Effect of momentum-dependent many-body interactions on the de Haas—van Alphen amplitude

J. Appel
I. Institut für Theoretische Physik, Universität Hamburg, D-2000 Hamburg 36, West Germany

D. Fay
Abteilung für Theoretische Festkörperphysik, Universität Hamburg, D-2000 Hamburg 36, West Germany
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The de Haas—van Alphen amplitude is calculated taking into account both the frequency *and* the momentum dependencies of the electron self-energy within the pole approximation to the electron spectral function. When we make the quasiparticle expansion of the self-energy, we find that the *same* effective mass enters both the amplitude and the electronic specific heat. The possibility of a discrepancy between these masses in nearly ferromagnetic systems is briefly discussed.

High-accuracy experimental data on the de Haas—van Alphen (dHvA) effect yield pertinent information about the electrons near the Fermi surface (FS). In the first place, the dHvA periods are determined by the Bloch-band structure through the cross-sectional areas of the *true* FS calculated by taking into account electron-electron exchange and correlation effects.[1] Secondly, the dHvA amplitude is governed by many-body effects. The renormalization of the amplitude factor due to electron-phonon interactions was formulated by Fowler and Prange[2] in terms of the frequency- and temperature-dependent electron self-energy which remains essentially unaffected by the magnetic field H. On this basis Engelsberg and Simpson[3] gave a detailed analysis of the strong-coupling effect that occurs in high magnetic fields when the cyclotron frequency $\omega_c \gg \omega_{\text{ph}}$ (equal to the characteristic phonon frequency) *and* the temperature T is small $x=2\pi^2 k_B T/\hbar\omega_c \ll 1$. In that case [where many Matsubara frequencies $\omega_\nu = 2\pi(\nu+1)k_B T$ lie within ω_c], the amplitude factor can deviate significantly from the "quasiparticle amplitude" $A^{(0)}=2x\exp[-(m^*/m)x]$ where m^* is the quasiparticle mass at zero temperature and zero frequency.[4–6] This deviation has been clearly observed in mercury by measuring the amplitude versus H at low temperature.[7]

In the theoretical investigations (cf. Refs. 2–6), the usual assumption is made that the electron self-energy is frequency dependent but not momentum dependent, that is, it is retarded in time but local in coordinate space. This assumption is justified for the electron-phonon interaction by virtue of its short-range nature. The self-energy has a weak momentum dependence, $\Sigma_{e\text{-ph}}(p,\omega) \propto p^{-1}$, so that for $p \simeq p_F$ (equal to the Fermi momentum) the effective mass m^* is determined solely by the frequency dependence of $\Sigma_{e\text{-ph}}(p_F,\omega)$.

In *simple* metals both the momentum and energy dependence of the electron self-energy, $\Sigma_{e\text{-}e}(p,\omega)$ due to the Coulomb interaction between the electrons, are important.[8] However, m^* only differs from m by the order of a few percent. For *transition* metals and their compounds in which the Coulomb interaction is strongly exchange enhanced and spin fluctuations are thus important, the mass enhancement can be significant. In spin-fluctuation theory the assumption is made that, in analogy to the phonon case, the momentum dependence of the self-energy is negligible. We will not make this assumption.

The following question arises: Assuming that $\Sigma_{e\text{-}e}$ is p dependent, does the dHvA amplitude *in the quasiparticle approximation* still have the form $A^{(0)}=2\times\exp[-(m^*/m)x]$, and is m^* identical with the specific-heat mass in Sommerfeld's γ? Note that we are not looking for deviations from quasiparticle behavior of the type considered in Ref. 3, i.e., we are primarily interested in the case where ω_c is small compared to ω_{ph} and ω_{SF}, if spin fluctuations are important.

We were motivated to investigate this question by detailed experimental observations of many cyclotron orbital areas on Pd by Dye *et al.*[9] using the dHvA effect. These authors concluded that the measured masses predict an electronic specific heat about 15% lower than observed. This discrepancy has apparently now disappeared.[10] In Pt, Nb, and noble metals, the fitting of the dHvA data to their Korringa-Kohn-Rostoker (KKR) parametrization of the Fermi-surface geometry leads to a prediction of specific-heat masses which are in good agreement with experiments. On the other hand, there is another metal with strong spin-fluctuation effects, $TiBe_2$,[11] where the observed dHvA masses are much smaller than the specific-heat mass.[12] As a first step in an investigation of the possibility of such discrepancies we consider the effect of the momentum dependence of $\Sigma_{e\text{-}e}$. Later we will briefly discuss another possibility.

The quasiparticle effective mass m^*, which is the "specific-heat" mass at low temperature,[13] is defined by the expansion of $\Sigma(p,\omega)$ near the FS,

$$\frac{m}{m^*} = \left| \frac{1+\dfrac{\partial\,\mathrm{Re}\Sigma(p,\omega)}{\partial p}}{1-\dfrac{\partial\,\mathrm{Re}\Sigma(p,\omega)}{\partial\omega}} \right|_{p=p_F,\ \omega=0} . \tag{1}$$

We write the e-e self-energy as

$$\Sigma_{e\text{-}e}(p,\omega) = \Sigma_x(p) + \Sigma_c(p,\omega) , \tag{2}$$

where Σ_x and Σ_c are the Hartree-Fock and correlation terms, respectively. In simple metals there are large contributions to the derivatives of $\Sigma_{e\text{-}e}$ with respect to both ω and p. The p dependence of $\Sigma_{e\text{-}e}$ is governed by Σ_x which yields the Hartree-Fock divergence of m^*. This is compensated for by the ω dependence of Σ_c.[8] This divergence difficulty can be avoided by including at least the static correlation effects with the help of a screened Coulomb potential when calculating the exchange self-energy $\Sigma_{e\text{-}e} \sim \Sigma_x^{\text{scr}}(p)$. We show later that a corresponding divergence does not occur in a Hartree-Fock evaluation of the dHvA amplitude.

A low-frequency, momentum-dependent contribution to $\Sigma_c(p,\omega)$ occurs in d-band metals that have a tendency to become itinerant ferromagnets or antiferromagnets. The exchange-enhanced e-e interaction gives rise to spin fluctuations which cause renormalization effects due to the emission and reabsorption of one or more virtual paramagnons. The spin-fluctuation model is not based on a fundamental theory of correlation effects as is Landau's quasiparticle theory. It does allow us, however, to calculate the effects of a well-defined class of particle-hole correlations thought to be the most important ones in nearly ferromagnetic metals at low frequencies and small momentum transfers. We note that although the Landau theory has been quite successful in liquid ^{3}He, it has failed in predicting, in a consistent manner, the renormalization effects for the electron gas in metals.[14] There is, in addition, the difficulty of extending the Landau f function to finite frequencies and momentum transfers. At this point let us assume that any spin-fluctuation effects are contained in $\Sigma_{e\text{-}e}(p,\omega)$. Later we comment on the nearly ferromagnetic case where the spin-fluctuation contributions dominate.

To evaluate the dHvA amplitude we start from the standard formula for the total electron density n. Using the notation of Ref. 2 (where $m\hbar\omega_c$ was set equal to 2), we have

$$n=\frac{m\hbar\omega_c}{\pi}\sum_{l=0}^{\infty}\int\frac{dp_z}{2\pi}\int\frac{d\omega}{2\pi}f(\omega)A(l,p_z,\omega)\ , \tag{3}$$

where

$$f(\omega)=\{\exp[(\omega-\mu)/k_BT]+1\}^{-1}\ ,$$

and $A(l,p_z,\omega)$ is the spectral weight function of the electrons whose orbital motion is quantized by a magnetic field H oriented in the z direction. The function $A(l,p_z,\omega)$ is obtained from the one in zero field when p^2 is replaced by

$$p_z^2+2m\hbar\omega_c(l+\tfrac{1}{2})\equiv p_z^2+p_\perp^2$$

and the sum over the Landau level quantum numbers l is defined by $2m\hbar\omega_c\sum_l\equiv dp_\perp^2$. By applying the Poisson formula[15] to Eq. (3), n is decomposed into a sum $n=\sum_r n_r$, where

$$n_r=(-1)^r\frac{m\hbar\omega_c}{\pi}\text{Re}\int_0^\infty dx\,\exp(2\pi irx)\times\int\frac{dp_z}{2\pi}\int\frac{d\omega}{2\pi}f(\omega)A(x-\tfrac{1}{2},p_z,\omega)\ . \tag{4}$$

The term n_r is the contribution of the rth harmonic of the dHvA oscillations;

$$n_r=-(\partial[\Omega_{\text{osc};r}/V]/\partial\mu)_{T,V}\ ,$$

where $\Omega_{\text{osc};r}$ is the rth harmonic of the oscillating part of the thermodynamic potential given by Luttinger.[1] In terms of the new integration variables,

$$2m\hbar\omega_c\int dx=\int dp_\perp^2=\pi^{-1}\int d^2p\ ,$$

Eq. (4) becomes

$$n_r=(-1)^r\text{Re}\int\frac{d^3p}{(2\pi)^3}\exp\left[\frac{i\pi rp_\perp^2}{m\hbar\omega_c}\right]\int\frac{d\omega}{2\pi}A(\epsilon_p,\omega)\ , \tag{5}$$

where $\epsilon_p=p^2/2m-\mu$. The momentum integration is converted to an energy (ϵ) integration by a standard procedure.[3] Then,

$$n_r=\frac{(-1)^r}{2}\text{Re}\int_{-\mu}^{\infty}\frac{d\epsilon}{2\pi}N(\epsilon)\left[\frac{\hbar\omega_c}{2r(\epsilon+\mu)}\right]^{1/2}\exp\left[\frac{2\pi ir(\epsilon+\mu)}{\hbar\omega_c}-\frac{i\pi}{4}\right]\int_{-\infty}^{\infty}d\omega\,f(\omega)A(\epsilon,\omega)\ , \tag{6}$$

where $N(\epsilon)$ is the unrenormalized density of states per spin. This is the general form of n_r containing the spectral function $A(\epsilon,\omega)$ which is determined by the p- and ω-dependent self-energy $\Sigma(\epsilon_p,\omega)$,

$$A(\epsilon,\omega)=\frac{\text{Im}\Sigma(\epsilon,\omega)}{[\omega-\epsilon-\text{Re}\Sigma(\epsilon,\omega)]^2+(\text{Im}\Sigma/2)^2}\ . \tag{7}$$

Using this form of A we cannot obtain a closed-form expression for the ω integration in Eq. (6). In order to proceed analytically, we make the pole approximation for A, that is, we assume that $\text{Im}\Sigma(\epsilon,\omega)=\text{constant}$ and take the limit $\text{Im}\Sigma=0$. Then we have

$$A(\epsilon,\omega)=2\pi\delta[\omega-\epsilon-\text{Re}\Sigma(\epsilon,\omega)]\ .$$

We are thus considering undamped quasiparticles and hence the effect of the p dependence of $\text{Im}\Sigma(p,\omega)$ is neglected. This is probably not a bad approximation since, as shown in Ref. 3, quasiparticle damping effects are not important for ω_c much smaller than the characteristic frequencies of the system (ω_{ph} or ω_{SF}). With the pole approximation, the ω integration in Eq. (6) yields

$$n_r=(-1)^r\pi\text{Re}\int_{-\mu}^{\infty}\frac{d\epsilon}{2\pi}N(\epsilon)\left[\frac{\hbar\omega_c}{2r(\epsilon+\mu)}\right]^{1/2}\exp\left[\frac{2\pi ir(\epsilon+\mu)}{\hbar\omega_c}-\frac{i\pi}{4}\right]f(\epsilon)\left[1-\left.\frac{\partial\,\text{Re}\Sigma(\epsilon,\omega)}{\partial\omega}\right|_{\omega=\eta_p}\right]^{-1}\ , \tag{8}$$

where η_p is the quasiparticle energy measured with respect to μ and given in terms of ϵ by the solution of the equation

$$\eta_p = \xi_p + \mathrm{Re}\Sigma(\xi_p, \eta_p) , \tag{9}$$

with $\xi_p = \epsilon_p - \mu$. To proceed with the ϵ integration we assume a parabolic band and use the relation

$$\frac{d\xi}{d\eta} = \frac{1 - \partial\, \mathrm{Re}\Sigma / d\eta}{1 + \partial\, \mathrm{Re}\Sigma / \partial\xi} .$$

Then Eq. (8) becomes

$$n_r = (-1)^r N(\epsilon_F) \left[\frac{\hbar\omega_c}{8r\epsilon_F} \right]^{1/2} \mathrm{Re} \left[\exp\left[\frac{2\pi i r \epsilon_F}{\hbar\omega_c} - \frac{i\pi}{4} \right] \int_{\eta(-\mu)}^{\infty} \frac{d\eta \exp[2\pi i r(\xi + \delta\mu)/\hbar\omega_c]}{[\exp(\eta/k_B T) + 1][1 + \partial\, \mathrm{Re}\Sigma(\xi,\eta)/\partial\xi]} \right] . \tag{10}$$

Here $\xi = \xi(\eta)$ is given by Eq. (9); for the case $\eta_p = 0$, we have $\delta\mu \equiv \mathrm{Re}\Sigma(\xi_F, 0) = \mu - \epsilon_F$, where $\epsilon_F = p_F^2/2m$. The basic assumption underlying Eq. (10) is the pole approximation, Eq. (7).

The rth harmonic of the magnetization, m_r, is given by integrating Eq. (10) with respect to μ and the differentiating with respect to H. We obtain

$$m_r = (-1)^r A_r \mathrm{Re} \left[\frac{i}{H} \frac{\hbar\omega_c N(\epsilon_F)}{2\pi} \left[\frac{\hbar\omega_c \epsilon_F}{8r^3} \right]^{1/2} \times \exp\left[\frac{2\pi i r \epsilon_F}{\hbar\omega_c} - \frac{i\pi}{4} \right] \right] , \tag{11}$$

where the amplitude A_r is given by the η integral in Eq. (10) multiplied by the factor $(2\pi i r/\hbar\omega_c)$. This result can be compared with Eq. (25) of Ref. 2. Closing the η integral in the upper half of the complex η plane yields

$$A_r = 2rx \sum_{\nu=0}^{\infty} \left[\frac{\exp[2\pi i r(\xi + \delta\mu)/\hbar\omega_c]}{1 + \partial\, \mathrm{Re}\Sigma(\xi,\eta)/\partial\xi} \right]_{\eta = i\omega_\nu} , \tag{12}$$

where ξ is given by Eq. (9) in terms of η.

The amplitude A_r is found immediately when we perform the usual expansion of $\Sigma(\xi,\eta)$ around its value at the FS, $\Sigma(p_F, 0)$. The result is given by Eq. (12) with the replacement

$$\frac{\xi + \delta\mu}{\hbar\omega_c} = \frac{i\omega_\nu}{\hbar\omega_c}(m^*/m) \tag{13}$$

in the exponent. Here m^*/m, defined by Eq. (2), is exactly equal to the specific-heat mass. Furthermore, the denominator in Eq. (12) is to be replaced by

$$1 + \left. \frac{\partial\, \mathrm{Re}\Sigma(\xi, 0)}{\partial\xi} \right|_{\xi_F} = Z^{-1}(m^*/m) , \tag{14}$$

where

$$Z = \left[1 - \frac{\partial\, \mathrm{Re}\Sigma(p_F, \omega)}{\partial\omega} \right]_{\omega=0}^{-1} \tag{15}$$

is the usual quasiparticle renormalization constant at the FS.

There are two cases where Σ depends on ξ (i.e., on p) only: the Hartree-Fock and the screened HF approximations. In the first case we use Eq. (12). The quasiparticle energy η is given by Eq. (9) with

$$\Sigma_x(\xi, 0) = \delta\mu + (e^2 m/\pi p_F)(\xi + \delta\mu) \ln | 4\epsilon_F/(\xi + \delta\mu) | , \tag{16}$$

assuming that $\xi + \delta\mu \ll \epsilon_F$; $\delta\mu = -\Sigma_x(\xi_{p_F}, 0)$. When $\xi + \delta\mu$ is found in terms of η, we can calculate the amplitude factor, A_r^{HF}, from Eq. (12) after substituting for $\partial\, \mathrm{Re}\Sigma/\partial\xi$ the quantity

$$\frac{\partial\Sigma_x(\xi, 0)}{\partial\xi} \doteq (e^2 m/\pi p_F)[\ln | 4\epsilon_F/(\xi + \delta\mu) | - 1] . \tag{17}$$

The resulting dHvA amplitude is well behaved, even at $T = 0$. A more realistic approximation to a p-dependent self-energy is obtained by screening the Coulomb potential in the self-energy with the Thomas-Fermi screening function. The result for the self-energy is

$$\Sigma_{scx}(\xi, 0) = (e^2 p_F/\pi) S_{scx}(\xi) , \tag{18}$$

where

$$S_{scx}(y) = -\left[1 + \left[\frac{1 - y^2 + y_0^2}{4y} \right] \ln\left[\frac{(1+y)^2 + y_0^2}{(1-y)^2 + y_0^2} \right] - \tan^{-1}\left[\frac{2y_0}{y^2 - 1 - y_0^2} \right] \right] . \tag{19}$$

Here $y = p/p_F$, $y_0 = p_{\mathrm{TF}}/p_F$, $\xi = \epsilon_F(y^2 - 1) + (e^2/\pi p_F) \times S_{scx}(y = 1)$, and $p_{\mathrm{TF}}/\hbar$ is the Thomas-Fermi screening wave vector. For $(\xi + \delta\mu)/\epsilon_F \ll 1, y_0$, we find the quasiparticle form of the amplitude, Eqs. (12)–(14), with $Z = 1$ and

$$\frac{m}{m^*} = 1 + \frac{me^2}{\pi p_F} \left[\frac{(y_0^2 + 2)}{4} \ln\left[\frac{y_0^2 + 4}{y_0^2} \right] - 1 \right] . \tag{20}$$

Finally, for a frequency-dependent self-energy part, $\mathrm{Re}\Sigma_{e\text{-}e}(p, \omega)$, such as that found in the plasma-pole approximation for the electron gas in simple metals,[16] we expect no deviations from the quasiparticle behavior of Eqs. (13)–(15). The instantaneous nature of the dynamically screened Coulomb interaction causes $\mathrm{Re}\Sigma_{e\text{-}e}$ to vary slowly with ω, on the scale of the plasma frequency ω_p.

From our results it seems reasonable to conclude that the momentum dependence *at the FS* of the self-energy does not lead to a deviation of the dHvA amplitude from quasiparticle behavior, i.e., there should be no difference in the dHvA and specific-heat masses due to this effect.

In view of the fact that such a discrepancy may exist in other systems (e.g., $TiBe_2$,[11] as previously mentioned), we would like to comment briefly on how this might occur in nearly ferromagnetic systems. We are not concerned here with the type of deviation from quasiparticle behavior discussed in Refs. 2 and 3, i.e., deviations due to quasiparticle damping effects not included in our pole approximation to the electron spectral weight function. This type of deviation is not likely to be important in most nearly ferromagnetic systems since the average spin-fluctuation (SF) energy is large compared with phonon energies and the condition $\omega_c \gg \omega_{SF}$ would be difficult to satisfy. Instead, we want to speculate about a possible deviation that could also occur within the pole approximation.

In Ref. 3, it was apparently concluded that SF effects (paramagnons) contribute to the dHvA amplitude in the same manner as phonons. The analogy between phonons and paramagons is, however, not as good as has often been assumed. In particular, due to the absence of Migdal's theorem for spin fluctuations, the one-paramagnon-exchange self-energy may be a rather poor approximation.[17,18] In the case of ^3He it was argued[18] that multiparamagnon processes could lead to a scaling, or "renormalization," of the quasiparticle renormalization constant Z in situations where the electron spectral function is integrated over a range of momenta rather than evaluated directly at the FS (as for the specific heat). The incoherent part of the spectral function, which is neglected in the pole approximation, was shown to give contributions that could be accounted for in a pole approximation by effectively *increasing* the magnitude of Z. If this effect occurs in the dHvA case, the factor Z occurring in the amplitude would be increased resulting in an effective mass *smaller* than the specific-heat mass.

Experimental measurement of the specific heat and the temperature dependence of the dHvA amplitude in nearly ferromagnetic metals would be helpful in clarifying these effects.

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$$\sum_{l=0} f(l+\tfrac{1}{2})$$

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