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On the thermodynamics of independent Landau electrons

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Abstract. The thermodynamic potential for independent electrons in a magnetic field is calculated by a method that arises from a more general Green function approach. Results are obtained in the weak field and the quantum limits.

The thermodynamics of a gas of independent Landau electrons has had a place in the literature for many years, having been studied by several distinct methods (Landau 1930, Shoenberg 1939, Sondheimer and Wilson 1951). With the acquisition of accurate frequency, amplitude and lineshape information even in the quantum limit (Barklie and Shoenberg 1975, Rode and Lowndes 1977) for both pure and alloy systems, theoretical methods which illuminate the behaviour of Landau electrons in a variety of environments have evolved. In particular, from a discussion of electron–phonon interactions an approach to this problem was developed in which the thermodynamic potential could be expressed in terms of interaction self-energies evaluated on the imaginary energy axis (Fowler and Prange 1965, Engelsberg and Simpson 1970), an approach further developed by the introduction of a simplifying integral technique (Wasserman and Bharatiya 1979) used in conjunction with Luttinger's formula (Luttinger 1960, 1961). Application of the method to the theory of the quantum limit in dilute alloys has further demonstrated its utility (Karniewicz 1980).

Although problems which involve electron interactions are of greatest interest in applying this approach, its application to even non-interacting cases introduces somewhat distinctive features to the evaluation of the thermodynamic potential, with the analysis in the high Landau level number region and the quantum limit being quite compact, as well as sharing some common features with the interacting case (Karniewicz 1980).

The thermodynamic potential for a non-interacting system of fermions may be written in terms of the Green function as

$$\Omega = -\frac{1}{\beta}\operatorname{Tr}\sum_n \ln[-G_0^{-1}(\mathrm{i}\tau_n)]$$

which may further be expressed as the sum of two contributions, each depending on the

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location of the imaginary energies $\tau_n = (2n+1)\pi/\beta$ (Wasserman and Bharatiya 1979),

$$\Omega_+ = -\frac{1}{\beta}\operatorname{Tr}\sum_n \int_b^{b+i\infty} \frac{ds}{s}\exp\{-s[\varepsilon(p,k_z,\sigma) - i\tau_n]\}, \qquad \tau_n > 0,$$

$$0 < b < 1,$$

$$\Omega_- = +\frac{1}{\beta}\operatorname{Tr}\sum_n \int_{b-i\infty}^{b} \frac{ds}{s}\exp\{-s[\varepsilon(p,k_z,\sigma) - i\tau_n]\}, \qquad \tau_n < 0,$$

$$\varepsilon(p,k_z,\sigma) = k_z^2/2m + \omega_c(p+\tfrac{1}{2}) + \sigma g\mu_B B - \gamma.$$

Here the $\operatorname{Tr} = (m\omega_c/2\pi^2)\int_{-\infty}^{\infty} dk_z \sum_{p=0}\sum_{\sigma=\pm 1/2}$, $\omega_c = eB/mc$ is the cyclotron frequency, m is the electron band effective mass, B is the magnetic field taken in the z direction, $\mu_B = e/2m_0c$ is the Bohr magneton and m_0 is the bare electron mass. The spin quantum number of the electron is σ, g is the electron g-factor, γ is the chemical potential and $\beta = (k_B T)^{-1}$ with k_B Boltzmann's constant and T the temperature.

In the limit $\omega_c < \gamma$ the Landau levels are closely spaced and the trace is taken to include these summed Landau quantum numbers immediately. The quantum limit condition, on the other hand, suggests a differently motivated treatment of the trace, as will be discussed below. With the trace and sum over thermal energies carried out, Ω_+ and Ω_- simply add to give

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

(This result is, of course, applicable to both field limits, but it does not prove to be convenient for analysis in the quantum limit.) We can proceed by developing the Mittag–Leffler expansion

$$\frac{\pi\operatorname{cosec}(\pi s/\beta)}{\sinh\lambda s} = \frac{\beta}{\lambda s^2} + \beta\sum_{k=-\infty}^{\infty}{}' \frac{(-1)^k}{(s-\beta k)\sinh\lambda\beta k} + i\pi\sum_{k=-\infty}^{\infty}{}' \frac{(-1)^{k+1}}{\lambda(s-k\pi i/\lambda)\sinh(k\pi^2/\lambda\beta)}$$

where $2\lambda = \omega_c$ and the prime in the summation indicates that the $k=0$ term is omitted. The Mittag–Leffler expansion can be integrated term by term, with the first giving, for $\lambda_0 < \gamma$, where $2\lambda_0 = g\mu_B B$

$$\Omega_1 = -\left(\frac{m}{2\pi}\right)^{3/2}\frac{[(\gamma+\lambda_0)^{5/2} + (\gamma-\lambda_0)^{5/2}]}{\Gamma(7/2)}.$$

In the second term we substitute

$$\frac{1}{s^{3/2}} = \frac{1}{\Gamma(3/2)}\int_0^{\infty} dx\, x^{1/2}\exp(-xs),$$

which allows the contour integration to be performed with the result

$$\Omega_2 = \frac{\omega_c}{2\Gamma(3/2)}\left(\frac{m}{2\pi\beta}\right)^{3/2}\sum_{k=1}^{\infty}\frac{(-1)^k}{\sinh\lambda\beta k}$$

$$\times\Bigg(e^{k\beta(\gamma+\lambda_0)}\int_{\beta(\gamma+\lambda_0)}^{\infty} e^{-kx}x^{1/2}\,dx + e^{k\beta(\gamma-\lambda_0)}\int_{\beta(\gamma-\lambda_0)}^{\infty} e^{-kx}x^{1/2}\,dx$$

$$+ e^{-k\beta(\gamma-\lambda_0)}\int_0^{\beta(\gamma+\lambda_0)} e^{kx}x^{1/2}\,dx + e^{-k\beta(\gamma-\lambda_0)}\int_0^{\beta(\gamma-\lambda_0)} e^{kx}x^{1/2}\,dx\Bigg).$$

Repeated integration by parts yields an asymptotic expansion in powers of $(\gamma\pm\lambda_0)^{1/2}$ of which the leading contribution is in the degenerate limit

$$\Omega_2 = -\frac{\omega_c}{\beta\Gamma(3/2)}\left(\frac{m}{2\pi}\right)^{3/2} \sum_{k=1}^{\infty} (-1)^{k+1}\left(\frac{(\gamma+\lambda_0)^{1/2}+(\gamma-\lambda_0)^{1/2}}{k \sinh \lambda\beta k}\right).$$

For $\beta\lambda \gg 1$ the sum contributes terms of order $e^{-\beta\lambda k}$, which may be neglected in comparison with a contribution arising from the third term of the Mittag–Leffler expansion evaluated below. For $\beta\lambda < 1$ we write

$$(\sinh \lambda\beta k)^{-1} = (\lambda\beta k)^{-1} - \frac{2}{\lambda\beta}\int_0^{\infty} dx \sin kx\left[\exp\left(\frac{\pi x}{\beta\lambda}\right)+1\right]^{-1}$$

whereupon Ω_2 becomes

$$\Omega_2 = \frac{[(\gamma+\lambda_0)^{1/2}+(\gamma-\lambda_0)^{1/2}]\omega_c}{\beta\Gamma(3/2)}\left(\frac{m}{2\pi}\right)^{3/2} \times\left[\sum_k (-1)^{k+1}\left(\frac{1}{\lambda\beta k^2}-\frac{2}{\lambda\beta k}\int_0^{\infty}\frac{\sin kx}{\exp(\pi x/\beta\lambda)+1}dx\right)\right].$$

The sum and the integral may be approximated by writing

$$\int_0^{\infty}\frac{\sin kx}{\exp(\pi x/\beta\lambda)+1}dx = \int_0^{\pi}\frac{\sin kx}{\exp(\pi x/\beta\lambda)+1}dx + \int_{\pi}^{\infty}\frac{\sin kx}{\exp(\pi x/\beta\lambda)+1}dx.$$

In comparison with the first integral on the right-hand side, the second is exponentially negligible. Summing the first over k and then extending the upper limit, we have

$$\int_0^{\infty}\frac{x}{\exp(\pi x/\beta\lambda)+1}dx = \frac{\beta^2\lambda^2}{12}$$

so that

$$\Omega_2 = -\frac{1}{6\beta^2\Gamma(3/2)}\left(\frac{m}{2\pi}\right)^{3/2}(\pi^2-\beta^2\lambda^2)[(\gamma+\lambda_0)^{1/2}+(\gamma-\lambda_0)^{1/2}].$$

Finally, the third term in the Mittag–Leffler expansion may be integrated by rewriting the integral as

$$\Omega_3 = -\frac{i\pi}{\beta\Gamma(3/2)}\left(\frac{m}{2\pi}\right)^{3/2} \sum_{k=-\infty}^{\infty}{}' (-1)^{k+1}\left(\sinh\frac{k\pi^2}{\beta\lambda}\right)^{-1} \times\left[\int_0^{\gamma+\lambda_0} dx\, x^{1/2}\exp\left((\gamma+\lambda_0-x)\frac{k\pi i}{\lambda}\right) + \int_0^{\gamma-\lambda_0} dx\, x^{1/2}\exp\left((\gamma-\lambda_0-x)\frac{k\pi i}{\lambda}\right)\right].$$

Then an integration by parts yields two terms, $\Omega_3 = \Omega_3^{(1)} + \Omega_2'$, where

$$\Omega_3^{(1)} = -\frac{\omega}{\beta\sqrt{2}\Gamma(3/2)}\left(\frac{m}{2\pi}\right)^{3/2} \times\sum_{k=1}^{\infty}\frac{(-1)^{k+1}\lambda^{1/2}}{k^{3/2}\sinh(k\pi^2/\beta\lambda)}\left[\cos\frac{\pi k(\gamma+\lambda_0)}{\lambda}C_2\left(\frac{k\pi(\gamma+\lambda_0)}{\lambda}\right)\right.$$

$$+\sin\frac{k\pi(\gamma+\lambda_0)}{\lambda}S_2\left(\frac{k\pi(\gamma+\lambda_0)}{\lambda}\right)+\cos k\pi\frac{(\gamma-\lambda_0)}{\lambda}C_2\left(\frac{k\pi(\gamma-\lambda_0)}{\lambda}\right)$$

$$+\sin\frac{k\pi(\gamma-\lambda_0)}{\lambda}S_2\left(\frac{k\pi(\gamma-\lambda_0)}{\lambda}\right)\Bigg]$$

where $C_2(u)$ and $S_2(u)$ are Fresnel integrals (Gautschi 1972). In the limit $\lambda_0<\gamma$ the Fresnel integrals converge rapidly to a constant and the usual de Haas–van Alphen harmonic series is recovered.

Finally

$$\Omega_2'=\frac{\omega}{\beta\Gamma(3/2)}\left(\frac{m}{2\pi}\right)^{3/2}\sum_{k=1}^{\infty}(-1)^{k+1}\frac{[(\gamma+\lambda_0)^{1/2}+(\gamma-\lambda_0)^{1/2}]}{k\sinh(k\pi^2/\beta\lambda)}$$

involves an infinite series much like that treated in Ω_2, except for the manner in which $\beta\lambda$ appears. In this case, when $\beta\lambda \ll 1$ the result is negligibly small, but when $\beta\lambda > 1$ we may use the same method as above to evaluate the sum and, moreover, obtain the same result.

In the quantum limit the separation between Landau levels is large and the differential susceptibility appears as a series of distinct peaks with, perhaps, spin-induced splitting or lineshape distortions. The procedure that suggests itself is the isolation of contributions from each spin-split Landau level and the eventual summation over all such contributions (Rode and Lowndes 1977). One might think of this as a regrouping of the de Haas–van Alphen harmonic series into a series that is more rapidly convergent in this limit. This analogy is drawn with some caution, since it is not clear that the susceptibility terms that contributed weak field variation when $\omega_c<\gamma$ will continue to do so in the quantum limit. Returning to our starting point, the sum over thermal energies and the integration over k_z are carried out. The sum over Landau levels and spin is delayed. The two contributions Ω_+ and Ω_- can again be added to give a single integral

$$\Omega=-\frac{\omega_c(2\pi m^3)^{1/2}}{2\pi i\beta}\sum_{p,\sigma}\int_{b-i\infty}^{b+i\infty}\pi\operatorname{cosec}\frac{\pi s}{\beta}\,e^{-s\bar{\varepsilon}}\,ds$$

where $\bar{\varepsilon}=(p+\frac{1}{2})\omega_c+\sigma g\mu_B B-\gamma$.

We again find a Mittag–Leffler expansion a convenient analytic tool:

$$\pi\operatorname{cosec}\frac{\pi}{\beta}s=\frac{\beta}{s}+2\beta s\sum_{k=1}^{\infty}\frac{(-1)^k}{(s^2-k^2\beta^2)},$$

which immediately allows us to express Ω as the sum of two groups of terms, one independent of temperature and the other containing the temperature corrections. Writing $\Omega=\Omega_0+\Omega_T$, we have then

$$\Omega_0=-\frac{\omega_c(2\pi m^3)^{1/2}}{2\pi i}\sum_{p,\sigma}\int_{b-i\infty}^{b+i\infty}\frac{e^{-s\bar{\varepsilon}}}{s^{5/2}}\,ds$$

and

$$\Omega_T=-\frac{\omega_c(2\pi m^3)^{1/2}}{\pi i}\sum_{p,\sigma}\sum_{k=1}^{\infty}(-1)^k\int_{b-i\infty}^{b+i\infty}\frac{e^{-s\bar{\varepsilon}}}{s^{1/2}(s^2-k^2\beta^2)}\,ds.$$

Evaluating the contour integral in Ω_0, we have

$$\Omega_0 = -\frac{4\omega_c}{3}\frac{(2m^3)^{1/2}}{\pi}\sum_{p,\sigma}\theta[-\bar{\varepsilon}]|\bar{\varepsilon}|^{3/2}, \qquad \theta(x) = \begin{cases} 0 & x<0, \\ 1 & x>0. \end{cases}$$

The step function, $\theta(x)$, signifies that as soon as a spin-split Landau level passes through the Fermi energy, i.e. $(p+\frac{1}{2})\omega_c + \sigma g \mu_B B > \gamma$, it no longer contributes to the thermodynamic potential. There may, however, be contributions in this 'extinction zone' from the low field side of the next higher Landau level (if there is one) or from a nearby spin state (if there is one). In the presence of impurity scattering this discontinuity is less drastic even at zero temperature, and the emerging lineshape is very sensitive to impurity scattering rates (Rode and Lowndes 1977, Karniewicz 1980). With decreasing magnetic field the low field sides of several peaks begin to overlap, for we are entering the region $\omega_c < \gamma$ where the harmonic analysis best describes the situation.

The finite-temperature contribution to the thermodynamic potential itself does not yield a convenient closed form; however, we continue the analysis with

$$(s^2 - k^2\beta^2)^{-1} = -\frac{1}{2k\beta}\left(\int_0^\infty e^{(s-k\beta)x}\,dx + \int_0^\infty e^{-(s+k\beta)x}\,dx\right),$$

and write $\Omega_T = \Omega_T^+ + \Omega_T^-$ where

$$\Omega_T^{\pm} = \frac{\omega_c}{2\pi i\beta}(2m^3\pi)^{1/2}\sum_{p,\sigma}\sum_k \frac{(-1)^k}{k}\int_0^\infty dx\, e^{-k\beta x}\int_{b-i\infty}^{b+i\infty} ds\, \frac{e^{-s[\bar{\varepsilon}\pm x]}}{s^{1/2}},$$

which yields, after doing the complex integration and the sum,

$$\Omega_T = -\frac{\omega_c}{\pi\beta}\left(\frac{m}{2\pi}\right)^{3/2}\sum_{p,\sigma}\int_0^\infty dx\, L(\beta x)[S_{1/2}(\bar{\varepsilon}+x) + S_{1/2}(\bar{\varepsilon}-x)]$$

where $S_{1/2}(\alpha) = \frac{1}{2}\sqrt{\pi}(|\alpha|-\alpha)^{1/2}/|\alpha|$ and $L(x) = \ln(1+e^{-x})$.

After integration by parts we have

$$\Omega_T = -\frac{\omega_c}{\pi}\left(\frac{m}{2\pi}\right)^{3/2}\sum_{p,\sigma}\int_0^\infty E(\beta x)[S_{3/2}(\bar{\varepsilon}+x) - S_{3/2}(\bar{\varepsilon}-x)]\,dx$$

where $E(x) = (e^x+1)^{-1}$ and $S_{3/2}(\alpha) = \sqrt{2\pi}(|\alpha|-\alpha)^{1/2}$, a form which is convenient for differentiation to obtain other thermodynamic variables.

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