Quasiparticle approach to the de Haas–van Alphen effect

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The oscillatory contribution to the thermodynamic grand potential for electrons in a magnetic field is calculated using an integral representation which conveniently yields the general amplitude result of Fowler and Prange. Linearization of the self-energy evaluated on the imaginary energy axis leads to a quasiparticlelike approximation which includes both impurity scattering and phonon effects.

Fowler and Prange[1] (FP) and Englesberg and Simpson[2] (ES) have shown that in some cases it is natural and convenient to express the thermodynamic potential of equilibrium statistical mechanics in terms of energies on an imaginary energy axis[3] instead of real energies, see, e.g., Soven.[4] In particular FP and ES both discuss application of this approach to studying the effects of electron-phonon coupling in the oscillatory part of the magnetic susceptibility of metals [de Haas–van Alphen (dHvA) effect]. Although their approaches differ formally, their results are essentially identical and each concludes that modification to the amplitude of the dHvA oscillations is contained in the self-energy due to electron-phonon effects which is imaginary when evaluated at points on the imaginary energy axis. (Both authors have finally carried out an analytic continuation of the self-energies from the real energy axis to the imaginary energy axis.)

We explore here an alternative formulation of the imaginary-energy-axis method which in a somewhat distinctive manner yields a convenient contour-integral representation for the total magnetic susceptibility of the free-electron gas, (i.e., self-energy terms zero) as well as the oscillatory part of the susceptibility with nonzero self-energy first given by FP.[1]

In keeping with FP and ES we focus on short-range interactions due to static impurities and phonons in which case the self-energies can be evaluated with magnetic-field-independent basis states and, as do Englesberg and Simpson, we begin with Luttinger's[5] expression for the leading contribution to at least the oscillatory part of the thermodynamic potential, Ω

$$\Omega_{\rm osc} = -\frac{1}{\beta}\operatorname{Tr}\sum_n \ln[-G^{-1}(i\tau_n)] \quad , \tag{1}$$

where $G(i\tau_n)$ is the electron Green's-function matrix[6] and

$$G^{-1}(i\tau_n) = G_0^{-1}(i\tau_n) - \Sigma(i\tau_n) \quad , \tag{2}$$

where

$$G_0^{-1}(i\tau_n) = i\tau_n - \epsilon(p,k_z,\sigma)$$

is a diagonal matrix. Here $\epsilon(p,k_z,\sigma)$ are the Landau levels with assumed band renormalized mass m

$$\epsilon(p,k_z,\sigma) = \frac{k_z^2}{2m} + \omega_c(p+\tfrac{1}{2}) + \sigma g \mu_{\rm B} B - \gamma \quad , \tag{3}$$

with $\omega_c = eB/mc$ as the cyclotron frequency, B is the magnetic field taken in the z direction, $\mu_{\rm B} = e/2m_0c$ is the Bohr magneton, $\sigma = \pm\frac{1}{2}$ is the spin quantum numbers of the electron, g is the electron-band g factor, γ is the chemical potential, m_0 is the bare-electron mass, and $\beta = (k_B T)^{-1}$ with $\tau_n = (2n+1)\pi/\beta$. $\Sigma(i\tau_n)$ is that part of the magnetic-field-dependent self-energy matrix which does not contain any oscillatory terms[5] and the trace is taken with respect to the matrix inside the logarithmic function. Procedures for evaluation of the trace in general cases where the Green's-function matrix has off-diagonal elements have been given by Luttinger[6]; however, for the present discussion we limit ourselves to diagonal matrices by using the arguments given by FP, Brailsford,[7] and Soven[4] for short-range impurity scattering and for electron-phonon interactions. These authors show that not only can the oscillatory contributions to the self-energy be neglected, but so can the entire magnetic field dependence; i.e., the self-energies can be calculated using field-independent states of the electron. Within the limitations imposed by these short-range conditions and with spin-dependent scattering ignored for now, the self-energy matrix is diagonal in the quantum numbers k_z, p, and σ. Hence we can write

$$\Omega_{\rm osc} = -\frac{1}{\beta}\operatorname{Tr}\sum_n \ln[\,\epsilon(p,k_z,\sigma - i\tau_n + \Sigma(k_z,k_\perp,i\tau_n)] \quad , \tag{4}$$

with

$$\operatorname{Tr} \equiv \frac{m\omega_c}{2\pi^2}\int_{-\infty}^{\infty} dk_z \sum_{p=0} \sum_{\sigma=\pm\frac{1}{2}} \quad .$$

Here $k_\perp$ is the wave-vector component transverse to the magnetic field direction which arises from using the field-independent electronic states in computing the self-energies. The $k_\perp$ contains "false" quantum numbers introduced by these basis states which may, however, be dealt with by defining a suitable orbital average over the Fermi surface.[8]

For convenience we drop the "osc" subscript and consider now the complex quantity $i\tau_n - \Sigma(k_z; i\tau_n)$, in particular, its imaginary part. If we treat the logarithm of Eq. (4) as a distribution we can construct the following integral representations applicable in the regions noted: when

$$\mathrm{Im}[i\tau_n - \Sigma(i\tau_n)] > 0 \ ,$$

$$\ln[\epsilon - i\tau_n + \Sigma(i\tau_n)] = \int_b^{b+i\infty} \frac{ds}{s} e^{-s[\epsilon - i\tau_n + \Sigma(i\tau_n)]}$$

and when

$$\mathrm{Im}[i\tau_n - \Sigma(i\tau_n)] < 0 \ ,$$

$$\ln[\epsilon - i\tau_n + \Sigma(i\tau_n)] = -\int_{b-i\infty}^{b} \frac{ds}{s} e^{-s[\epsilon - i\tau_n + \Sigma(i\tau_n)]} \ . \quad (5)$$

Here b is real and positive, and the contour lies just to the right of the imaginary axis. From the spectral representation of the self-energy function[3]

$$\Sigma(i\tau_n) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega \Gamma(\omega)}{i\tau_n - \omega}, \quad \Gamma(\omega) \geqslant 0 \ .$$

We note that

$$\mathrm{Im}\Sigma(i\tau_n) = \frac{-\tau_n}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega \Gamma(\omega)}{\tau_n^2 + \omega^2} \ ,$$

so $\mathrm{Im}\Sigma(i\tau_n) < 0$ when $\tau_n > 0$ and $\mathrm{Im}\Sigma(i\tau_n) > 0$ when $\tau_n < 0$. We then can partition Ω as a sum of contributions from $\tau_n > 0$ and from $\tau_n < 0$ which we call Ω_+ and Ω_-, respectively, i.e.,

$$\Omega_+ = -\frac{1}{\beta} \mathrm{Tr} \sum_n \int_b^{b+i\infty} \frac{ds}{s} e^{-s[\epsilon(p,k_z,\sigma) - i\tau_n + \Sigma(k_z, i\tau_n)]} \quad (\tau_n > 0) \ ,$$

$$\Omega_- = \frac{1}{\beta} \mathrm{Tr} \sum_n \int_{b-i\infty}^{b} \frac{ds}{s} e^{-s[\epsilon(p,k_z\sigma) - i\tau_n + \Sigma(k_z, i\tau_n)]} \quad (\tau_n < 0) \ . \quad (6)$$

To clarify the objectives of the method we note that for free electrons the trace and sum over τ_n can be easily done, for with Re $s > 0$ we have the following:

$$\int_{-\infty}^{\infty} dk_z \, e^{-sk_z^2/2m} = \left[\frac{2m\pi}{s}\right]^{1/2} ,$$

$$\sum_{p=0}^{\infty} e^{-s\omega_c(p+\frac{1}{2})} = \left[2\sinh\frac{2\omega_c}{2}\right]^{-1} \ .$$

Furthermore, when

$$\tau_n > 0, \quad \mathrm{Im}s > 0 \ ,$$

$$\sum_{n=0}^{\infty} e^{is(2n+1)\frac{\pi}{\beta}} = -\left[2i\sin\frac{s\pi}{\beta}\right]^{-1} ,$$

and when

$$\tau_n < 0, \quad \mathrm{Im}s < 0 \ ,$$

$$\sum_{n=0}^{\infty} e^{-is(2n+1)\frac{\pi}{\beta}} = \left[2i\sin\frac{s\pi}{\beta}\right]^{-1} \ .$$

The two integrals Ω_+ and Ω_-, may now be summed to give a contour integral representation for free-Landau electrons[9]

$$\Omega = \frac{m\omega_c}{2\pi^{3/2}} \frac{(2m)^{1/2}}{2\pi i} \times \int_{b-i\infty}^{b+i\infty} e^{s\gamma} \frac{\pi}{\beta} \frac{\csc(\pi s/\beta) \times 2\cosh(\frac{1}{2} g\mu_B Bs)}{s^{3/2}\sinh(\frac{1}{2}s\omega_c)} \ , \quad (7)$$

where $\cosh\frac{1}{2}(g\mu_B Bs)$ arises from the spin sum. As an aside it is mentioned that this integral is surprisingly easy to evaluate and has been studied for both its oscillatory and nonoscillatory contributions to the magnetic susceptibility.[9,10]

In the more general case when $\Sigma(i\tau_n) \neq 0$ we find, after performing the Landau level and spin sum,

$$\Omega_+ = -\frac{1}{\beta} \frac{m\omega_c}{2\pi^2} \sum_n \int_{-\infty}^{\infty} dk_z \int_b^{b+i\infty} ds \frac{\exp\{-s[k_z^2/2m - \gamma - i\tau_n + \Sigma(k_z, i\tau_n)]\}}{s\sinh(\frac{1}{2}s\omega_2)} \cosh(\tfrac{1}{2} g\mu_B Bs) \quad (8)$$

and

$$\Omega_- = \frac{1}{\beta} \frac{m\omega_c}{2\pi^2} \sum_n \int_{-\infty}^{\infty} dk_z \int_{b-i\infty}^{b} ds \frac{\exp\{-s[k_z^2/2m - \gamma - i\tau_n + \Sigma(k_z; i\tau_n)]\}}{s\sinh(s\omega_c/2)} \cosh(\tfrac{1}{2} g\mu_B Bs) \ .$$

The FP-ES result can be directly obtained by asymptotically extracting the oscillatory behavior. This is done by deforming the contours in Ω_+ and Ω_- to encircle the zeros of $\sinh\frac{1}{2}(s\omega_c)$ at $s=2\pi ir/\omega_c$, $r\neq 0$. Using the residue theorem we then have

$$\Omega_\pm=-\frac{m\omega_c}{\pi^2\beta}\sum_n\int_{-\infty}^{\infty}dk_z\sum_{r=1}\frac{(-1)^r}{r}\exp\left[\pm\frac{2\pi ir}{\omega_c}\left[\frac{k_z^2}{2m}-\gamma-i\tau_n+\Sigma(k_z;i\tau_n)\right]\right]\cos\left[\frac{g\mu_B\pi Br}{\omega_c}\right] . \tag{9}$$

Finally Ω_+ and Ω_- can be combined to give, with all $\tau_n>0$,

$$\Omega=-\frac{2m\omega_c}{\pi^2\beta}\sum_n\int_{-\infty}^{\infty}dk_z\sum_{r=1}^{\infty}\frac{(-1)^r}{r}\cos\frac{2\pi r}{\omega_c}\left[\frac{k_z^2}{2m}-\gamma+\mathrm{Re}\Sigma(k_z;i\tau_n)\right]$$
$$\times\exp\left[-\frac{2\pi r}{\omega_c}[\tau_n-\mathrm{Im}\Sigma(k_z;i\tau_n)]\right]\cos\left[\frac{g\mu_B\pi Br}{\omega_c}\right] . \tag{10}$$

Apart from a remaining k_z integration, this is the FP-ES result. It shows conveniently how the dHvA effect separates contributions from the real and imaginary part of the self-energy for a short-range interaction, when the self-energy is evaluated on the imaginary energy axis.

When the self-energy is specified the sum over n can be numerically done as has been demonstrated by FP for model phonon interactions and ES for realistic phonon interactions. FP also noted that at sufficiently high temperature ($k_BT>>\omega_c$) only the first term in the sum contributes significantly. On the other hand if the self-energies do not vary too rapidly along the imaginary energy axis they can be expanded to linear order and the n sum readily approximated. This leads to an extension of the FP high-temperature result which, by further examination, can be brought into the quasiparticle form. To simplify the presentation we ignore the real part of the self-energy which only serves to modify the dHvA frequency and locate the extremal orbits.

The k_z integration is generally approximated by a method of stationary phase to give

$$\Omega=-2\frac{(m\omega_c)^{3/2}}{\pi^2\beta}\sum_n\sum_{r=1}^{\infty}\frac{(-1)^r}{r^{3/2}}\cos\left[\frac{2\pi r\gamma}{\omega_c}-\frac{\pi}{4}\right]e^{-(2\pi r/\omega_c)[\tau_n-\mathrm{Im}\Sigma(0;i\tau_n)]}\cos\left[\frac{\pi g\mu_B rB}{\omega_c}\right] , \tag{11}$$

or, for the dominant term in the magnetization

$$M=4\frac{m^{3/2}\omega_c^{1/2}\gamma}{\beta\pi B}\sum_n\sum_r\frac{(-1)^r}{r^{1/2}}\sin\left[\frac{2\pi r\gamma}{\omega_c}-\frac{\pi}{4}\right]e^{-(2\pi r/\omega_c)[\tau_n-\mathrm{Im}\Sigma(0;i\tau_n)]}\cos\left[\frac{\pi g\mu_B rB}{\omega_c}\right] , \tag{12}$$

where $k_z=0$ is, in this case, the extremal dHvA orbit. With the τ_n sum yet to do we apply the Poisson sum formula to the grand potential,

$$\sum_{n=0}^{\infty}f\left[i(2n+1)\frac{\pi}{\beta}\right]=\sum_{\nu=-\infty}^{\infty}\int_0^{\infty}dy\, f\left[i(2y+1)\frac{\pi}{\beta}\right]e^{-2\pi i\nu y}$$

and assuming differentiability expand $\mathrm{Im}\Sigma((2y+1)(\pi/\beta)i)$ to linear order about $y=0$,

$$\mathrm{Im}\Sigma((2y+1)(\pi/\beta)i)=\mathrm{Im}\Sigma(i\tau_0)+\frac{2\pi y}{\beta}\frac{\partial}{\partial\tau_0}\mathrm{Im}\Sigma(i\tau_0) ,$$

where $\tau_0=\pi/\beta$. The dHvA amplitude for each harmonic becomes

$$\sum_{\nu=-\infty}^{\infty}e^{-(2\pi r/\omega_c)[\tau_0-\mathrm{Im}\Sigma(i\tau_0)]}\int_0^{\infty}dy\, e^{-2\pi i\nu y}\exp\left[-\frac{4\pi r\tau_0}{\omega_c}\left[1-\frac{\partial}{\partial\tau_0}\mathrm{Im}\Sigma(i\tau_0)\right]y\right] . \tag{13}$$

The y integration yields for the amplitude of the rth harmonic

$$e^{-(2\pi r/\omega_c)[\tau_0-\mathrm{Im}\Sigma(i\tau_0)]}\sum_{\nu=-\infty}^{\infty}\left[2\pi i\nu+\frac{4\pi r\tau_0}{\omega_c}\left[1-\frac{\partial}{\partial\tau_0}\mathrm{Im}\Sigma(i\tau_0)\right]\right] , \tag{14}$$

where the infinite sum over ν is an expansion of

$$\left\{1-\exp\left[-\frac{4\pi r\tau_0}{\omega_c}\left[1-\frac{\partial}{\partial\tau_0}\mathrm{Im}\Sigma(i\tau_0)\right]\right]\right\}^{-1} . \tag{15}$$

To this approximation then the amplitude of the rth harmonic is

$$\frac{e^{-(2\pi r/\omega_c)[\tau_0 - \mathrm{Im}\Sigma(i\tau_0)]}}{1-\exp\left[-\frac{4\pi r}{\omega_c}\tau_0\left(1-\frac{\partial}{\partial\tau_0}\mathrm{Im}\Sigma(i\tau_0)\right)\right]} \;. \tag{16}$$

The oscillatory part of the thermodynamic potential is then

$$\Omega = -2\left(\frac{m\omega_c}{\pi^2\beta}\right)^{3/2}\sum_{r=1}\frac{(-1)^r}{r^{3/2}}\cos\left(\frac{2\pi r\gamma}{\omega_c}-\frac{\pi}{4}\right)\cos\left(\frac{\pi g\mu_B rB}{\omega_c}\right)\frac{e^{-(2\pi r/\omega_c)[\tau_0 - \mathrm{Im}\Sigma(i\tau_0)]}}{1-\exp\left[-\frac{4\pi r}{\omega_c}\tau_0\left(1-\frac{\partial}{\partial\tau_0}\mathrm{Im}\Sigma(i\tau_0)\right)\right]} \;. \tag{17}$$

For the particular self-energy contributions considered here we have first the electron-phonon term[2]

$$\Sigma_{e-p}(i\tau_0) = -i\tau_0\lambda \;, \tag{18}$$

where λ, the dHvA orbital average electron-phonon enhancement factor is defined as

$$\lambda = \int_0^\infty \frac{d\omega}{\omega}[|g(\omega)|^2 F(\omega)] \;,$$

with $g(\omega)$ the coupling constant and $F(\omega)$ the phonon density of states. At low temperature we also have

$$\frac{\partial}{\partial\tau_0}\mathrm{Im}\Sigma_{e-p}(i\tau_0) \cong -\lambda \;.$$

For impurity scattering we can use the spectral representation with $\Gamma(\vec{k},\omega)$ expressed in terms of the forward-scattering t matrix;

$$\Gamma(\vec{k},\omega) = 2\pi N_i \sum_q |\tau_{\vec{k},\vec{q}}|^2 \delta(\omega - \epsilon_{\vec{q}}) \;, \tag{19}$$

with N_i the number of scattering sites. Taking $k_z = 0$ as extremal and orbital averaging this becomes

$$\mathrm{Im}\Sigma_{\mathrm{imp}}(0,i\tau_0) = -\frac{\tau_0}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{\Gamma(\omega)}{\tau_0^2 + (\omega-\gamma)^2} \;,$$

which upon going to zero temperature gives

$$\lim_{\tau_0\to 0}\mathrm{Im}\Sigma_{\mathrm{imp}}(0,i\tau_0) = -\tfrac{1}{2}\Gamma(\gamma) \;, \tag{20}$$

the usual temperature independent zero-temperature result.[4,7] Thus the rth harmonic of the amplitude is

$$A_r = \frac{e^{-(\pi r/\omega_c)\Gamma(\gamma)}\,e^{-(2\pi r/\omega_c)\tau_0 m^*/m}}{1-\exp\left[-\frac{4\pi r}{\omega_c}\tau_0\left(\frac{m^*}{m}-\frac{\partial}{\partial\tau_0}\mathrm{Im}\Sigma_{\mathrm{imp}}(i\tau_0)\right)\right]} \;, \tag{21}$$

where $m^*/m = \lambda + 1$, with m^* the electron effective mass, and $(2\pi k_B)^{-1}\Gamma(\gamma)$ is defined as the Dingle temperature. Despite its seeming inadequacy if compared to the full ES calculation it is not inconsistent with their results. When real parts of self-energies are included Eq. (21) will differ somewhat from Soven.[4]

Spin-dependent scattering can formally be treated if it is noted that the spin scattering self-energy is a matrix and therefore the initial Green's function must first be diagonalized in spin coordinates. This step allows the trace to be readily performed and the remaining argument is identical to that given above.[11]

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