Landau Diamagnetism: A $T = 0$ Calculation

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The ground state energy of a three dimensional free Fermi gas of electrons in a uniform applied magnetic field is computed. By considering how the ground state energy varies as a function of the applied magnetic field, one obtains a $T = 0$ derivation of the Landau diamagnetic susceptibility and the de Hass − van Alphen oscillations of the magnetization density. This $T = 0$ calculation provides a straightforward approach to understanding the basic physical phenomena behind these two important effects.

INTRODUCTION

The diamagnetic magnetic susceptibility χ of a free Fermi gas of electrons in a uniform applied magnetic field $\mathbf{H}$ is due to the changing nature of the single particle energy eigenstates in the plane perpendicular to $\mathbf{H}$, reflecting the orbital motion of the electrons under the influence of the magnetic field. As originally computed by Landau, the standard calculation of this effect is done at finite temperature T, summing the grand canonical partition function over the quantum numbers k_z, k_x, and integer n that label the eigenstates in the magnetic field. The chemical potential that appears in the Fermi occupation function remains constant and the sum over n is approximated by using the Euler summation formula. Finally one must demonstrate that the magnetization density M and susceptibility χ computed at constant chemical potential μ are equal to the desired M and χ under the true physical condition of constant electron density n_e. The calculation is involved and requires familiarity with important concepts from statistical mechanics. It is easy to lose sight of the underlying basic physics leading to the effect.

As an alternative to this standard approach, here we present a calculation of the Landau diamagnetic susceptibility carried out at zero temperature, $T = 0$. The calculation is conceptually straightforward and simple, involving only the basic ideas familiar from the $\mathbf{H} = 0$ Sommerfeld model. Specifically, the Landau level eigenstate structure of motion in the plane perpendicular to $\mathbf{H}$ is used to construct the full three dimensional density of states $g(\epsilon)$ in the presence of the magnetic field. One finds that the periodic Landau level structure leads to periodic van Hove singularities in $g(\epsilon)$. The density of states is then integrated to determine the Fermi energy ϵ_F as a function of H for an electron gas of fixed density $n_e = \int_0^{\epsilon_F} d\epsilon g(\epsilon)$. We find that, as a function of $1/H$, ϵ_F oscillates about the zero field value ϵ_{F0} with a period of $\Delta(1/H) = 2\mu_0/\epsilon_{F0}$, where μ_0 is the Bohr magneton. Knowing $g(\epsilon)$ and ϵ_F for finite H, we then integrate to compute the ground state energy density $u = \int_0^{\epsilon_F} d\epsilon g(\epsilon)\epsilon$. From the dependence of the ground state energy on magnetic field we compute the magnetic susceptibility, $\chi = -\partial^2 u/\partial H^2$, and recover Landau's result. A side product of this $T = 0$ approach is the calculation of the de Haas − van Alphen oscillations of the magnetization density that are physically present in the system whenever $k_\mathrm{B}T \ll \mu_0 H$. In particular, we find how the amplitude of these oscillations grows as H increases.

The above steps involve only elementary mathematics, resulting in finite sums that are evaluated numerically, and a numerical solution of an implicit equation that is easily accomplished on any modern computer. What is lacking in analytical exactness is compensated for by the conceptual simplicity of our approach that highlights the basic physics: the variation of the density of states and the Fermi energy in response to turning on the magnetic field. In the following discussion, quantities with a subscript "0" are evaluated at $H = 0$, while those without such subscript are at finite $H > 0$.

DENSITY OF STATES

Consider a free electron moving in three dimensional space. We can partition its energy ϵ into two pieces: its kinetic energy $\epsilon_\perp$ in the xy plane and its kinetic energy ϵ_z along the $\hat{z}$ axis,

$$\epsilon = \epsilon_\perp + \epsilon_z \ . \tag{1}$$

The density of single particle states per unit volume, per energy, $g(\epsilon)$, can then be written as the convolution of the two dimensional density of states per unit area $g_\perp(\epsilon_\perp)$ and the one dimensional density of states per unit length $g_z(\epsilon_z)$,

$$g(\epsilon) = 2\int_0^\epsilon d\epsilon_\perp g_\perp(\epsilon_\perp) g_z(\epsilon - \epsilon_\perp) \ , \tag{2}$$

where the factor of 2 counts the spin degeneracy. For $\epsilon_z = \hbar^2 k_z^2/2m$, one has $g_z(\epsilon_z)d\epsilon_z = 2d|k_z|/(2\pi)$, yielding,

$$g_z(\epsilon_z) = \frac{1}{\pi}\frac{d|k_z|}{d\epsilon_z} = \frac{1}{2\pi}\sqrt{\frac{2m}{\hbar^2\epsilon_z}} \ . \tag{3}$$

The density of states can thus be expressed as,

$$g(\epsilon) = \frac{1}{2\pi}\sqrt{\frac{2m}{\hbar^2}}\int_0^\epsilon d\epsilon_\perp \frac{2g_\perp(\epsilon_\perp)}{\sqrt{\epsilon - \epsilon_\perp}} \ . \tag{4}$$

For the ordinary case of a free electron in the absence of an applied magnetic field, $\epsilon_\perp = \hbar^2(k_x^2 + k_y^2)/2m$, and the two dimensional density of states is the constant $g_\perp(\epsilon_\perp) = m/(2\pi\hbar^2)$. Inserting this in Eq. (4) gives the familiar density of states $g_0(\epsilon)$,

$$g_0(\epsilon) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\epsilon} \ . \tag{5}$$

Now consider turning on a uniform applied magnetic field $\mathbf{H} = H\hat{z}$. The motion in the xy plane is then quantized into Landau levels with a discrete energy spectrum $\hbar\omega_c(n + \frac{1}{2})$, $n = 0, 1, 2, \ldots$, with the cyclotron frequency $\omega_c = eH/mc$. The degeneracy of each Landau level is $H/(2\phi_0)$, where $\phi_0 = hc/2e$ is the flux quantum. The two dimensional density of states is then given by,

$$g_\perp(\epsilon_\perp) = \frac{H}{2\phi_0}\sum_{n=0}^{\infty}\delta\left(\epsilon_\perp - \hbar\omega_c\left(n + \frac{1}{2}\right)\right) \ . \tag{6}$$

Inserting the above into Eq. (4) then gives,

$$g(\epsilon) = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\hbar\omega_c\sum_{n=0}^{n_{\max}}\frac{1}{\sqrt{\epsilon - \hbar\omega_c(n + \frac{1}{2})}} \tag{7}$$

where $n_{\max}$ is the largest integer such that $\hbar\omega_c(n_{\max} + 1/2) < \epsilon$. Defining the Fermi energy of the system in zero magnetic field as ϵ_{F0}, and defining the dimensionless energy variable $x = \epsilon/\hbar\omega_c$, we can compare Eqs. (5) and (7) rewriting them as,

$$g_0(\epsilon) = \frac{g_0(\epsilon_{F0})}{\sqrt{x_0}}\sqrt{x} \tag{8}$$

$$g(\epsilon) = \frac{g_0(\epsilon_{F0})}{\sqrt{x_0}}\frac{1}{2}\sum_{n=0}^{n_{\max}}\frac{1}{\sqrt{x - n - \frac{1}{2}}} \ , \tag{9}$$

where $x_0 = \epsilon_{F0}/\hbar\omega_c$. In Fig. 1 we plot $\bar{g}_0(\epsilon) \equiv g_0(\epsilon)/c_0$ and $\bar{g}(\epsilon) \equiv g(\epsilon)/c_0$ vs x, where $c_0 \equiv g_0(\epsilon_{F0})/\sqrt{x_0}$. We see that the finite field density of states $g(\epsilon)$ oscillates about zero field density of states $g_0(\epsilon)$, with van Hove singularities $1/\sqrt{x - x_n}$ at values $x_n = n + \frac{1}{2}$. These van Hove singularities are the manifestation of the two dimensional discrete Landau level structure on the three dimensional density of states.

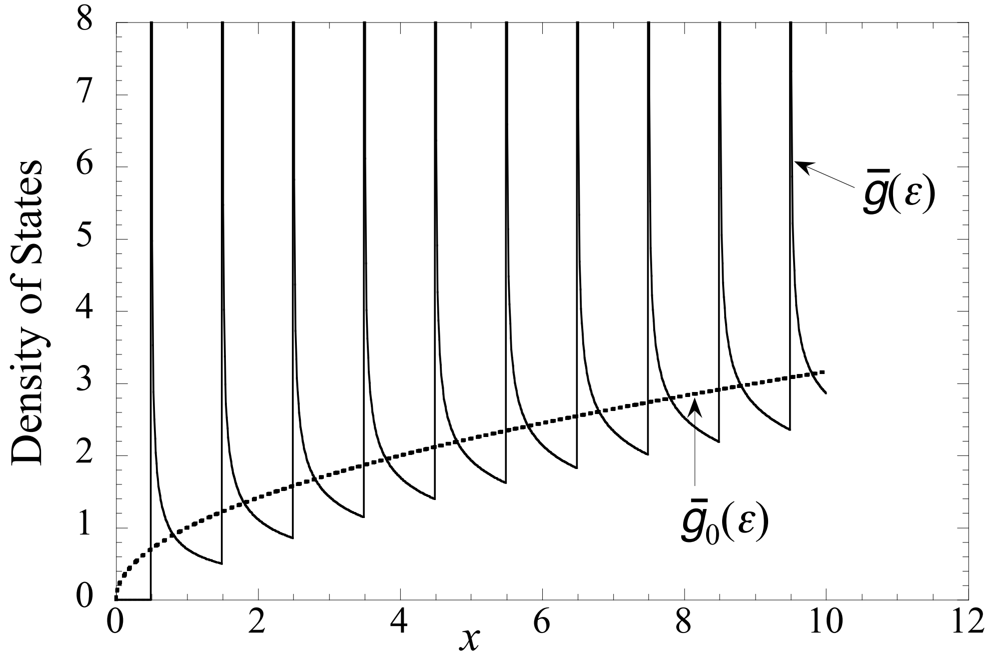

FIG. 1: Normalized density of states $\bar{g}_0(\epsilon) = g_0(\epsilon)/c_0$ for zero applied magnetic field (dotted line), and $\bar{g}(\epsilon) = g(\epsilon)/c_0$ for finite applied magnetic field H (solid line), where $c_0 \equiv g_0(\epsilon_{F0})/\sqrt{x_0}$ (see text), vs $x = \epsilon/\hbar\omega_c$, where $\omega_c = eH/mc$ is the cyclotron frequency. In the finite field H, $\bar{g}(\epsilon)$ has van Hove singularities $\sim 1/\sqrt{x - x_n}$ at $x_n = n + 1/2$.

INTEGRATED DENSITY OF STATES AND THE FERMI ENERGY

Next we define the integrated density of states,

$$G(\epsilon) = \int_0^\epsilon d\epsilon' g(\epsilon') \quad . \tag{10}$$

For the cases of zero and finite magnetic field we then get respectively,

$$G_0(\epsilon) = g_0(\epsilon_{F0})\epsilon_{F0} \, \frac{2}{3} \left(\frac{x}{x_0}\right)^{3/2} \tag{11}$$

$$G(\epsilon) = g_0(\epsilon_{F0})\epsilon_{F0} \, \frac{1}{(x_0)^{3/2}} \sum_{n=0}^{n_{\max}} \sqrt{x - n - \frac{1}{2}} \quad . \tag{12}$$

The Fermi energy is then determined by the condition that,

$$G(\epsilon_F) = n_e \quad , \tag{13}$$

where n_e is the density of electrons. For zero field, Eq. (11) then gives the familiar result,

$$g(\epsilon_{F0}) = \frac{3}{2} \frac{n_e}{\epsilon_{F0}} \quad . \tag{14}$$

When a magnetic field is turned on, the density of electrons n_e remains constant, but the Fermi energy must shift due to the change in the density of states $g(\epsilon)$. We can denote,

$$\epsilon_F = \epsilon_{F0} + \delta\epsilon \quad , \tag{15}$$

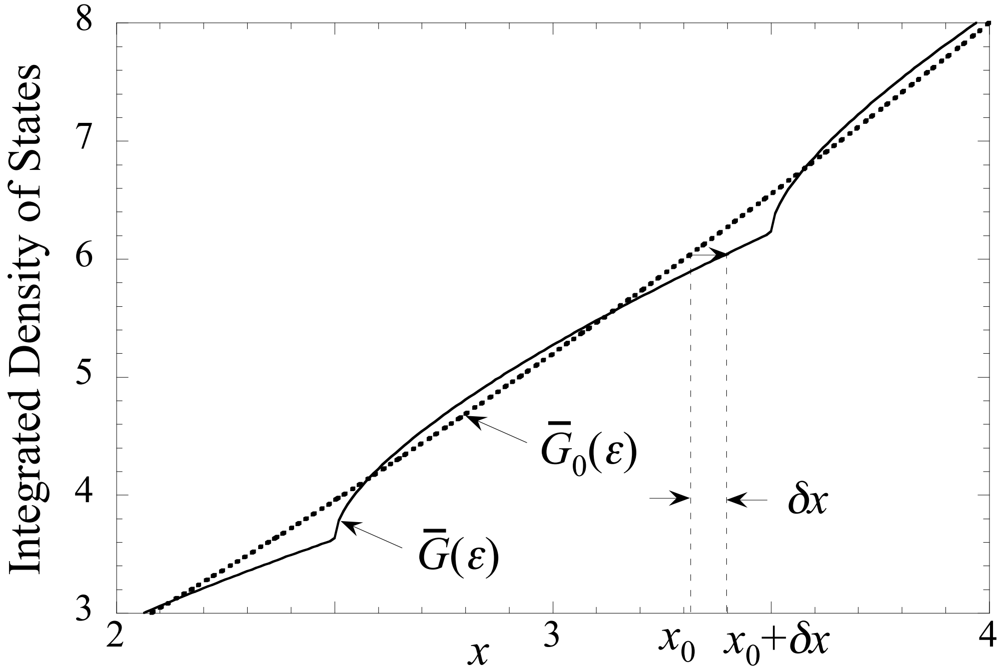

FIG. 2: Normalized integrated density of states $\bar{G}_0(\epsilon) = G_0(\epsilon)/C_0$ for zero applied magnetic field (dotted line), and $\bar{G}(\epsilon) = G(\epsilon)/C_0$ for finite applied magnetic field H (solid line), where $C_0 \equiv (2/3)g_0(\epsilon_{F0})\epsilon_{F0}/(x_0)^{3/2}$ (see text), vs $x = \epsilon/\hbar\omega_c$, where $\omega_c = eH/mc$ is the cyclotron frequency. If x_0 corresponds to the Fermi energy at $H = 0$, the Fermi energy at finite H is given by $x_0 + \delta x$, where δx is determined by $\bar{G}(x_0 + \delta x) = \bar{G}_0(x_0)$, as shown graphically.

where $\delta\epsilon$ is this shift in the Fermi energy, and is determined by the condition,

$$G(\epsilon_{F0} + \delta\epsilon) = G_0(\epsilon_{F0}) = n_e \ . \tag{16}$$

We illustrate this graphically in Fig. 2, where we plot $\bar{G}_0(\epsilon) \equiv G_0(\epsilon)/C_0$ and $\bar{G}(\epsilon) \equiv G(\epsilon)/C_0$ vs x, where $C_0 = (2/3)g_0(\epsilon_{F0})\epsilon_{F0}/(x_0)^{3/2}$. If $x_0 = \epsilon_{F0}/\hbar\omega_c$ gives the Fermi energy in zero magnetic field, then the Fermi energy at finite field is obtained by finding the value x such that $G(x) = G_0(x_0)$, as shown in the figure. Using Eqs. (11) and (12) we can rewrite the condition of Eq. (16) as,

$$\frac{3}{2}\frac{1}{(x_0)^{3/2}}\sum_{n=0}^{n_{\max}}\sqrt{x_0 + \delta x - n - \frac{1}{2}} = 1 \ , \tag{17}$$

where $\delta x = \delta\epsilon/\hbar\omega_c$, and $n_{\max}$ is the largest integer such that $n_{\max} + \frac{1}{2} < x_0 + \delta x$. For fixed x_0, the left hand side of Eq. (17) is a monotonically increasing function of δx, and it is therefore straightforward to sum the series numerically and determine the value of δx that satisfies this condition using the numerical method of bisection on the interval $\delta x \in [-1, 1]$. We plot the resulting solution for δx vs x_0 in Fig. 3. We see that δx decreases as x_0 increases (i.e. H decreases) and oscillates with a period of $\Delta x_0 = 1$.

GROUND STATE ENERGY AND LANDAU DIAMAGNETIC SUSCEPTIBILITY

We are now in position to compute the ground state energy of the electron gas in a magnetic field, and from that the Landau diamagnetic susceptibility. Let u be the total energy per unit volume of an electron gas with Fermi energy ϵ_F. We have,

$$u = \int_0^{\epsilon_F} d\epsilon g(\epsilon)\epsilon = (\hbar\omega_c)^2 \int_0^{x_F} dx g(x) x \ . \tag{18}$$

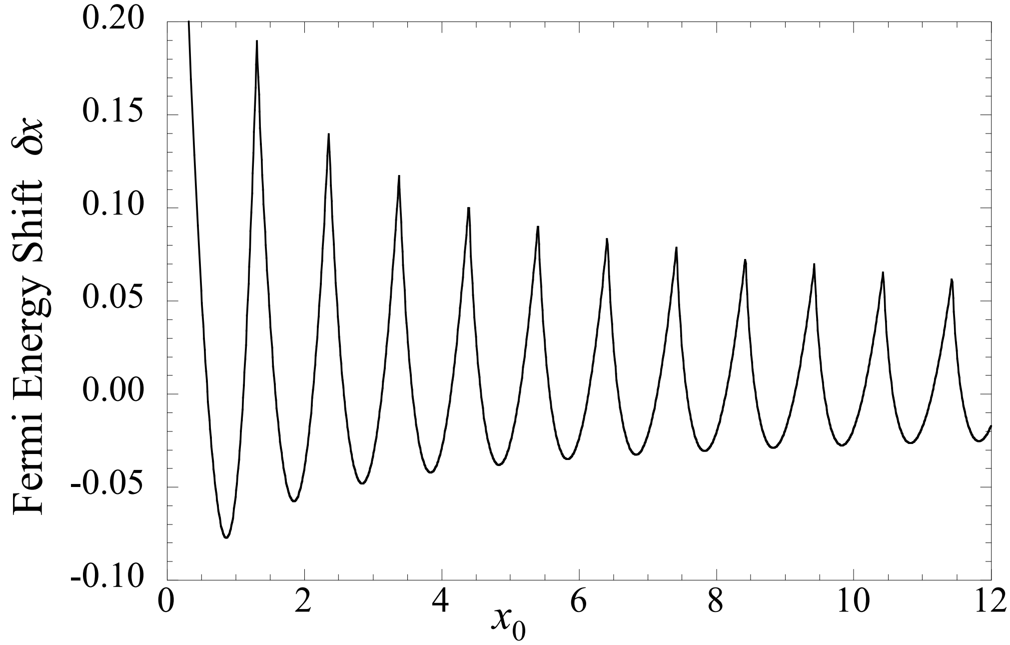

FIG. 3: Shift in Fermi energy upon turning on a magnetic field H, $\delta x = \delta\epsilon/\hbar\omega_c$, vs Fermi energy in zero magnetic field $x_0 = \epsilon_{F0}/\hbar\omega_c$, where $\omega_c = eH/mc$ is the cyclotron frequency. δx oscillates with period $\Delta x_0 = 1$.

Using Eqs. (8) and (9) we the get for the zero and finite magnetic field cases respectively,

$$u_0 = \frac{2}{5}\frac{g_0(\epsilon_{F0})}{\sqrt{x_0}}(\hbar\omega_c)^2 x_0^{5/2} = \frac{3}{5}n\epsilon_{F0} \tag{19}$$

$$u = \frac{1}{3}\frac{g_0(\epsilon_{F0})}{\sqrt{x_0}}(\hbar\omega_c)^2 \sum_{n=0}^{n_{\max}}(x_F + 2n + 1)\sqrt{x_F - n - \frac{1}{2}} \tag{20}$$

and so,

$$\frac{u}{u_0} = \frac{5}{6}\frac{1}{(x_0)^{5/2}}\sum_{n=0}^{n_{\max}}(x_0 + \delta x + 2n + 1)\sqrt{x_0 + \delta x - n - \frac{1}{2}} \tag{21}$$

where $\epsilon_F/\hbar\omega_c \equiv x_F = x_0 + \delta x$.

Using our result for δx obtained from Eq. (17), we substitute into the above equation and plot $(u - u_0)/u_0$ vs x_0 in Fig. 4. We plot to relatively large values of x_0 here, as compared to the earlier figures, in order to see how $(u - u_0)/u_0$ decays to zero as it must at large $x_0 = \epsilon_{F0}/\hbar\omega_c$, since $x_0 \to \infty$ corresponds to $H \to 0$. We see that $(u - u_0)/u_0$ displays small oscillations with period $\Delta x_0 = 1$ about an overall decay. Fitting to a quadratic decay α/x_0^2, we find an excellent fit using the numerical value $\alpha = 0.10418$. This is further illustrated in Fig. 5 where we plot $(u - u_0)/u_0$ vs. $1/x_0^2$ and see oscillations about a perfect straight line. Our numerical results above thus give,

$$u = u_0\left[1 + \frac{\alpha}{x_0^2}[1 + q(x_0)]\right] , \tag{22}$$

where $q(x_0)$ gives the oscillations about the $1/x_0^2$ decay. We plot $q(x_0)$ vs x_0 in Fig. 6. We see that it oscillates about zero with a period $\Delta x_0 = 1$, while the amplitude of oscillation decays as $\alpha'/\sqrt{x_0}$. A numerical fit to the maxima of $q(x_0)$ gives the value $\alpha' = 0.50216$. We thus can write,

$$u = u_0\left[1 + \frac{\alpha}{x_0^2} + \frac{\bar{\alpha}}{x_0^{5/2}}\bar{q}(x_0)\right] , \tag{23}$$

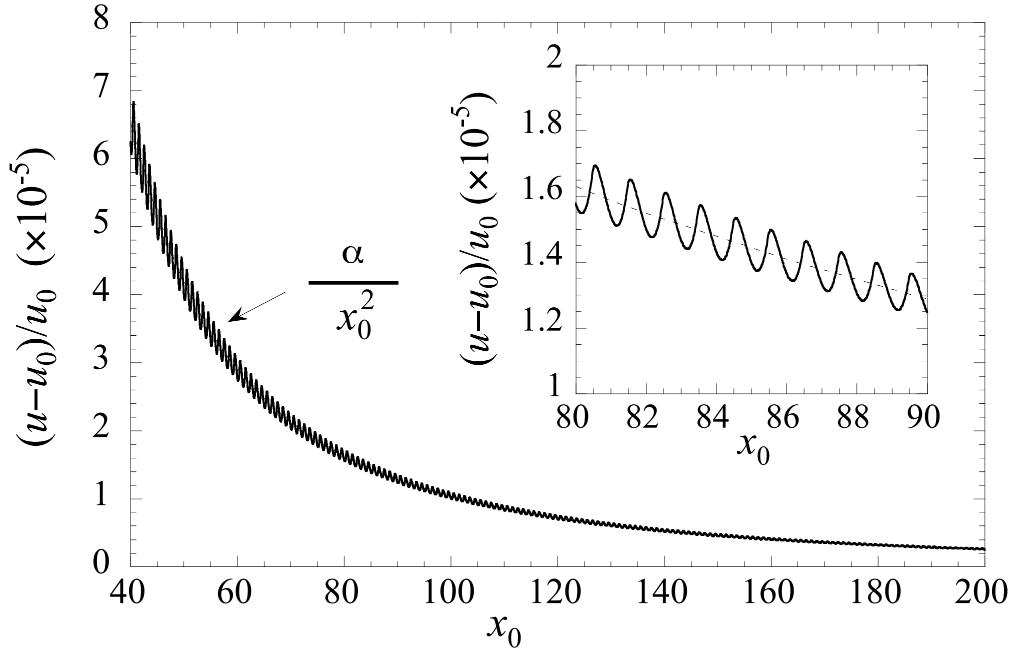

FIG. 4: Relative energy change $(u - u_0)/u_0$ upon turning on a finite magnetic field H vs $x_0 = \epsilon_{F0}/\hbar\omega_c$, where ϵ_{F0} is the Fermi energy for $H = 0$ and $\omega_c = eH/mc$ is the cyclotron frequency. The dashed line is a fit to α/x_0^2 and gives the value $\alpha = 0.10418$. The inset is a blow-up detailing the oscillations with period $\Delta x_0 = 1$.

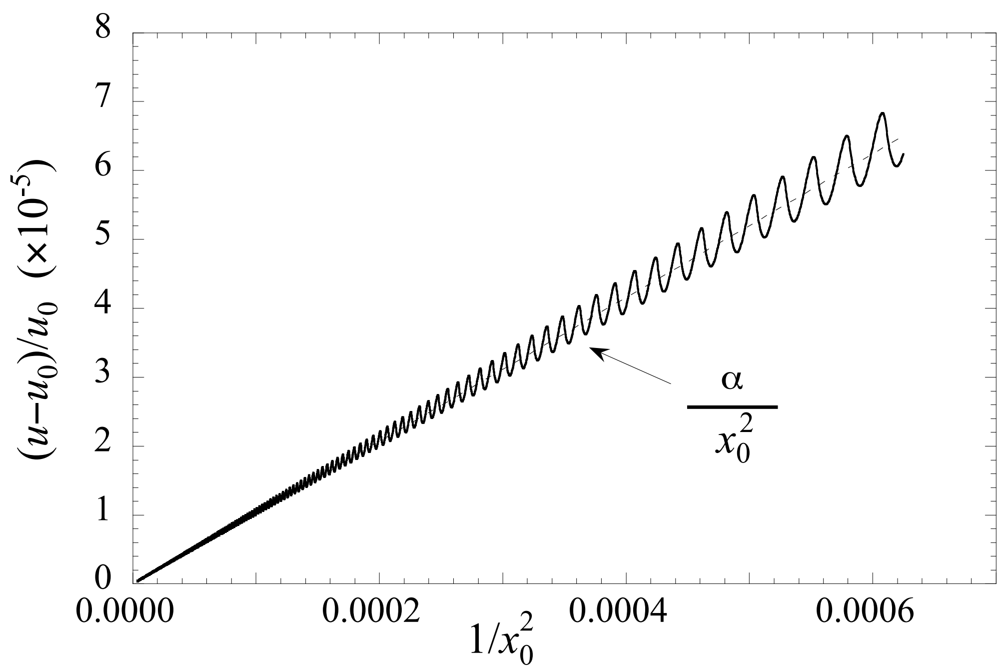

FIG. 5: Relative energy change $(u - u_0)/u_0$ upon turning on a finite magnetic field H vs $1/x_0^2 = (\hbar\omega_c/\epsilon_{F0})^2$, where ϵ_{F0} is the Fermi energy for $H = 0$ and $\omega_c = eH/mc$ is the cyclotron frequency. The straight dashed line is a fit to α/x_0^2, with $\alpha = 0.10418$.

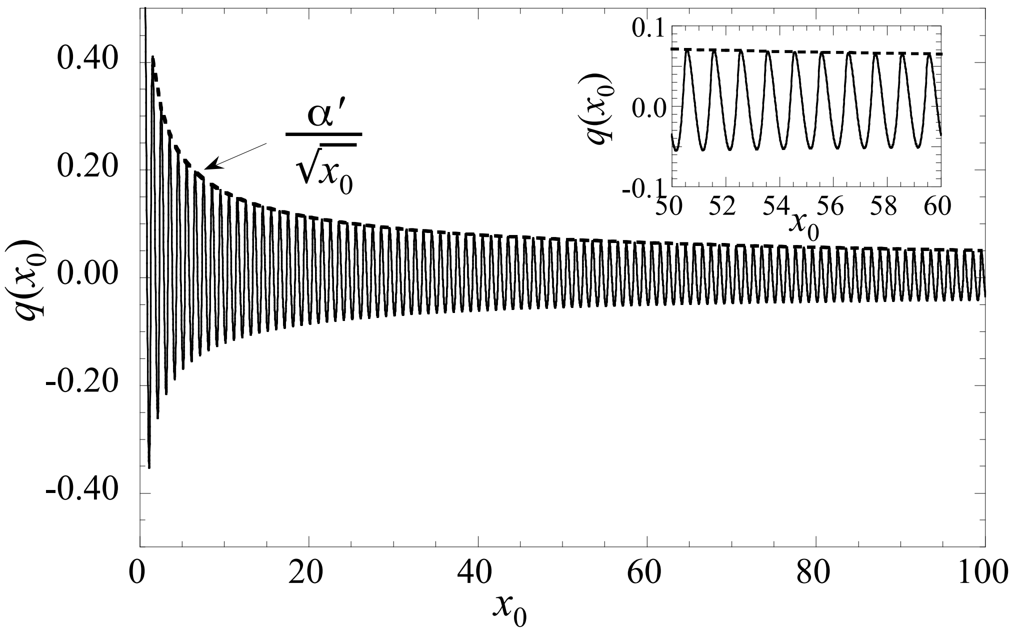

FIG. 6: Oscillations $q(x_0)$ vs $x_0 = \epsilon_{F0}/\hbar\omega_c$, where ϵ_{F0} is the Fermi energy for $H = 0$ and $\omega_c = eH/mc$ is the cyclotron frequency. The dashed line is a fit of the maxima to the form $\alpha'/\sqrt{x_0}$ and gives the value $\alpha' = 0.50216$. The inset is a blow-up detailing the oscillations with period $\Delta x_0 = 1$.

where $\bar{\alpha} \equiv \alpha\alpha' = 0.052315$, and $\bar{q}(x_0) \equiv \sqrt{x_0}q(x_0)/\alpha'$ oscillates with constant unit amplitude and period $\Delta x_0 = 1$. Using $u_0 = (3/5)n\epsilon_{F0}$, $g_0(\epsilon_{F0}) = (3/2)n/\epsilon_{F0}$, $x_0 = \epsilon_{F0}/\hbar\omega_c$, $\omega_c = eH/mc$, and $\mu_0 \equiv e\hbar/(2mc)$ the Bohr magneton, we can rewrite the above as,

$$u = u_0 + \alpha\frac{8}{5}g_0(\epsilon_{F0})\mu_0^2 H^2 + \bar{\alpha}\frac{8}{5}g(\epsilon_{F0})\sqrt{\frac{2}{\epsilon_{F0}}}\mu_0^{5/2}H^{5/2}\bar{q}(\epsilon_{F0}/2\mu_0 H) \ . \tag{24}$$

The magnetization density M and the magnetic susceptibility χ are defined by,

$$M = -\frac{\partial u}{\partial H}, \quad \chi = \left.\frac{\partial M}{\partial H}\right|_{H=0} \tag{25}$$

The term $\bar{q}$ in Eqs. (23) and (24) therefore results in oscillations of the magnetization density as a function of magnetic field with a period $\Delta x_0 = 1$, or $\Delta(1/H) = 2\mu_0/\epsilon_{F0} = 2e/(\hbar c k_{F0}^2)$, where the last result follows from $\mu_0 = \hbar e/2mc$ and $\epsilon_{F0} = \hbar^2 k_{F0}^2/2m$, with k_{F0} the Fermi wavevector at $H = 0$. These are the well known de Haas $-$ van Alphen oscillations. Moreover, our $T = 0$ calculation finds that oscillations in M/H grow in amplitude as H increases as $\sim H^{1/2}$.

At finite temperature $k_B T > \hbar\omega_c$, the oscillations due to $\bar{q}$ will be washed out. The magnetic susceptibility is then given by the second term on the right hand side of Eq. (24). One thus gets,

$$\chi = -\alpha\frac{16}{5}g_0(\epsilon_{F0})\mu_0^2 = -0.3334 g_0(\epsilon_{F0})\mu_0^2 \ , \tag{26}$$

where we have used $\alpha = 0.10418$ from our numerical fit. This should be compared to Landau's analytic calculation which yields $\chi = -(1/3)g_0(\epsilon_{F0})\mu_0^2$.