivative of the Fermi function times some exponential function of the self-energy. The derivative of the Fermi function will pick out that part of the function multiplying it evaluated at the Fermi surface. However, both the real and imaginary parts of the electron self-energy have rather large temperature variations even when evaluated at the Fermi surface. The imaginary part changes its temperature behavior completely in going from low to high temperatures (T^3 for $T \ll \omega_{\rm Debye}$, and T for $T \gg \omega_{\rm Debye}$). Such variation is completely absent in the DHVA amplitude for mercury[7] where, because of the strong coupling between electrons and phonons and the low-lying phonon mode,[6] we should expect rather extreme deviations from free-particle behavior. The result (2.14) for the thermodynamic potential can be used to obtain all of the oscillatory magnetic properties. We will, however, focus attention on the magnetization $M = -\partial\Omega/\partial H$. In taking the derivative of $\Omega_{\rm osc}$ with respect to field, the dominant contribution (to order ω_c/μ) comes from the oscillatory term $e^{2\pi i k\mu/\omega_c}$,

$$\frac{M_{\rm osc}}{V} = -\frac{m^{3/2}\omega_c^{1/2}}{\pi^2}\,\frac{\mu}{H}\,\mathrm{Re}\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{1/2}}\times\exp\left(\frac{2\pi i k\mu}{\omega_c}-\frac{\pi i}{4}\right)\cos\left(\frac{\pi k g}{2}\frac{m}{m_0}\right)\times\int_{-\infty}^{\infty}dx\,(e^{\beta x}+1)^{-1}\exp\{(2\pi i k/\omega_c)[x-\Sigma_0(x)+i\Gamma_0(x)]\}. \quad (2.15)$$

This result is consistent with the expression (25) obtained by Fowler and Prange.[2]

Closing the integral of (2.15) in the upper half-plane and defining the analytic continuation of the full-electron self-energy onto the imaginary axis

$$\zeta(\omega_n) = i\Sigma_0(i\omega_n)\,, \quad (2.16)$$

we obtain for the oscillatory magnetization

$$\frac{M_{\rm osc}}{V} = -\frac{2}{\pi}\left(\frac{e}{2c}\right)^{3/2}H^{1/2}\left(\frac{\mu}{\omega_c}\right)k_B T\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{1/2}}\times\cos\left(\pi k\frac{g}{2}\frac{m}{m_0}\right)\sin\left(\frac{2\pi k\mu}{\omega_c}-\frac{\pi}{4}\right)\times\sum_{n=0}^{\infty}\exp\{(-2\pi k/\omega_c)[\omega_n+\zeta(\omega_n)]\}. \quad (2.17)$$

III. ELECTRON SELF-ENERGY

In this section we will consider the electron self-energy within the theory of electron-phonon interactions and prove the theorem which is used in evaluating the amplitude of the DHVA oscillations. We will then go on to consider briefly the case of electron-electron interactions for nearly ferromagnetic systems.

We have stated in Sec. II that we need only consider the nonoscillatory part of the electron self-energy. However, there is still the question of the field dependence of the self-energy. Fowler and Prange[2] have given arguments to show that the entire field dependence of the self-energy may be neglected. In the Appendix we show that within the constant-coupling Einstein model, the nonoscillatory part of the second-order self-energy has no field dependence. For this particular model the field dependence is negligible to the same order as the vertex corrections, namely, $(m/M)^{1/2}$ (square root of the electron-to-ion mass ratio). We will continue our analysis neglecting the field dependence of the self-energy. Using the definition (2.16) we write the function $\zeta(\omega_n)$ in an integral representation which may be evaluated once the product of the electron-phonon coupling interaction $\alpha^2(\nu)$ and the phonon density of states $F(\nu)$ has been obtained, e.g., by use of superconducting tunneling data,[6,13]

$$\zeta(\omega_n) = i\int_0^{\infty}d\nu\,\alpha^2(\nu)\,F(\nu)\times\int_{-\infty}^{\infty}d\epsilon\left(\frac{1-f(\epsilon)+n(\nu)}{i\omega_n-\epsilon-\nu}+\frac{f(\epsilon)+n(\nu)}{i\omega_n-\epsilon+\nu}\right), \quad (3.1)$$

where $f(\epsilon)$ and $n(\nu)$ are the Fermi and Bose distribution functions, respectively. The analysis proceeds by first closing the ϵ integration in the upper half-plane:

$$\int_{-\infty}^{\infty}d\epsilon\left(\frac{1-f(\epsilon)+n(\nu)}{i\omega_n-\epsilon-\nu}+\frac{f(\epsilon)+n(\nu)}{i\omega_n-\epsilon+\nu}\right) = -\pi i\left[4\nu k_B T\left(\sum_{m=0}^{\infty}[(2\pi m k_B T)^2+\nu^2]^{-1}+\sum_{m=1}^{n}[(2\pi m k_B T)^2+\nu^2]^{-1}\right)-2n(\nu)-1\right]. \quad (3.2)$$

However, one may prove that

$$4\nu k_B T\sum_{m=0}^{\infty}\frac{1}{(2\pi m k_B T)^2+\nu^2}-2n(\nu)-1 = \frac{2k_B T}{\nu}\,. \quad (3.3)$$

Hence (3.1) becomes

$$\zeta(\omega_n, T) = \pi k_B T \int_0^\infty d\nu \frac{2\alpha^2(\nu) F(\nu)}{\nu} \times \left\{1 + 2 \sum_{m=1}^{n} \left[1 + \left(\frac{2\pi m k_B T}{\nu}\right)^2\right]^{-1}\right\}, \tag{3.4}$$

which is the generalized Fowler-Prange theorem that we use to evaluate the amplitude in the DHVA effect. For $n=0$ we obtain the limited form of the theorem first given by Fowler and Prange[2]:

$$\zeta(\pi k_B T, T) = \pi k_B T \int_0^\infty d\nu \frac{2\alpha^2(\nu) F(\nu)}{\nu} = \pi k_B T \lambda, \tag{3.5}$$

where λ may also be defined by the equations[4,10,13,16]

$$\lambda = -\frac{\partial \Sigma(\omega)}{\partial \omega}\bigg|_{\omega=0, T=0} \equiv \frac{m^*}{m} - 1 . \tag{3.6}$$

We will return to these results in Sec. IV, which includes numerical work using the phonon spectrum of mercury.

We now consider briefly the case of nearly ferromagnetic systems. The model chosen for the electron-electron interactions is the same short-range interaction that was chosen originally.[9,11] The diagrams summed in Ω' are the closed loops and ladders, also chosen originally[9,11] (the closed loops, or σ_z fluctuations were omitted in Ref. 9) and in the work of Amit, Kane, and Wagner.[17] The Hartree single-particle energies have the term

$$+\tfrac{1}{2} I (N_\sigma - N_{-\sigma})$$

added to (2.4) as, e.g., given in Ref. 11. This term may be combined with the term $\frac{1}{2}\sigma g \mu_B H$ in (2.4) to give a magnetic term in the single-particle energies:

$$\tfrac{1}{2}\sigma g \mu_B H/(1-\bar{I}), \tag{3.7}$$

where $\bar{I} = IN(0)$ and $N(0)$ is the density of states at the Fermi surface for a single spin. This equation follows on using the fact that the magnetization is given as

$$M = \tfrac{1}{2}\sigma g \mu_B (N_\sigma - N_{-\sigma}) = \chi H = (\tfrac{1}{2} g \mu_B)^2 \frac{2N(0)}{1 - IN(0)} H \tag{3.8}$$

and substituting for $(N_\sigma - N_{-\sigma})$ in the expression for the single-particle energy. If the Hartree term of (3.8) rather than the noninteracting term of (2.4) is kept in the analysis the resulting "spin splitting factor" is

$$\cos\left(\frac{\pi k g}{2} \frac{m}{m_0} \frac{1}{1-\bar{I}}\right) . \tag{3.9}$$

Thus the argument of the spin splitting factor is enhanced by the same amount as the electronic spin susceptibility. This result was also given by Bychkov and Gorkov[1] on the basis of Fermi liquid theory arguments.

The rest of the analysis for the case of nearly ferromagnetic systems follows through in analogy with the electron-phonon case. The temperature dependence of the electron self-energy cannot be neglected, but we do neglect its magnetic field dependence. The neglect of the field dependence is consistent with the model calculations[11]; however, experiments[18] indicate a greater sensitivity of nearly ferromagnetic alloys to the application of a field than the model predicts.

The final result is a formula for Ω_{osc} of the same form as (2.14) with (3.9) replacing the unenhanced spin splitting factor and the spin fluctuation contribution to the self-energy replacing that of the electron-phonon interaction. This result implies that if one could do DHVA amplitude measurements on a series of nearly ferromagnetic alloys as, for example, Ni-Rh or Pd-Ni, one should see the same changes in mass enhancement of the cyclotron frequency as observed in the γ value obtained by specific-heat experiments.[19]

IV. NUMERICAL RESULTS

In this section we will use superconducting tunneling data to present the results of numerical work on the DHVA amplitude for a low-mass orbit in mercury. From Eq. (2.17), considering only the first harmonic in the sum, i.e., $k=1$, we may define an amplitude

$$A = \sum_{n=0}^{\infty} \exp\{-(2\pi/\omega_c)[\omega_n + \zeta(\omega_n)]\}. \tag{4.1}$$

This amplitude contains all the effects of the electron-phonon interactions. We will consider the behavior of A as a function of temperature and magnetic field.

For temperatures high compared to the cyclotron frequency, i.e., $x \gg 1$, where

$$x = 2\pi^2 k_B T/\omega_c , \tag{4.2}$$

only the first term in the series for A will contribute significantly. However, we have seen in (3.5) that

$$\zeta(\pi k_B T, T) = \pi k_B T \lambda = \pi k_B T (m^*/m - 1),$$

so that

$$A = \exp\left(-\frac{2\pi^2 k_B T}{\omega_c} \frac{m^*}{m}\right) = e^{-(m^*/m)x}, \quad \text{for } x \gg 1 \tag{4.3}$$

a result first given by Fowler and Prange.[2]

If we plot $\ln A$ as a function of temperature, then at high temperatures we will obtain a straight line

of gradient proportional to m^*/m. We now define an amplitude A^0 for free particles of mass m^* by

$$A^0 = [2\sinh(2\pi^2 k_B T/\omega_c^*)]^{-1}, \tag{4.4}$$

from which we see that the high-temperature limit of A is identical to A^0. As has been pointed out previously,[1-3] we find that the electron-phonon enhancement factor does enter the amplitude of the oscillation,[20] while the oscillation frequency $(k\mu H/\omega_c)$ is *not* affected by the electron-phonon interaction, since the electron self-energy at the Fermi surface is negligible.

For temperatures such that $x \lesssim 1$, terms other than the first contribute to the sum (4.1); it is these terms which will cause A to differ from A^0. We have not been able to obtain an analytic form for A (even when using an Einstein model for the phonon spectrum), but we can make some qualitative remarks. From Eq. (3.4) we note that

$$\zeta(\omega_n, T) \lesssim (2n+1)\lambda\pi k_B T, \tag{4.5}$$

and hence

$$A \geq \sum_{n=0}^{\infty} \exp[-(2\pi/\omega_c)(\omega_n + \lambda\omega_n)],$$

i.e., $$A \geq A^0. \tag{4.6}$$

To maximize these deviations, using Eqs. (3.4) and (4.1), we see that for a given temperature we require a large magnetic field to increase the number of terms in the series (4.1) and small phonon frequencies to increase the ratio $2m\pi k_B T/\nu$ in the expression for $\zeta(\omega_n, T)$. This latter condition is most favorable in mercury, with its low-frequency phonon mode.

Using a computer program and the experimental phonon density of states for mercury, shown in Fig. 1, we have calculated the amplitude (4.1) as

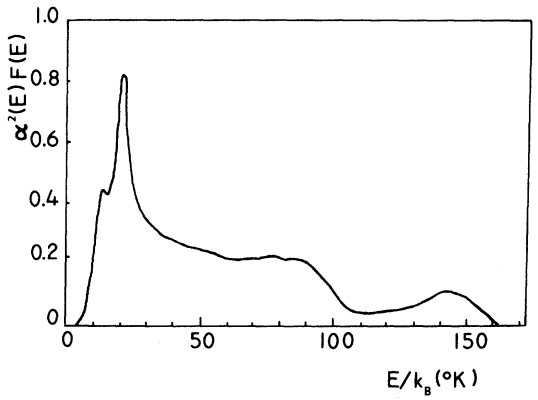

FIG. 1. The product of the electron-phonon coupling interaction and the phonon density of states $\alpha^2 F$ as a function of energy for mercury, taken from the work of McMillan and Rowell (Ref. 6).

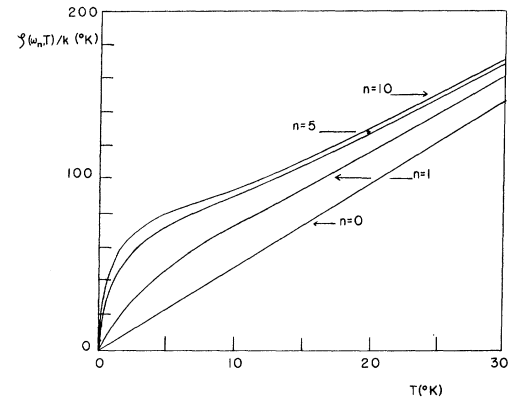

FIG. 2. The analytically continued electron self-energy in mercury evaluated at $\omega_n = (2n+1)\pi T$ as a function of temperature for $n = 0, 1, 5, 10$.

a function of temperature, for various values of the magnetic field. In Fig. 2 we have plotted the analytically continued self-energy $\zeta(\omega_n, T)$ in mercury, as given by Eq. (3.4), for several different values of n.

The results of the calculations indicate that, except at the highest fields, deviations from free-particle behavior are small and unlikely to be detectable. We show, in Fig. 3, two cases of the amplitude as a function of temperature for mercury. We plot $\ln A_c$ and $\ln A^0{}_c$ against temperature, where

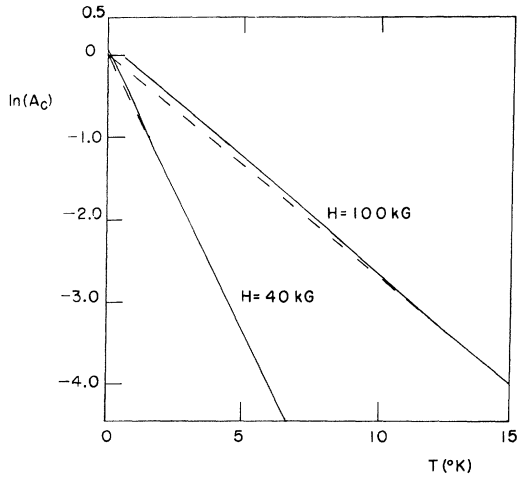

FIG. 3. The temperature dependence of the amplitude of the DHVA oscillations in mercury:

$$A_c = [1 - e^{-(2m^*/m)x}] \sum_{n=0}^{\infty} \exp\{-(2\pi/\omega_c)[\omega_n + \zeta(\omega_{n,T})]\},$$

where $x = 2\pi^2 k_B T/\omega_c$. A cyclotron mass $m^* = 0.183$ is used. The dashed lines correspond to free-particle behavior.

$$A_c = A(1 - e^{-(2m^*/m)x}) \qquad (4.7)$$

and $A^0{}_c = A^0[1 - e^{-(2m^*/m)x}] = e^{-(m^*/m)x}$.

The effect of the factor $[1 - e^{-(2m^*/x)x}]$ introduced in (4.7) is to make $\ln A^0{}_c$ a linear function of temperature for all temperatures, and $\ln A_c$ will show deviations from this straight line.

We use a cyclotron mass (that is, the band mass times the electron-phonon enhancement m^*/m) of 0.183, corresponding to a β orbit in mercury. The first case, for a field of 40 kG, shows a maximum deviation of about 5%, but seen only at the lowest temperatures. These values of magnetic field and cyclotron mass correspond fairly closely to experiments of Palin, who found no appreciable deviations from linear behavior over the temperature range 1–10 °K. The second case, also plotted in Fig. 3, for a field of 100 kG and a cyclotron mass of 0.183 shows deviations of up to 15% over a range of temperature to about 10 °K. However, for much of this range $\ln A_c$ looks close to a straight line, corresponding to a cyclotron mass only 5% different from the true cyclotron mass. Hence, in order to see the deviations unambiguously, one would have to perform an experiment over a broad temperature range up to and including the region where the deviations disappear ($x > 1$). In Fig. 4, we show the deviations for $H = 100$ kG on a larger scale. The curve does not quite reach $T = 0$ because for temperatures such that $x \ll 1$, the summation (4.1) converges only very slowly and eventually becomes unmanageable. However, within an Einstein model and for fields such that ω_c is not large compared with the Einstein frequency, we are able to expand A about its $T = 0$ value, given by Fowler and Prange[2] [their Eq. (35)], and obtain a smooth curve for A over the full temperature range.

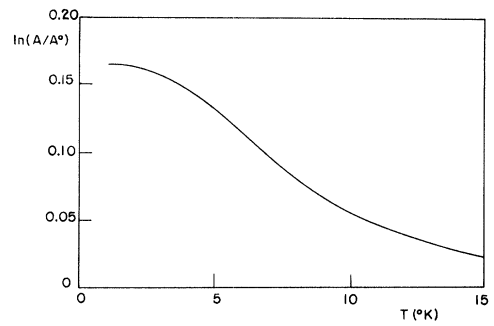

FIG. 4. The deviations, $\ln(A/A^0)$ for a cyclotron mass of 0.183 and a magnetic field of 100 kG, shown on a larger scale; the curve does not reach $T = 0$ because of the slow convergence of the summation (4.1) at low temperatures.

Although Palin did not carry out an experiment in quite such extreme conditions as those of the second case, he still found no significant deviation from linearity (i.e., quasiparticle behavior) in an experiment at 82 kG over a range from 4–17 °K for a cyclotron mass of about 0.187. Our calculations suggest that the amplitude should deviate by up to about 10% from linearity under these conditions, but the consequent change of slope on a logarithmic plot would probably have been too slight for unambiguous experimental observation.

ACKNOWLEDGMENTS

We should like to thank Professor J. Wilkins for bringing Palin's experiments to our attention and Dr. D. Schoenberg, C. J. Palin, and Dr. J. Vanderkooy, who kindly discussed their experimental work with us before publication. Dr. W. McMillan sent the results of his work with Dr. J. Rowell on the phonon density of states in mercury. We would also like to thank Dr. W. Brinkman, Professor J. Hopfield, and Professor M. Wortis for helpful discussions.

APPENDIX

In this Appendix we calculate the shift in thermodynamic potential to second order in the electron-phonon coupling constant. We use an Einstein spectrum, i.e., constant phonon frequency ω_0, and a wave-vector–independent coupling constant g. For this special model all the integrals may be evaluated analytically.

To carry out the perturbation calculation in a magnetic field we consider the creation and annihilation operators that describe electrons in their eigenstates in a magnetic field rather than in the usual plane wave states. The noninteracting electron Hamiltonian in this representation is

$$H^0{}_{\rm el} = \sum_{l,p_z,\sigma} \epsilon_{p_z,l,\sigma}\, c^+_{p_z,l,\sigma}\, c_{p_z,l,\sigma}, \qquad (A1)$$

where the single-particle electron energies $\epsilon_{p_z,l,\sigma}$ were given in (2.4). The phonons and density fluctuations are assumed to be uncoupled from the magnetic field so that the noninteracting phonon Hamiltonian is

$$H^0{}_{\rm ph} = \sum_k \omega_0\, a^+_k a_k. \qquad (A2)$$

The interaction term is taken to be the usual Fröhlich Hamiltonian, which in the plane wave description is

$$H' = \sum_{p,p',\sigma} \frac{g}{(2\omega_0)^{1/2}}\, c^+_{p',\sigma}\, c_{p,\sigma}\,(a_{p'-p} + a^+_{p-p'}). \qquad (A3)$$

We now convert to the magnetic field eigenoperators and insert the matrix element of a plane wave between the magnetic field oscillator eigenfunctions

$\psi_l(r)$:

$$M_{ll'}(\vec{q}) = \int d\vec{r}\, \psi_l^*(r)\, e^{i\vec{q}\cdot\vec{r}}\, \psi_{l'}(r). \quad \text{(A4)}$$

The integral may be evaluated and the result is as given by Brailsford[8] [Eq. (A8)]. Excluding the momentum δ function on the y and z momenta the result is

$$|M_{ll'}(q_\perp)| = \alpha^{(l'-l)/2} e^{-\alpha/2} (l!/l'!)^{1/2} L_l^{l'-l}(\alpha), \quad \text{(A5)}$$

where $\alpha = q_\perp^2/2m\omega_c$, $q_\perp^2 = q_x^2 + q_y^2$, and L_l^m is an associated Laguerre polynomial. For $l' < l$, l and l' in (A5) are interchanged. The interaction term in the Hamiltonian is thus written

$$H' = \sum_{\substack{l,l',p_z \\ \sigma,\vec{q}}} M_{l,l'}(q_\perp) \frac{g}{(2\omega_0)^{1/2}} c^+_{l',p_z+q_z,\sigma} \times c_{l,p_z,\sigma}(a_q + a^+_{-q}). \quad \text{(A6)}$$

We may now write the second-order shift in the thermodynamic potential as

$$\Delta\Omega^{(2)} = L_x L_y \frac{m\omega_c}{2\pi} \frac{1}{2\beta^2} \sum_{\omega_{n_1}\omega_{n_2}} \sum_{l,l',p_z,\vec{q},\sigma} \times |M_{l,l'}(q_\perp)|^2 g^2 \frac{1}{i\omega_{n_1} - \epsilon} \frac{1}{i\omega_{n_2} - \epsilon'} \frac{1}{(\omega_{n_2} - \omega_{n_1})^2 - \omega_0^2}. \quad \text{(A7)}$$

Since we have chosen the coupling constant and phonon frequency to be independent of wave vector, the only place $q_\perp$ occurs is in the matrix element $|M_{ll'}(q_\perp)|^2$. The sum over $q_\perp$ is just the orthogonality integral for the Laguerre polynomial:

$$\sum_{q_x,q_y} |M_{ll'}(q_\perp)|^2 = (m\omega_c/2\pi) L_x L_y. \quad \text{(A8)}$$

Now we follow the steps (2.7)–(2.10) as in Sec. II to revert back to the usual momentum variables:

$$\Delta\Omega^{(2)} = \frac{1}{2\beta^2} \sum_{\omega_{n_1}\omega_{n_2}} \sum_{p,q,\sigma} g^2 \left(1 + 4\sum_{k=1}^{\infty} (-1)^k \times \cos\frac{2\pi k \epsilon_\perp}{\omega_c} + 4 \sum_{k,k'=1}^{\infty} (-1)^{k+k'} \cos\frac{2\pi k \epsilon_\perp}{\omega_c} \times \cos\frac{2\pi k' \epsilon'_\perp}{\omega_c}\right) \frac{1}{i\omega_{n_1} - \epsilon} \frac{1}{i\omega_{n_2} - \epsilon'} \frac{1}{(\omega_{n_2} - \omega_{n_1})^2 - \omega_0^2}, \quad \text{(A9)}$$

where $\epsilon \equiv \epsilon(p)$ and $\epsilon' \equiv \epsilon(p+q)$.

The first term in the large parentheses of (A9) (the term 1) represents the shift of the thermodynamic potential in the absence of a magnetic field. The second term of (A9) [the term $4\sum_{k=1}^{\infty}(-1)^k \times \cos 2\pi k \epsilon_\perp/\omega_c$] is just the expansion of (2.3) to second order. The third term in the large parenthesis of (A9) (the term with the product of two oscillatory factors) represents the oscillatory field dependence of the self-energy. We may evaluate this term using the method of stationary phase on both the $\cos\theta$ and $\cos\theta'$ integrals, and we obtain a term which is smaller in magnitude by $(\omega_c/\mu)^{1/2}$ than the second term.

To show that the second term is the expansion of (2.3), we perform the ω_{n_1} and ω_{n_2} sums by converting to integrals and obtain

$$\Delta\Omega^{(2)} = -\sum_{p,q,\sigma} \frac{g^2}{2\omega_0} \left[2\sum_{k=1}^{\infty} (-1)^k \cos\frac{2\pi k \epsilon_\perp}{\omega_c} \times \frac{1}{2\pi i} \int_c dz \frac{f(z)}{z-\epsilon} \left(\frac{n(\omega_0) + f(\epsilon')}{z - \epsilon' + \omega_0} + \frac{n(\omega_0) + 1 - f(\epsilon')}{z - \epsilon' - \omega_0}\right)\right]. \quad \text{(A10)}$$

This result is identical to that obtained by expanding (2.3) to second order in the coupling constant, as may be verified by noting that the second-order self-energy is

$$\Sigma^{(2)}(\epsilon_p, i\omega_n) = \sum_q \frac{g^2}{2\omega_0} \left(\frac{n(\omega_0) + f(\epsilon_{p+q})}{i\omega_n - \epsilon_{p+q} + \omega_0} + \frac{n(\omega_0) + 1 - f(\epsilon_{p+q})}{i\omega_n - \epsilon_{p+q} - \omega_0}\right). \quad \text{(A11)}$$

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*Work started while one of the authors (S.E.) was senior research fellow at Imperial College, London, England and the other author (G.S.) held a SRC student scholarship there.

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PHYSICAL REVIEW B VOLUME 2, NUMBER 6 15 SEPTEMBER 1970

Low-Energy Electron Diffraction from Liquid Hg: Multiple Scattering, Scattering Factor, and Attenuation*

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(Received 2 March 1970)

The elastic scattering of electrons from liquid Hg has been measured for energies between 100 and 500 eV and for scattering angles between 60° and 170°. The observed scattering is remarkably similar to that from Hg vapor; a model calculation shows that the differences between the liquid and vapor scattering are due to multiple scattering and inelastic processes. The analysis shows that (i) higher-order multiple scatterings are strongly attenuated by inelastic processes; (ii) approximately half the observed integrated intensity has been scattered only once; (iii) for back angles, the atomic scattering factor is essentially the same for the atoms in the liquid and the vapor; and (iv) attenuation coefficients for elastic electrons are of the order of several tenths of a reciprocal angstrom.

I. INTRODUCTION

The difficulties in developing a satisfactory understanding of low-energy electron diffraction are well known and arise because of the strong interactions between the electron and the crystal.[1] Because of the large elastic cross section, multiple scattering must be important, and most current theoretical work aims to develop dynamic theories in which either band-structure calculations are extended to the energies of the incident electron[2] or, equivalently, in which the multiple scattering is treated explicitly in a self-consistent way.[3] In these theoretical treatments one needs either the lattice potential or the related atomic scattering factor, neither of which has generally been available from experiment. The inelastic interactions are also strong and have an important effect on the elastic scattering. They have been included in some recent calculations,[1,4] usually in a phenomenological way. Little experimental information is available about the attenuation of the elastic beams due to inelastic processes.

It is the purpose of this paper to report the results and interpretation of experiments on the low-energy electron scattering from liquid Hg. These experiments allow reasonably direct estimates of the multiple-scattering contribution, of the inelastic absorption coefficient, and of the atomic scattering factor.

An earlier paper[5] reported a generally applicable method to measure what was called the square of the effective atomic scattering factor, $|f(\theta, E)|^2_{\mathrm{eff}}$. In that work the elastic scattering of low-energy electrons from the surface of a Ni crystal at elevated temperatures was measured as a function of the scattering angle 2θ for various angles of incidence. The observed scattered intensity could be divided into two parts, one part which depended on the crystal structure and its orientation and a second part which did not. This latter part, which is dominant at high temperatures, gives the angular dependence of $|f(\theta, E)|^2_{\mathrm{eff}}$. After correction