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Free energy for harmonically bound fermions in a magnetic field

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Abstract. An analytic expression is obtained for the free energy of fermions bound in an anisotropic harmonic potential in the presence of an arbitrary magnetic field, at a finite temperature. The specific heat and the magnetic moment are readily calculated. Our results consist of two parts, a steady part and an oscillatory one. The latter is similar to the well known de Haas-van Alphen oscillation, but persists in the absence of a magnetic field. Applications of our results to the nuclear shell model and surface effects of solids are briefly discussed.

1. Introduction

Exactly soluble models often lead to qualitative and useful results, although they may not be accurate enough quantitatively. One of the most familiar and widely used models in physics as well as physical chemistry is that of the harmonic oscillator (Moshinsky 1969). The shell model is certainly a cornerstone in modern nuclear physics. A harmonic oscillator system has been used with enormous success to model the nuclear vibrational and electronic motions in complex molecular systems and to provide a basis for interpreting molecular spectra, chemical kinetics, and both inter- and intramolecular energy transfer phenomena.

The Schrödinger equation for systems with either isotropic or anisotropic harmonic oscillation potentials without magnetic field is soluble exactly, and it is also well known that the energy levels of an electron in the absence of potential barrier are quantised into Landau levels by an external magnetic field. The problem of the combination of isotropic harmonic potential and magnetic field was solved by Papadopoulos (1971) and Chanmugam *et al* (1972). Later the results were extended to an anisotropic harmonic potential (Datta and Richardson 1977) and an arbitrary quadratic potential (Davies 1985). The energy eigenvalues of the systems mentioned above are found to be those of an anisotropic harmonic oscillator in the absence of magnetic field, with frequencies that depend on the original natural frequencies and the applied magnetic field. This simple model has been applied to the calculations of Kemp's magneto-emission process (Kemp 1970) in magnetic white dwarfs (Chanmugam *et al* 1972) and the magneto-optical absorption spectroscopy and Faraday effect (Datta and Richardson 1977).

In the early work by Papadopoulos (1971), Boltzmann statistics are used to evaluate the partition function of a canonical ensemble of harmonically bound particles, which is then applied to the discussion of the magnetisation of an ionic lattice. Zero-temperature Fermi statistics was also considered by Papadopoulos and the steady part of the nuclear magnetisation in the shell model obtained.

The purpose of this paper is to extend the Fermi statistics of the system to finite temperature. As we shall soon see, apart from a steady term in the free energy, there is a de Haas-van Alphen-like oscillatory term, which even persists when the applied magnetic field vanishes.

The technique that we shall employ is the Sondheimer-Wilson (SW) Laplace transform method (Sondheimer and Wilson 1951), which relates Boltzmann statistics to Fermi statistics by the Laplace transform. In appendix 1, we present an alternative derivation of the SW result—which we consider is more physically appealing—as well as a discussion of the same.

2. The free energy

First of all we shall review the basic features of a harmonically bound fermion in a uniform magnetic field. The Hamiltonian of this system is the following:

$$H=\frac{1}{2M}\left(-\mathrm{i}\hbar\nabla-\frac{e}{c}\boldsymbol{A}\right)^2+\tfrac{1}{2}M(\omega_1^2x^2+\omega_2^2y^2+\omega_3^2z^2)-\gamma\boldsymbol{S}\cdot\boldsymbol{B} \tag{1}$$

where $\nabla\times\boldsymbol{A}=\boldsymbol{B}$ is the magnetic field and oriented in an arbitrary direction, ω_1, ω_2 and ω_3 are the natural frequencies of the oscillator, M and e are the mass and the charge of the fermion, $\boldsymbol{S}$ is the spin of the fermion and γ is the gyromagnetic ratio.

It has been shown (Davies 1985) that the eigenenergies of Hamiltonian (1) without the last spin-dependent term are, in general,

$$E_{lmn}=(l+\tfrac{1}{2})\hbar\Omega_1+(m+\tfrac{1}{2})\hbar\Omega_2+(n+\tfrac{1}{2})\hbar\Omega_3. \tag{2}$$

Here $l, m, n=0, 1, 2, \ldots, \Omega_1$, Ω_2 and Ω_3 are the eigenfrequencies which depend on the natural frequencies, and on both the magnitude and direction of the magnetic field. Needless to say $\Omega_i(i=1, 2, 3)$ must approach ω_i when the magnetic field goes to zero. In the case $\omega_1=\omega_2=\omega_3\equiv\omega$, where we have an isotropic harmonic oscillator, the eigenfrequencies can be determined as follows: $\Omega_{1,2}=(\omega^2+\omega_L^2)^{1/2}\pm\omega_{\mathrm{L}}$, $\Omega_3=\omega$, where $\omega_{\mathrm{L}}=eB/2MC$ is the Larmor frequency and the direction of the magnetic field has been chosen to be the z axis.

It is easy to extend Davies' result to the case of fermions with arbitrary spin $s/2$, where s is a positive odd integer. The eigenenergies of Hamiltonian (1) are the following:

$$E_{lmn\sigma}=E_{lmn}-\gamma S_{\mathrm{B}}B \tag{3}$$

where S_{B} is the spin component along the direction of $\boldsymbol{B}$, $S_{\mathrm{B}}=(-s/2)\hbar$, $(-s/2+1)\hbar, \ldots, (s/2)\hbar$ and $B=|\boldsymbol{B}|$.

As a direct consequence of (3), the Boltzmann partition function of a canonical ensemble of such systems can be written as

$$Z(\beta)=Z_1(\beta,\Omega_1)Z_1(\beta,\Omega_2)Z_1(\beta,\Omega_3)Q_s(\beta) \tag{4}$$

where $\beta=1/kT$ is the inverse temperature and

$$Z_1(\beta,\omega)=[2\sinh(\beta\hbar\omega/2)]^{-1} \tag{5}$$

is the partition function of a one-dimensional harmonic oscillator with frequency ω (Wilson 1965). $Q_s(\beta)$ is a factor introduced by spin:

$$Q_s(\beta) = \sum_{S_B=(-s/2)\hbar}^{(s/2)\hbar} \exp(\beta\gamma S_B B)$$
$$= \sinh\left(\frac{(s+1)\beta\mu_s B}{2}\right)\left[\sinh\left(\frac{\beta\mu_s B}{2}\right)\right]^{-1} \qquad (6)$$

where $\mu_s \equiv \gamma\hbar$.

The free energy of this ensemble with Fermi–Dirac statistics can be evaluated from the known Boltzmann partition function by the Sondheimer–Wilson Laplace transform technique (1951), which is discussed below and in appendix 1.

If one defines a function $\phi(E)$ by

$$\frac{Z(\beta)}{\beta^2} \equiv L_\beta[\phi(E)] = \int_0^\infty \phi(E)\,e^{-\beta E}\,dE \qquad (7)$$

or

$$\phi(E) \equiv L_E^{-1}\left(\frac{Z(\beta)}{\beta^2}\right)$$
$$= \frac{1}{2\pi i}\int_{C-i\infty}^{C+i\infty} \frac{Z(\beta)}{\beta^2}\,e^{\beta E}\,d\beta \qquad (8)$$

where the real number C is chosen such that every singular point of $Z(\beta)/\beta^2$ stays on the left-hand side of C, then the Fermi–Dirac free energy is given by

$$F = N\mu + \int_0^\infty \phi(E)\frac{\partial f(E)}{\partial E}\,dE. \qquad (9)$$

Here L and L^{-1} in (7) and (8) denote the Laplace transform and its inverse, respectively, $f(E)$ is the Fermi–Dirac distribution function:

$$f(E) = \frac{1}{\exp[\beta(E-\mu)]+1} \qquad (10)$$

where μ is the Fermi energy, which is determined by the number of particles N. As we shall see later (equation (A1.7)), the second derivative of the function $\phi(E)$ is just the density of states.

The Laplace inverse in (8) can be carried out by using (4) and (5) for our system. The result consists of a steady part and an oscillatory part. Basically, the behaviour of the Boltzmann partition function near $\beta = 0$ determines the steady part, whereas the singularities along the imaginary axis of β plane introduce the oscillatory part. Since the orders of the singularities depend on whether (i) Ω_1, Ω_2 and Ω_3 are all different, (ii) any two frequencies are equal, the third is different, (iii) three frequencies are all the same, separate derivations and expressions are needed for the oscillatory term in the above three cases. The detailed proof is put in appendix 2. In general the results can be written as the following:

$$\phi(E) = \phi_{st}(E) + \phi_{os}(E) \qquad (11)$$

where the steady part

$$\phi_{st}(E) = \frac{(s+1)}{\hbar^3\Omega_1\Omega_2\Omega_3}\left(\tfrac{1}{24}E^4 - \tfrac{1}{2}d_1E^2 + d_2\right) \qquad (12)$$

with

$$d_1 = a_1 - b_1 \tag{13}$$

$$a_1 = \tfrac{1}{24}\hbar^2(\Omega_1^2+\Omega_2^2+\Omega_3^2) \tag{14}$$

$$b_1 = (\mu_s B)^2[(s+1)^2-1]/24 \tag{15}$$

and

$$d_2 = a_2 + b_2 - a_1 b_1 \tag{16}$$

$$a_2 = \frac{7\hbar^4}{5760}(\Omega_1^4+\Omega_2^4+\Omega_3^4) - \frac{\hbar^4}{574}(\Omega_1^2\Omega_2^2+\Omega_2^2\Omega_3^2+\Omega_3^2\Omega_1^2) \tag{17}$$

$$b_2 = (\mu_s B)^4[3(s+1)^4 - 10(s+1)^2 + 7]/5760. \tag{18}$$

First we consider the case (i) where Ω_1, Ω_2 and Ω_3 are all different. The oscillatory part is the following:

$$\begin{aligned}\phi_{os}(E) = {}& \frac{\hbar\Omega_1}{8}\sum_{l=1}^{\infty}\frac{(-1)^l}{(l\pi)^2}\frac{R(\Omega_1)\cos(2l\pi E/\hbar\Omega_1)}{\sin(l\pi\Omega_2/\Omega_1)\sin(l\pi\Omega_3/\Omega_1)} \\ & + \frac{\hbar\Omega_2}{8}\sum_{l=1}^{\infty}\frac{(-1)^l}{(l\pi)^2}\frac{R(\Omega_2)\cos(2l\pi E/\hbar\Omega_2)}{\sin(l\pi\Omega_3/\Omega_2)\sin(l\pi\Omega_1/\Omega_2)} \\ & + \frac{\hbar\Omega_3}{8}\sum_{l=1}^{\infty}\frac{(-1)^l}{(l\pi)^2}\frac{R(\Omega_3)\cos(2l\pi E/\hbar\Omega_3)}{\sin(l\pi\Omega_1/\Omega_3)\sin(l\pi\Omega_2/\Omega_3)}\end{aligned} \tag{19}$$

where the R factors are due to spin:

$$R(\omega) = \sin\left(\frac{(s+1)l\pi\mu_s B}{\hbar\omega}\right)\left[\sin\left(\frac{l\pi\mu_s B}{\hbar\omega}\right)\right]^{-1}. \tag{20}$$

Thus we have obtained the function $\phi(E)$ for three different frequencies. The next thing we shall do is to use (9) to calculate the free energy. In general, the integration in (9) has to be carried out numerically. But if $\mu \gg kT$, we are able to obtain a closed analytic expression, as follows (see appendix 3 for details):

$$F = N\mu + F_{st} + F_{os} \tag{21}$$

where

$$F_{st} = -\phi_{st}(\mu) - \frac{(s+1)\pi^2(kT)^2}{6\hbar^3\Omega_1\Omega_2\Omega_3}\left(\frac{\mu^2}{2} - d_1 + o[10^{-2}(kT)^2]\right) \tag{22}$$

and

$$\begin{aligned}F_{os} = {}& \frac{kT}{4}\sum_{l=1}^{\infty}\frac{(-1)^{l-1}}{l}\left(\frac{R(\Omega_1)\cos(2l\pi\mu/\hbar\Omega_1)}{\sinh(2\pi^2 lkT/\hbar\Omega_1)\sin(l\pi\Omega_2/\Omega_1)\sin(l\pi\Omega_3/\Omega_1)}\right. \\ & + \frac{R(\Omega_2)\cos(2l\pi\mu/\hbar\Omega_2)}{\sinh(2\pi^2 lkT/\hbar\Omega_2)\sin(l\pi\Omega_3/\Omega_2)\sin(l\pi\Omega_1/\Omega_2)} \\ & \left. + \frac{R(\Omega_3)\cos(2l\pi\mu/\hbar\Omega_3)}{\sinh(2\pi^2 lkT/\hbar\Omega_3)\sin(l\pi\Omega_1/\Omega_3)\sin(l\pi\Omega_2/\Omega_3)}\right).\end{aligned} \tag{23}$$

We shall also write down the results for F_{os} in cases (ii) and (iii), saving the detailed proof in the appendices.

When any two frequencies are equal, but differ from the third, we denote the two equal frequencies by Ω and the third by ω. In this case, the oscillatory free energy takes the following form:

$$F_{\rm os}=\frac{kT}{4}\sum_{l=1}^{\infty}\frac{(-1)^{l-1}}{l}\frac{R(\omega)\cos(2l\pi\mu/\hbar\omega)}{\sinh(2\pi^2lkT/\hbar\omega)\sin^2(l\pi\Omega/\omega)}$$
$$+\frac{kT}{2}\sum_{l=1}^{\infty}\frac{R(\Omega)}{l\sinh(2\pi^2lkT/\hbar\Omega)\sin(l\pi\omega/\Omega)}$$
$$\times\left\{\left[\frac{\mu_sB}{2\hbar\Omega}G(\Omega)+\frac{1}{l\pi}+\left(\frac{\omega}{2\Omega}\right)\cot\left(\frac{l\pi\omega}{\Omega}\right)\right]\cos\left(\frac{2l\pi\mu}{\hbar\Omega}\right)+\frac{\mu}{\hbar\Omega}\sin\left(\frac{2l\pi\mu}{\hbar\Omega}\right)\right\} \tag{24}$$

where another spin factor is defined by

$$G(\Omega)=\frac{\sin(sl\pi\mu_sB/\hbar\Omega)}{\sin(l\pi\mu_sB/\hbar\Omega)\sin((s+1)l\pi\mu_sB/\hbar\Omega)}-\cot\left(\frac{(s+1)l\pi\mu_sB}{\hbar\Omega}\right). \tag{25}$$

In the case where $\Omega_1=\Omega_2=\Omega_3\equiv\Omega$, the corresponding result is

$$F_{\rm os}=kT\sum_{l=1}^{\infty}\frac{(-1)^{l-1}R(\Omega)}{l\sinh(2\pi^2lkT/\hbar\Omega)}\left\{\left[\left(\frac{\mu_sB}{2\hbar\Omega}\right)+\frac{1}{l\pi}\right]\left(\frac{\mu}{\hbar\Omega}\right)\sin\left(\frac{2l\pi\mu}{\hbar\Omega}\right)\right.$$
$$\left.+\left[\left(\frac{\mu_sB}{2\hbar\Omega}\right)\frac{G(\Omega)}{l\pi}-\frac{1}{8}\left(\frac{\mu_sB}{\hbar\Omega}\right)D(\Omega)-\frac{1}{2}\left(\frac{\mu}{\hbar\Omega}\right)^2+\frac{1}{8}+\frac{3}{4(l\pi)^2}\right]\cos\left(\frac{2l\pi\mu}{\hbar\Omega}\right)\right\} \tag{26}$$

where

$$D(\Omega)=(s+1)^2+2(s+1)\cot\left(\frac{l\pi\mu_sB}{\hbar\Omega}\right)\cot\left(\frac{l\pi(s+1)\mu_sB}{\hbar\Omega}\right)$$
$$-\operatorname{cosec}^2\left(\frac{l\pi\mu_sB}{\hbar\Omega}\right)-\cot^2\left(\frac{l\pi\mu_sB}{\hbar\Omega}\right). \tag{27}$$

3. Discussions

We have obtained a closed expression for the free energy of a canonical ensemble of anisotropic harmonic oscillators in a magnetic field by using Fermi–Dirac statistics. Our result consists of two parts: steady and oscillatory ones. The physical quantities of the system, such as specific heat, magnetic susceptibility, etc, can be calculated by using standard thermodynamical relations. It is straightforward, but very lengthy. We would rather make the following simple observations than writing down these results explicitly.

Similar to the free energy, other thermodynamical quantities of the system also contain oscillatory terms, and therefore show the de Haas–van Alphen-like oscillations when the temperature of the magnetic field of the system varies. Since the eigenfrequencies (Ω) reduce to the natural frequencies (ω) when the magnetic field vanishes, this oscillatory behaviour of the specific heat, for instance, persists even in the absence of a magnetic field.

Because of the factor $x_j/\sinh(lx_j)$, where $x_j = 2\pi^2 kT/\hbar\Omega_j$, $j = 1, 2, 3$, in front of each oscillatory term, the oscillation amplitudes are maximum when $x_j \sim 1$ which is

$$kT \sim 0.1\hbar\Omega_j \qquad j = 1, 2, 3. \tag{28}$$

In the nuclear shell model, $\hbar\Omega_j \sim$ MeV, and (17) shows that the oscillation is most significant when $T \sim 10^9$ K. The harmonic oscillator potential model considered above is a useful approximation when one considers the effects of the surface barrier of solids (Wang and O'Connell 1986).

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Appendix 1. An alternative derivation of the Sondheimer–Wilson results

The original proof of SW is rather mathematical. Here we shall show how the function $\phi(E)$ is introduced physically. As we shall soon see, the second derivative of the function $\phi(E)$ is just the density of states of the system.

Consider a system with energy levels $E_0 < E_1 < E_2 \ldots$. The Boltzmann partition function of a canonical ensemble of such a system is given by

$$Z(\beta) = \sum_{i=0}^{\infty} d_i \exp(-E_i\beta) \tag{A1.1}$$

where d_i is the degeneracy of the ith energy level. In terms of the density of states

$$g(E) = \sum_{i=0}^{\infty} d_i\delta(E - E_i) \tag{A1.2}$$

we may substitute $\int_0^{+\infty} g(E)\,dE$ for $\Sigma_{i=0}^{\infty} d_i$, if we choose $E_0 \geqslant 0$:

$$Z(\beta) = \int_0^{\infty} e^{-E\beta} g(E)\,dE$$

$$= L_\beta[g(E)] \tag{A1.3}$$

where L_β denotes Laplace transform with variable β. The inverse of (A1.3) is as follows:

$$g(E) = L_E^{-1}[Z(\beta)]. \tag{A1.4}$$

Here L_E^{-1} is the Laplace inverse with a variable E.

In Fermi–Dirac statistics the free energy of the ensemble is given by

$$F = N\mu - \frac{1}{\beta}\sum_{i=0}^{\infty} d_i \ln\{1 + \exp[\beta(\mu - E_i)]\}$$

$$= N\mu - \frac{1}{\beta}\int_0^{\infty} \ln\{1 + \exp[\beta(\mu - E)]\} g(E)\,dE. \tag{A1.5}$$

If one defines

$$\phi(E)=L_E^{-1}\left(\frac{Z(\beta)}{\beta^2}\right)$$
$$=\frac{1}{2\pi\mathrm{i}}\int_{C-\mathrm{i}\infty}^{C+\mathrm{i}\infty}\frac{Z(\beta)}{\beta^2}\mathrm{e}^{\beta E}\,\mathrm{d}\beta \tag{A1.6}$$

one has the following relation:

$$\partial^2\phi/\partial E^2=g(E). \tag{A1.7}$$

It is easy to verify the following expressions for $\phi(E)$ and its derivative $\partial\phi/\partial E$ by combining (A1.6) and (A1.1):

$$\phi(E)=\sum_{i=0}^{\infty}d_i(E-E_i)\theta(E-E_i) \tag{A1.8}$$

and

$$\frac{\partial\phi}{\partial E}=\sum_{i=0}^{\infty}d_i\theta(E-E_i) \tag{A1.9}$$

where $\theta(x)$ is the step function:

$$\theta(x)=\begin{cases}1 & x>0\\ 0 & x\leqslant 0.\end{cases} \tag{A1.10}$$

From (A1.2), (A1.8) and (A1.9) we find that, for any $\varepsilon_0\leqslant E_0$,

$$\phi(\varepsilon_0)=\left.\frac{\partial\phi}{\partial E}\right|_{E=\varepsilon_0}=g(\varepsilon_0)=0. \tag{A1.11}$$

Hence

$$\int_{\varepsilon_0}^{+\infty}\phi(E)\frac{\partial f}{\partial E}\,\mathrm{d}E=\phi(E)f(E)|_{\varepsilon_0}^{\infty}-\int_{\varepsilon_0}^{+\infty}\frac{\partial\phi}{\partial E}f(E)\,\mathrm{d}E$$
$$=\frac{1}{\beta}\int_{\varepsilon_0}^{+\infty}\frac{\partial\phi}{\partial E}\,\mathrm{d}(\ln\{1+\exp[\beta(\mu-E)]\})$$
$$=\frac{1}{\beta}\frac{\partial\phi}{\partial E}\ln\{1+\exp[\beta(\mu-E)]\}_{\varepsilon_0}^{\infty}$$
$$-\frac{1}{\beta}\int_{\varepsilon_0}^{\infty}\ln\{1+\exp[\beta(\mu-E)]\}\frac{\partial^2\phi}{\partial E^2}\,\mathrm{d}E$$
$$=-\frac{1}{\beta}\int_0^{\infty}\ln\{1+\exp[\beta(\mu-E)]\}g(E)\,\mathrm{d}E \tag{A1.12}$$

which we identify as the second term in the free energy given by (A1.5).

Combination of (A1.5) and (A1.12) gives

$$F=N\mu+\int_{\varepsilon_0}^{+\infty}\phi(E)\frac{\partial f}{\partial E}\,\mathrm{d}E. \tag{A1.13}$$

Since (A1.14) is true for any $\varepsilon_0\leqslant E_0$, a special choice $\varepsilon_0=0$ gives the sw relation (equation (7)).

In order to see the physical meaning of $\phi(E)$ more clearly, we now consider absolute zero temperature, where

$$\partial f / \partial E = -\delta(E - \mu_0) \tag{A1.14}$$

and μ_0 is the Fermi energy at absolute zero. The free energy at zero temperature, F_0 say, is obtained by using (7) and (A1.14):

$$F_0 = N\mu_0 - \phi(\mu_0). \tag{A1.15}$$

In addition, μ_0 can be found by using the general relation $\partial F/\partial \mu = 0$, which is now simply (see (A1.13) and (A1.14))

$$N = \partial \phi / \partial E|_{E=\mu_0}. \tag{A1.16}$$

Another example we shall consider here is the one we met in the text. We have obtained the exact expression for the function $\phi(E)$, for a system of anisotropic harmonic oscillators with an arbitrary (but uniform) magnetic field ((9)-(13)). It follows from (A1.7) that the density of state of this system can be calculated by simply taking the second derivative of the function $\phi(E)$. The steady part of the density of state agrees with that obtained via the semiclassical expansion technique (Bhaduri and Ross 1971). The oscillatory part is singular, but when the energy spacing is much smaller than the energy scale of the problem, the Fermi energy, say, the oscillatory part (see (12)), is very small and can be ignored.

Appendix 2. Proof for equations (9)-(13)

The combination of (3), (4) and (6) gives

$$\phi(E) = \frac{1}{2\pi i} \int_{C-i\infty}^{C+i\infty} d\beta \frac{Q_s(\beta)\, e^{E\beta}}{8\beta^2 \sinh(\beta\hbar\Omega_1/2) \sinh(\beta\hbar\Omega_2/2) \sinh(\beta\hbar\Omega_3/2)}. \tag{A2.1}$$

To carry out the integration in (A2.1), we choose the contour shown in figure 1 and rewrite the integral as follows:

$$\frac{1}{2\pi i} \int_{C-i\infty}^{C+i\infty} d\beta = \sum \gamma - \frac{1}{2\pi i} \int_{\substack{R_c \\ R_c \to +\infty}} d\beta - \frac{1}{2\pi i} \int_{\substack{\sigma \\ \delta \to 0}} d\beta \tag{A2.2}$$

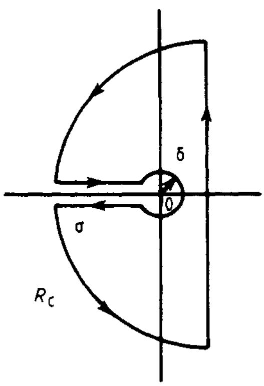

Figure 1. The closed contour used in the evaluation of the integral appearing in (A2.1).

where the second term vanishes and γ is the residue of the integrand. As we shall soon see, the first term oscillates, whereas the third is steady. We shall start with the third term.

We observe that

$$\chi(\sinh\chi)^{-1} = 1 - \frac{\chi^2}{6} - \frac{13}{360}\chi^4 + O(\chi^6) \qquad \text{when } \chi \to 0. \tag{A2.3}$$

Hence

$$\frac{\beta^3(\hbar^3\Omega_1\Omega_2\Omega_3/8)Q_s(\beta)}{\sinh(\hbar\Omega_1\beta/2)\sinh(\hbar\Omega_2\beta/2)\sinh(\hbar\Omega_3\beta/2)} = (s+1)(1 - d_1\beta^2 + d_2\beta^4) + o(\beta^6) \qquad \text{when } \beta \to 0 \tag{A2.4}$$

where d_1 and d_2 are given by (13)-(18). If we derive a new function by

$$P(\beta) \equiv \frac{Q_s(\beta)}{8\beta^2\sinh(\hbar\Omega_1\beta/2)\sinh(\hbar\Omega_2\beta/2)\sinh(\hbar\Omega_3\beta/2)} - \frac{(s+1)}{\hbar^3\Omega_1\Omega_2\Omega_3}\left(\frac{1}{\beta^5} - \frac{d_1}{\beta^3} + \frac{d_2}{\beta}\right) \tag{A2.5}$$

from (A2.4) we know that $P(\beta)$ vanishes when β goes to zero. Also, the last term in (A2.2) can be written in terms of $P(\beta)$:

$$\frac{1}{2\pi i}\int_{\sigma \atop \delta\to 0} \frac{Q_s(\beta)\,e^{E\beta}\,d\beta}{8\beta^2\sinh(\hbar\Omega_1\beta/2)\sinh(\hbar\Omega_2\beta/2)\sinh(\hbar\Omega_3\beta/2)} = \frac{1}{2\pi i}\int_{\sigma \atop \delta\to 0} P(\beta)\,d\beta + \frac{(s+1)}{\hbar^3\Omega_1\Omega_2\Omega_3}\frac{1}{2\pi i}\int_{\sigma \atop \delta\to 0}\left(\frac{1}{\beta^5} - \frac{d_1}{\beta^3} + \frac{d_2}{\beta}\right)e^{E\beta}\,d\beta. \tag{A2.6}$$

Since $P(\beta) \to 0$ as $\beta \to 0$, its integration along the small circle in σ vanishes as $\delta \to 0$. Furthermore, since the x axis is not a branch cut for $P(\beta)$, the integrations in opposite directions along the x axis cancel. So the first term on the right-hand side of (A2.6) is zero. The second term can be readily evaluated from the following representation of a Γ function:

$$\frac{1}{\Gamma(Z)} = -\frac{1}{2\pi i}\int_\sigma e^t\,t^{-Z}\,dt. \tag{A2.7}$$

This result will show that the last term in (A2.2) reduces to the steady part ϕ_{st}, which is given by (12).

Next we turn to calculate the first term in (A2.2). We begin with case (i), where the three frequencies in (A2.2) are all different and all singularities of the integrand are of the first order.

Since $\sinh(\hbar\Omega_j\beta/2)$ vanishes at $\beta_{l,j} = (2\pi l/\hbar\Omega_j)i$, where $j = 1, 2, 3$, and $l = \pm 1, \pm 2, \ldots$, the residue at $\beta_{l,1}$, say, is

$$\gamma_{l,1} = \frac{\hbar\Omega_1}{16(l\pi)^2}\frac{Q_s(\beta_{l,1})\exp[(2l\pi E/\hbar\Omega_1 + l\pi)i]}{\sin(l\pi\Omega_2/\Omega_1)\sin(l\pi\Omega_3/\Omega_1)}. \tag{A2.8}$$

By changing Ω_1 to Ω_2, Ω_2 and Ω_3 to Ω_3 and Ω_1 in (A2.8), one obtains $\gamma_{l,2}$ and $\gamma_{l,3}$.

It is easy to verify that the summation of all the residues gives the oscillatory part of $\phi(E)$:

$$\sum_{l=\pm 1}^{\pm\infty} \sum_{j=1}^{3} \gamma_{l,j} = \phi_{\text{os}} \tag{A2.9}$$

where ϕ_{os} is defined in (19).

When any two frequencies in (A2.1) are the same, but the third is different, we denote the two equal frequencies by Ω and the third by ω. Hence the residues at $\beta_{l,1} = 2\pi l\mathrm{i}/\hbar\omega$, where $l = \pm 1, \pm 2, \ldots$, are still given by the RHS of (A2.8), with Ω_2, Ω_3 replaced by Ω and Ω_1 replaced by ω. The singularities of $\beta_l = 2\pi l\mathrm{i}/\hbar\Omega$ are second order and the residues are

$$\gamma_l = -\frac{Q_s(\beta_l)\exp[(2\pi lE/\hbar\Omega)\mathrm{i}]}{8\sin(l\pi\omega/\Omega)(l\pi)^2}\left(\frac{Q_s'(\beta_l)}{Q_s(\beta_l)} + \frac{\hbar\Omega}{l\pi} + \cot\left(\frac{l\pi\omega}{\Omega}\right) + \frac{E}{\mathrm{i}}\right) \tag{A2.10}$$

where the prime denotes differentiation with respect to β_l.

It is straightforward to show that $Q_s'(\beta_l)/Q_s(\beta_l)$ is equal to $\mu_s BG(\Omega)/2$, where $G(\Omega)$ is given by (25). Hence the function $\phi_{\text{os}}(E)$ in this case can be written as follows:

$$\begin{aligned}
\phi_{\text{os}}(E) &= \sum_{l=\pm 1}^{\pm\infty} \gamma_{l,1} + \sum_{l=\pm 1}^{+\infty} \gamma_l \\
&= \frac{\hbar\omega}{8}\sum_{l=1}^{\infty} \frac{(-1)^l}{(l\pi)^2}\frac{R(\omega)\cos(2l\pi E/\hbar\omega)}{\sin^2(l\pi\Omega/\omega)} \\
&\quad - \frac{\hbar\Omega}{4}\sum_{l=1}^{\infty} \frac{R(\Omega)}{(l\pi)^2\sin(l\pi\omega/\Omega)}\left\{\left[\left(\frac{\mu_s B}{2\hbar\Omega}\right)G(\Omega) + \frac{1}{l\pi}\right.\right. \\
&\quad \left.\left. + \left(\frac{\omega}{2\Omega}\right)\cot\left(\frac{l\pi\omega}{\Omega}\right)\right]\cos\left(\frac{2l\pi E}{\hbar\Omega}\right) + \left(\frac{E}{\hbar\Omega}\right)\sin\left(\frac{2l\pi E}{\hbar\Omega}\right)\right\}.
\end{aligned} \tag{A2.11}$$

In case (iii), where all three frequencies in (A2.1) are equal, we denote this frequency by Ω. The singularities at $\beta_l = 2\pi l\mathrm{i}/\hbar\Omega$ are now of the third order, so the calculations of the residues are more tedious, but still straightforward. The result is

$$\begin{aligned}
\gamma_l &= \frac{(-1)^l Q_s(\beta_l)\exp(E\beta_l)}{\beta_l^2(\hbar\Omega)^3} \\
&\quad \times\left(\frac{EQ_s'(\beta_l)}{Q_s(\beta_l)} - \frac{2E}{\beta_l} - \frac{2Q_s'(\beta_l)}{\beta_l Q_s(\beta_l)} + \frac{Q_s''(\beta_l)}{2Q_s(\beta_l)} + \frac{E^2}{2} + \frac{3}{\beta_l^2} - \frac{(\hbar\Omega)^2}{8}\right).
\end{aligned} \tag{A2.12}$$

One can reduce $Q_s''(\beta_l)/2Q_s(\beta_l)$ to $(\mu_s B)^2 D(\Omega)/8$, where $D(\Omega)$ is given by (27). Summing up all the residues, we finally obtain

$$\begin{aligned}
\phi_{\text{os}}(E) &= \frac{(\hbar\Omega)}{2}\sum_{l=1}^{\infty}\frac{(-1)^l R(\Omega)}{(l\pi)^2}\left\{\left[\left(\frac{\mu_s B}{2\hbar\Omega}\right) + \frac{1}{l\pi}\right]\left(\frac{E}{\hbar\Omega}\right)\sin\left(\frac{2l\pi E}{\hbar\Omega}\right)\right. \\
&\quad + \left[\left(\frac{\mu_s B}{2\hbar\Omega}\right)\frac{G(\Omega)}{l\pi} - \frac{1}{8}\left(\frac{\mu_s B}{\hbar\Omega}\right)^2 D(\Omega) - \frac{1}{2}\left(\frac{E}{\hbar\Omega}\right)^2\right. \\
&\quad \left.\left. + \frac{1}{8} + \frac{3}{4(\pi l)^2}\right]\cos\left(\frac{2l\pi E}{\hbar\Omega}\right)\right\}.
\end{aligned} \tag{A2.13}$$

Appendix 3. The proof of equations (14)–(16)

Since $\partial f/\partial E$ is very close to $-\delta(E-\mu)$ at low temperatures ($kT \ll \mu$), the steady part F_{st} can be readily calculated from the following formula (Wilson 1965):

$$\int_0^{+\infty} \phi_{st}(E)\frac{\partial f}{\partial E}\,dE = -\phi_{st}(\mu) - \frac{\pi^2}{6}(kT)^2\phi_{st}^{(2)}(\mu) - \frac{7\pi^4}{360}(kT)^4\phi_{st}^{(4)}(\mu) - \dots. \tag{A3.1}$$

To evaluate the oscillatory part F_{os} we need the following integration:

$$I_j = \int_0^{\infty} \cos\left(\frac{2l\pi E}{\hbar\Omega_j}\right)\frac{\partial f}{\partial E}\,dE. \tag{A3.2}$$

We cannot use (A3.1) in this case, since the cos function oscillates around μ, so we do it in the following fashion:

$$I_j = -\mathrm{Re}\left(\exp(\mathrm{i}2l\pi\mu/\hbar\Omega_j)\beta\int_0^{\infty}\frac{\exp[2\mathrm{i}l\pi(E-\mu)/\hbar\Omega_j]\,dE}{\{\exp[(E-\mu)\beta/2]+\exp[-(E-\mu)\beta/2]\}^2}\right)$$

$$= -\frac{1}{2}\mathrm{Re}\left(\exp(\mathrm{i}2l\pi\mu/\hbar\Omega_j)\int_{-\beta\mu/2}^{\infty}\frac{\exp(4\pi\mathrm{i}lZ/\beta\hbar\Omega_j)}{\cosh^2 Z}\,dZ\right) \tag{A3.3}$$

where Re{ } means the real part of { }. The lower limit of the integral can be replaced by $-\infty$ when $\beta\mu = \mu/kT \gg 1$. Then the path of the integration can be closed by the upper semicircle and the integral can be evaluated by the sum of the residues of the second-order poles at $Z = \mathrm{i}(n+\frac{1}{2})\pi$, $n = 0, 1, 2, \dots$. Replacing Z by $y = Z - \mathrm{i}(n+\frac{1}{2})\pi$, and putting $\cosh Z = \mathrm{i}(-1)^n \sinh y$, one obtains

$$\int_{-\infty}^{+\infty}\frac{\exp(4\pi l\mathrm{i}Z/\beta\hbar\Omega_j)}{\cosh^2 Z}\,dZ$$

$$= -\sum_{n=0}^{\infty}\exp[-\pi^2 2l(2n+1)/\beta\hbar\Omega_j]\oint\frac{\exp(4\pi\mathrm{i}ly/\beta\hbar\Omega_j)}{\sinh^2 y}\,dy$$

$$= \left(-\frac{\exp(-2\pi^2 l/\beta\hbar\Omega_j)}{1-\exp(-4\pi^2 l/\beta\hbar\Omega_j)}\right)\left(-\frac{8\pi^2 l}{\beta\hbar\Omega_j}\right)$$

$$= \frac{4\pi^2 l/\hbar\Omega_j\beta}{\sinh(2\pi^2 l/\beta\hbar\Omega_j)}. \tag{A3.4}$$

Thus

$$I_j = -\frac{2\pi^2 l/\beta\hbar\Omega_j}{\sinh(2\pi^2 l/\beta\hbar\Omega_j)}\cos\left(\frac{2l\pi\mu}{\hbar\Omega_j}\right). \tag{A3.5}$$

Substituting (A3.5) with $j = 1, 2, 3$, into

$$F_{os} = \int_0^{\infty}\phi_{os}\frac{\partial f}{\partial E}\,dE \tag{A3.6}$$

where ϕ_{os} is given by (19), we finally obtain (23).

When only two frequencies are equal, we have to evaluate F_{os} using $\phi_{os}(E)$ given by (A2.11). We need another integral given by

$$I = \int_0^{\infty} E\sin\left(\frac{2l\pi E}{\hbar\Omega}\right)\frac{\partial f}{\partial E}\,dE. \tag{A3.7}$$

We can obtain I by the following arguments. Since E does not oscillate around μ, only $\sin(2l\pi E/\hbar\Omega)$ on the RHS of (A3.7) needs the above special treatment. If we consider the imaginary part of the RHS in (A3.3) we have

$$\int_0^\infty \sin\left(\frac{2l\pi E}{\hbar\Omega}\right)\frac{\partial f}{\partial E}\mathrm{d}E = -\frac{2\pi^2 l/\beta\hbar\Omega}{\sinh(2\pi^2 l/\beta\hbar\Omega)}\sin\left(\frac{2l\pi\mu}{\hbar\Omega}\right). \tag{A3.8}$$

Hence when $kT \ll \mu$,

$$\begin{aligned} I &= \mu\int_0^\infty \sin\left(\frac{2l\pi E}{\hbar\Omega}\right)\frac{\partial f}{\partial \Omega}\mathrm{d}E \\ &= -\frac{2\pi^2 l\mu/\beta\hbar\Omega}{\sinh(2\pi^2 l/\beta\hbar\Omega)}\sin\left(\frac{2l\pi\mu}{\hbar\Omega}\right). \end{aligned} \tag{A3.9}$$

In fact, one can calculate (A3.7) by observing that $I = -(\hbar\Omega/2\pi)\,\partial I_j/\partial l$, where I_j is given by (A3.2), with Ω_j replaced by Ω. One will find that both results agree well when $kT \ll \mu$.

Similarly, one needs

$$\begin{aligned} J &= \int_0^\infty E^2\cos\left(\frac{2l\pi E}{\hbar\Omega}\right)\frac{\partial f}{\partial E}\mathrm{d}E \\ &= -\frac{\mu^2 2\pi^2 l/\beta\hbar\Omega}{\sinh(2\pi^2 l/\beta\hbar\Omega)}\cos\left(\frac{2l\pi\mu}{\hbar\Omega}\right) \end{aligned} \tag{A3.10}$$

to calculate F_{os} via $\phi_{os}(E)$ given by (13) in the case where three frequencies are the same. One can also evaluate the integral J by observing that $J = -(\hbar\Omega/2\pi)^2\,\partial^2 I_j/\partial l^2$.

Combinations of (A3.9) and (A2.11), (A3.10) and (A2.13) give (24) and (26), respectively.

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