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Surface statistical thermodynamics and magnetic susceptibility in the infinite-barrier model

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The effects of a planar bounding surface on the statistical thermodynamics of a semi-infinite solid-state electron gas in a magnetic field normal to the surface are examined. The boundary condition of specular reflection for an infinite-barrier model is employed. Contributions proportional to surface area are determined for particle number N_s, grand thermodynamic potential W_s, internal energy E_s, magnetization M_s, and specific heat C_s. Surface Landau diamagnetic effects are studied in all regimes of magnetic field strength: Low monotonic magnetic field effects and surface de Haas–van Alphen oscillations are treated at low to intermediate field strengths. We also examine the surface statistical thermodynamic functions in the quantum high-field limit (all electrons in the lowest Landau level). All are analyzed in the degenerate regime, including finite-temperature corrections to the exact zero-temperature results. Nondegenerate quantum magnetic-field effects in N_s, W_s, E_s, M_s, and C_s are also treated in this study.

I. INTRODUCTION

This work is undertaken to determine the statistical thermodynamics and magnetic susceptibility of a bounded, semi-infinite, solid-state plasma in a quantizing magnetic field. In particular, we examine surface-related features for specular reflection of electrons at a planar boundary whose "infinite" potential barrier is much larger than the Fermi thermal energy. Wang and O'Connell[1] have recently focused attention on the role of boundaries in Landau diamagnetism, a problem of historical significance which was first examined by Teller,[2] who calculated the magnetic-field-induced current of an electron gas along an impenetrable wall [infinite-barrier model (IBM)]. This calculation was reexamined by Ohtaka and Moriya[3] and Jancovici.[4] Another approach to the study of surface effects in Landau diamagnetism by examining the thermodynamic potential for an electron gas contained in a hard-wall enclosure (IBM) has an equally long history,[5–10] beginning with the work of Papapetrou.[11–13] A survey of these various approaches to the IBM model is given in Refs. 14–31. A physically different model, in which the hard wall is replaced by a harmonic confinement potential, was first analyzed by Darwin.[5] This model has been investigated and elaborated from various points of view; a representative sampling of the literature may be found in Refs. 6–10. Another important aspect of this problem occurs for confining potentials which are smoothly variable, so that a semiclassical expansion in powers of $\hbar$, the thermal wavelength, or an equivalent parameter can be used. Such calculations were apparently first surveyed by Saenz and O'Rourke[32] and subsequently extended by Jennings and Bhaduri,[33] and by Wang and O'Connell.[1]

In this paper, we employ the infinite-barrier model for the planar surface bounding a semi-infinite solid-state plasma, and treat all regimes of normal magnetic field strength, including surface de Haas–van Alphen oscillatory phenomena for low and intermediate magnetic fields along with monotonic magnetic field effects in the degenerate case, as well as the quantum strong-field limit (in which only the lowest Landau state is occupied). Finite-temperature effects are discussed below the degeneracy temperature as well as above, and nondegenerate quantum magnetic field effects are also examined. In general, we consider quantum effects which may be large, as in the case where the Landau-level separation exceeds the Fermi energy, as well as the weak-field case. We present useful closed-form representations for the surface contributions to the grand potential W_s, internal energy E_s, magnetization M_s, and specific heat C_s, as well as the particle number N_s (where the subscript s denotes an areal density at the surface) in a comprehensive treatment.

II. GENERAL FORMULATION AND APPLICATION TO THE NONDEGENERATE CASE

In earlier work[34–37] pertaining to the thermodynamic Green's function[38] of a bounded semi-infinite solid-state plasma in a magnetic field $\mathbf{H}=H\hat{\mathbf{z}}$ normal to the planar surface, the quantum-mechanical grand-canonical-ensemble-averaged expression for the density $\rho(z)$ (uncorrelated) was found to be

$$\rho(z)=\frac{1}{(2\pi)^{3/2}}\int_0^\infty d\omega\frac{f_0(\omega)}{\hbar^3}\int_{-i\infty\mp\delta}^{i\infty\mp\delta}\frac{ds}{2\pi i}e^{\omega s}\frac{(m)^{3/2}\hbar\omega_c\cosh(\mu_0 Hs)}{s^{1/2}\sinh(\hbar\omega_c s/2)}[1-\exp(-2mz^2/\hbar^2 s)]\ . \tag{1}$$

Here $f_0(\omega)$ is the temperature-dependent Fermi distribution, $1/\beta$ is the thermal energy k_BT, ζ is chemical potential, ω_c is the cyclotron frequency, μ_0 is the Bohr magneton, m is the electron effective mass, and z is depth into the medium from an origin at the surface. The s integration is along the standard inverse–Laplace-transform contour. The total number N is readily obtained by integrating with respect to z:

$$N=A\int_0^\infty dz\,\rho(z)=N_VV+N_sA\ , \tag{2}$$

where V is the volume of the medium and A is its surface area. Using (1), the volume density is

$$N_V=\frac{1}{(2\pi)^{3/2}}\times\int_0^\infty d\omega\frac{f_0(\omega)}{\hbar^3}\int\frac{ds}{2\pi i}e^{s\omega}\frac{m^{3/2}\hbar\omega_c\cosh(\mu_0Hs)}{s^{1/2}\sinh(\hbar\omega_c s/2)}\ , \tag{3}$$

and the equivalent surface density is obtained from the z integration:

$$N_s=-\frac{1}{8\pi}\int_0^\infty\frac{f_0(\omega)}{\hbar^2}\int\frac{ds}{2\pi i}e^{s\omega}m\hbar\omega_c\frac{\cosh(\mu_0Hs)}{\sinh(\hbar\omega_c s/2)}\ . \tag{4}$$

It is advantageous to note that the analytical structure of the surface density N_s is identical to the analytical structure of the two-dimensional density expression $\rho(\text{2D})$:[34]

$$N_s=-\tfrac{1}{4}\rho(\text{2D})\ , \tag{5}$$

in regard to functional dependence on chemical potential. [Of course, the chemical potential involved in N_s is determined by the bulk density, unlike that of ρ(2D), which is determined by the sheet density.] The integrals representing ρ(2D) have been exhaustively analyzed,[36] and this provides a wealth of information concerning N_s and related quantities.

The expression for total number, as given by Eq. (2), has well-known thermodynamic relations to the grand potential W (logarithm of the grand partition function) and internal energy E in accordance with

$$N=\beta^{-1}\left[\frac{\partial W}{\partial\zeta}\right]_\beta \tag{6a}$$

and

$$E=-\left[\frac{\partial W}{\partial\beta}\right]_{\beta\zeta}\ . \tag{6b}$$

The specific heat for fixed geometry V, A is readily obtained as

$$C=\left[\frac{\partial E}{\partial T}\right]_{V,A}\ , \tag{7}$$

and the magnetization M is given by

$$M=\beta^{-1}\left[\frac{\partial W}{\partial H}\right]_{\beta,\zeta}\ . \tag{8}$$

Thus, integration of Eqs. (6a) and (6b) using Eq. (2) yields surface thermodynamic relations, after separation of the corresponding well-known bulk thermodynamic relations. For the surface density of the grand potential W_s, we have

$$N_s=\beta^{-1}\left[\frac{\partial W_s}{\partial\zeta}\right]_\beta\to W_s=\beta\int_{-\infty}^{\zeta}d\zeta'\,N_s(\zeta')\qquad\text{(holding }\beta\text{ fixed)}\ . \tag{9}$$

Our problem is to evaluate W_s explicitly by performing the ζ' integral of Eq. (9), and then determine the surface density of internal energy E_s in accordance with

$$E_s=-\left[\frac{\partial W_s}{\partial T}\right]_{\zeta\beta}\ , \tag{10}$$

and to use this to obtain the surface density of specific heat C_s from

$$C_s=\left[\frac{\partial E_s}{\partial T}\right]_A\ , \tag{11}$$

and finally we shall examine the surface density of magnetization M_s in the form

$$M_s=\beta^{-1}\left[\frac{\partial W_s}{\partial H}\right]_{\beta,\zeta}\ . \tag{12}$$

Having the relation $N_s=-\frac{1}{4}\rho(\text{2D})$ we can in fact simply transcribe results from Ref. 36 to this analysis, just multiplying by the factor $(-\frac{1}{4})$.

We shall focus attention of the zero-temperature limit first, since the finite-temperature result for any of the 2D integrals $G(\beta;\zeta)$ at hand may be obtained from the exact relation[36]

$$G(\beta;\zeta)=\int_0^{\infty} du\,(-\partial f_0/\partial u)G(\beta\to\infty;\ \zeta\to u)\ , \tag{13}$$

where $G(\beta\to\infty;\zeta)$ is the zero-temperature limit. This formula is especially convenient for low-temperature corrections in the degenerate case, since standard approximation procedures yield[39]

$$G(\beta;\zeta)=G(\beta\to\infty;\zeta)+\sum_{n=1}^{\infty} a_n (kT)^{2n}\frac{\partial^{2n}G(\beta\to\infty;\zeta)}{\partial\zeta^{2n}}\ , \tag{14a}$$

where

$$a_n=\left[2-\frac{1}{2^{2(n-1)}}\right]z(2n)\ , \tag{14b}$$

and $z(2n)$ denotes the Riemann zeta function. This representation is not useful above the degeneracy temperature, in which case it is more convenient to employ Eq. (4), noting that $f_0(\omega)\to e^{\zeta\beta}e^{-\omega\beta}$, and evaluate the ω and s integrations as Laplace transform and inverse Laplace transform with the result (nondegenerate case)

$$N_s=-\frac{e^{\zeta\beta}m\hbar\omega_c}{8\pi\hbar^2}\frac{\cosh(\mu_0 H\beta)}{\sinh(\hbar\omega_c\beta/2)}\ . \tag{15}$$

We shall illustrate the procedures outlined above, exploiting the simplicity of the nondegenerate case. Employing Eq. (9) with Eq. (15), we obtain W_s as

$$W_s=-\frac{e^{\zeta\beta}m\hbar\omega_c}{8\pi\hbar^2}\frac{\cosh(\mu_0 H\beta)}{\sinh(\hbar\omega_c\beta/2)}\ , \tag{16}$$

and using Eq. (10) for E_s, we have

$$E_s=\frac{e^{\zeta\beta}m\omega_c}{8\pi\hbar\sinh(\hbar\omega_c\beta/2)}\left[(\hbar\omega_c/2)\frac{\cosh(\mu_0 H\beta)\cosh(\hbar\omega_c\beta/2)}{\sinh(\hbar\omega_c\beta/2)}-(\mu_0 H)\sinh(\mu_0 H\beta)\right]\ . \tag{17}$$

Differentiation of E_s with respect to temperature T gives C_s [Eq. (11)] as

$$\begin{aligned}C_s=-k_B\beta^2\frac{m\omega_c}{8\pi\hbar}e^{\beta\zeta}\Bigg[&-(\mu_0 H)\frac{\zeta\sinh(\mu_0 H\beta)}{\sinh(\beta\hbar\omega_c/2)}+\frac{\zeta\hbar\omega_c}{2}\frac{\cosh(\beta\mu_0 H)\cosh(\beta\hbar\omega_c/2)}{\sinh^2(\beta\hbar\omega_c/2)}\\&-(\mu_0 H)^2\frac{\cosh(\beta\mu_0 H)}{\sinh(\beta\hbar\omega_c/2)}+(\mu_0 H)\frac{\hbar\omega_c}{2}\frac{\sinh(\beta\mu_0 H)\cosh(\beta\hbar\omega_c/2)}{\sinh^2(\beta\hbar\omega_c/2)}\\&+\frac{\hbar\omega_c}{2}\frac{\mu_0 H\sinh(\beta\mu_0 H)\cosh(\beta\hbar\omega_c/2)+(\hbar\omega_c/2)\cosh(\beta\mu_0 H)\sinh(\beta\hbar\omega_c/2)}{\sinh^2(\beta\hbar\omega_c/2)}\\&-\frac{\hbar\omega_c}{2}\cosh(\beta\mu_0 H)\cosh(\beta\hbar\omega_c/2)\hbar\omega_c\frac{\cosh(\beta\hbar\omega_c/2)}{\sinh^3(\beta\hbar\omega_c/2)}\Bigg]\ ,\end{aligned} \tag{18}$$

and M_s is obtained using Eq. (12) as

$$M_s=\frac{1}{\beta}\left[\frac{e^{\beta\zeta}m\omega_c/H}{8\pi\hbar}\frac{\cosh(\beta\mu_0 H)}{\sinh(\beta\hbar\omega_c/2)}+\frac{e^{\beta\zeta}m\omega_c}{8\pi\hbar}\beta\mu_0\frac{\sinh(\beta\mu_0 H)}{\sinh(\beta\hbar\omega_c/2)}-e^{\beta\zeta}\frac{m\omega_c}{8\pi\hbar}\frac{\cosh(\beta\mu_0 H)}{\sinh^2(\beta\hbar\omega_c/2)}\frac{\beta\hbar\omega_c}{2H}\cosh(\beta\hbar\omega_c/2)\right]\ . \tag{19}$$

It is noteworthy that the classical limit $\hbar\to 0$ is devoid of magnetic field effects, with $N_s=-m\exp(\beta\zeta)/(4\pi\hbar^2\beta)=W_s$; $E_s=-m\exp(\beta\zeta)/(4\pi\hbar^2\beta^2)=N_s/\beta$; $C_s=-k_B\zeta m\exp(\beta\zeta)/(4\pi\hbar^2)$, and $M_s=0$. It is clear that equipartition is not applicable to E_s (especially with N_s negative); on the other hand, the Bohr–van Leeuwen theorem is satisfied by $M_s=0$ for the classical limit, since the quantum magnetic field parameters vanish. Although classical magnetic field parameters need not vanish, they produce no magnetization for the geometry considered.

III. SURFACE THERMODYNAMICS BELOW THE DEGENERACY TEMPERATURE

As indicated above, it suffices to consider the zero-temperature limit. In this, we need only transcribe results from Ref. 36, multiplying by the factor $-\frac{1}{4}$. We shall cite exact results, as well as three cases of special interest: (A) spin splitting equal to Landau-level separation ($\mu_0 H=\omega_c/2$), (B) zero spin ($\mu_0 H=0$), and (C) low magnetic field ($\zeta\gg\omega_c$) ($\hbar\to 1$). Of course, the quantum strong-field limit, in which only the lowest Landau level is occupied ($\omega_c>\zeta$), is incorporated into the exact result. For lower fields ($\zeta>\omega_c$), de Haas–van Alphen (dHvA) oscillations are also in the exact result, and we will exhibit such structure.

For N_s we find the following zero-temperature results:

$$N_s=-\frac{m\omega_c}{8\pi}(n_+ + n_-) \tag{20}$$

is exact, and results for cases (A), (B), and (C) are given by

$$N_s^{(A)}=-\frac{m\omega_c}{8\pi}(2n_- + 1)\ , \tag{20a}$$

$$N_s^{(B)} = -\frac{m\omega_c}{4\pi}n' , \tag{20b}$$

$$N_s^{(C)} = -\frac{m\zeta}{4\pi} , \tag{20c}$$

where $n_\pm = \lfloor \zeta/\omega_c \pm \mu_0 H/\omega_c + \frac{1}{2} \rfloor_I$ and $\lfloor x \rfloor_I$ designates the maximum integer less than or equal to x (Fig. 1). The average of $n_\pm$ is given by

$$(n_\pm)_{\text{av}} = \frac{\zeta}{\omega_c} \pm \frac{\mu_0 H}{\omega_c} , \tag{21}$$

and $n' = n_+ = n_-$ for zero spin (case B). For W_s at $T=0$, we obtain

$$W_s = -\frac{\beta m\omega_c}{16\pi}[\, 2n_+(\zeta+\mu_0 H) + 2n_-(\zeta-\mu_0 H) - \omega_c(n_+^2 + n_-^2)] , \tag{22}$$

$$W_s^{(A)} = -\frac{\beta m\omega_c}{8\pi}[\, \zeta(2n_- + 1) - \omega_c n_-(n_- + 1)] , \tag{22a}$$

$$W_s^{(B)} = -\frac{\beta m\omega_c}{8\pi}[2\zeta n' - \omega_c(n')^2] , \tag{22b}$$

$$W_s^{(C)} = -\frac{\beta m}{8\pi}[\zeta^2 + (\mu_0 H)^2] . \tag{22c}$$

For E_s we find it convenient to note that

$$E_s = -\frac{m\omega_c}{2\pi}\left[\omega_c\frac{\partial}{\partial\omega_c} + \mu_0 H\frac{\partial}{\partial(\mu_0 H)}\right]\frac{2\pi}{\beta m\omega_c}W_s , \tag{23}$$

and thus for E_s at $T=0$ we find

$$E_s = -\frac{m\omega_c}{16\pi}[\omega_c(n_+^2 + n_-^2) - 2\mu_0 H(n_+ - n_-)] , \tag{24}$$

$$E_s^{(A)} = -\frac{m\omega_c^2}{8\pi}[n_-(n_- + 1)] , \tag{24a}$$

$$E_s^{(B)} = -\frac{m\omega_c^2}{8\pi}(n')^2 , \tag{24b}$$

$$E_s^{(C)} = -\frac{m}{8\pi}[\zeta^2 - (\mu_0 H)^2] . \tag{24c}$$

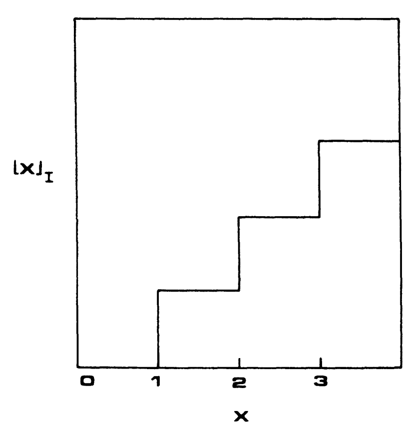

FIG. 1. The maximum-integer step function ($\lfloor x \rfloor_I$) designating the maximum integer less than or equal to x.

For the magnetic moment M_s at zero temperature, we note that

$$M_s = \frac{2W_s}{\beta H} - \frac{\zeta N_s}{H} , \tag{25}$$

and we obtain M_s as follows:

$$M_s = -\frac{m\omega_c}{8\pi H}[\zeta(n_+ + n_-) + 2\mu_0 H(n_+ - n_-) - \omega_c(n_+^2 + n_-^2)] , \tag{26}$$

$$M_s^{(A)} = -\frac{m\omega_c}{8\pi H}[\zeta(2n_- + 1) - 2\omega_c n_-(n_- + n_+)] , \tag{26a}$$

$$M_s^{(B)} = -\frac{m\omega_c}{4\pi H}[\zeta n' - \omega_c(n')^2] , \tag{26b}$$

$$M_s^{(C)} = -\frac{m\mu_0^2}{4\pi}H . \tag{26c}$$

All the results presented here involve the staircase "step" function $\lfloor x \rfloor_I$ which is obviously oscillatory in the dHvA sense about its average value. To make this explicit, we note that introducing $x = y + \frac{1}{2}$, we have $\lfloor y + \frac{1}{2} \rfloor_I = y - [y]_{\text{per}}$, where $[y]_{\text{per}}$ is the periodic linear sawtooth function $[y]_{\text{per}} = y$ in the fundamental interval $-\frac{1}{2} \le y \le \frac{1}{2}$, with periodic extension outside, as shown in Fig. 2. The dHvA oscillations are evident in this closed-form solution, but further confirmation may be had by exhibiting $[y]_{\text{per}}$ in terms of a Fourier sine series:[34]

$$[y]_{\text{per}} = \sum_{n=1}^{\infty}{}' \frac{(-1)^{n+1}}{\pi n}\sin(2\pi n y) . \tag{27}$$

Considering the specific heat, it is necessary to examine nonzero temperature. We employ Eq. (13) and its low-

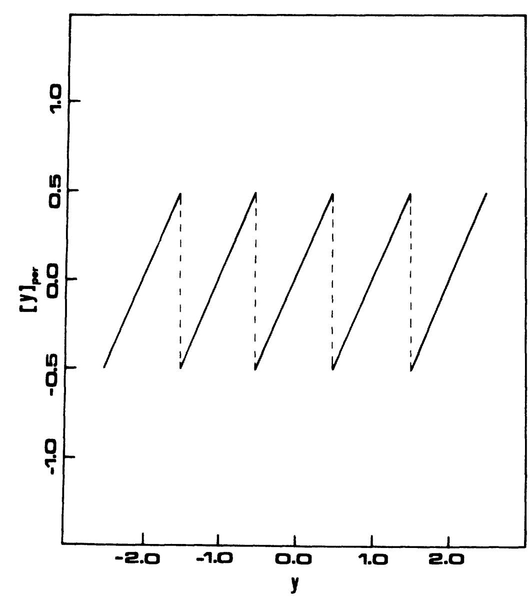

FIG. 2. The periodic linear sawtooth function $[y]_{\text{per}} = y$ in the fundamental interval $-\frac{1}{2} \le y \le \frac{1}{2}$, with periodic extension outside.

temperature expansion Eq. (14) (retaining only the leading term for $T\neq 0$). While Eq. (13) is exact, it is unwieldy. On the other hand, Eq. (14) is restricted in validity to cases for which the function $G(\beta\to\infty;\zeta)$ is nonsingular and nonrapidly varying. This is clearly not true for the steplike behavior of $\lfloor x\rfloor_I$, when ζ crosses a Landau level. In view of this, we exclude such cases from consideration, and treat only the quantum strong-field limit and the low magnetic field limit. In the quantum strong-field limit, all the dependence of E_s on ζ occurs through $n_{\pm}$, and barring Landau-level crossings, E_s is constant with $n_{\pm}$, so that $\partial E_s/\partial\zeta\to 0$ and the temperature-correction terms in Eq. (14) are null for E_s, whence $C_s=\partial E_s/\partial T\to 0$ in this case. This is to say that at high fields, $C_s\to 0$, unless we admit thermal excitations across Landau levels. The low-field limit has monotonic magnetic field dependence for E_s, since even at higher magnetic fields, an averaging procedure gives (dropping spin for the moment)

$$\left\langle n'=\left\lfloor \frac{\zeta}{\omega_c}+\frac{1}{2}\right\rfloor_I\right\rangle_{\text{av}}\to(n')_{\text{av}}=\frac{\zeta}{\omega_c}\ , \tag{28}$$

with which we obtain ($\mu_0\to 0$)

$$E_s^{(B)}=-\frac{m\omega_c^2}{8\pi}(n')^2\to E_s^{(C)}=-\frac{m\zeta^2}{8\pi}\ . \tag{29}$$

Thus, the low-field result, which does not in fact involve the field, extends to somewhat higher fields in an average sense. Since the applicable result is independent of magnetic field strength, what we have is the zero-field limit. It yields C_s as

$$C_s^{\text{LF}}=\tfrac{1}{4}k_B\beta^2 m\left\{-\frac{2}{\beta^3}\int_{-i\infty+\delta}^{i\infty+\delta}\frac{dt}{2\pi i}\frac{e^{\beta\zeta t}}{t^2\sin(\pi t)}+\frac{1}{\beta^2}\int_{-i\infty+\delta}^{i\infty+\delta}\frac{dt}{2\pi i}\frac{\zeta t e^{\beta\zeta t}}{t^2\sin(\pi t)}\right\}\ . \tag{30}$$

An alternative procedure may be employed to yield in-

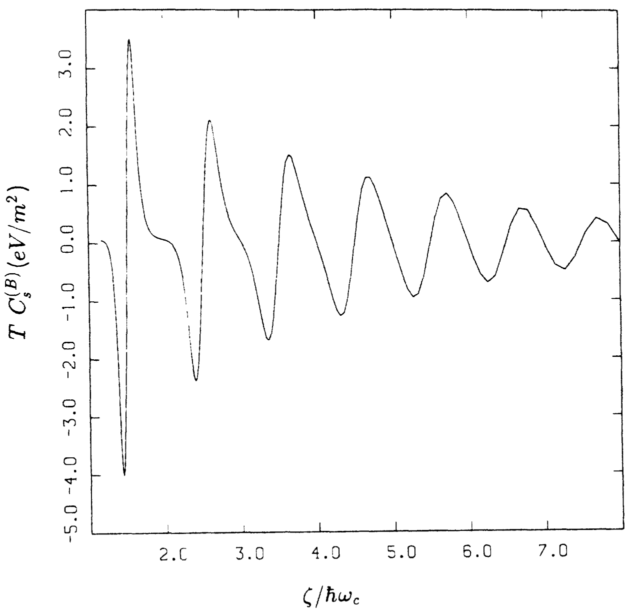

FIG. 3. dHvA oscillatory part of the surface specific heat $C_{s(\text{dHvA})}^{(B)}$ (plotted as $TC_s^{(B)}$) vs $\zeta/\hbar\omega_c$ for density $\rho=10^{16}\ \text{cm}^{-3}$, $m=0.0665m_e$.

formation concerning temperature dependence and specific heat associated with the dHvA oscillatory component of E_s due to thermal excitation of electrons across Landau levels. Proceeding from the exact integral representation for E_s given in Ref. 36, Eq. (7), we have (ignoring spin):

$$E_s^{(B)}=-\frac{m\omega_c^2}{16\beta}\int_{-i\infty+\delta}^{i\infty+\delta}\frac{ds}{2\pi i}\frac{e^{st}}{\sin(\pi s/\beta)}\frac{\cosh(\omega_c s/2)}{\sinh^2(\omega_c s/2)}\ , \tag{31}$$

and

$$C_s^{(B)}=-\frac{m\omega_c^2}{16}\int\frac{ds}{2\pi i}e^{st}\left\{\frac{k_B}{\sin(\pi s k_B T)}-\frac{\pi k_B^2 Ts\cos(\pi s k_B T)}{\sin^2(\pi s k_B T)}\right\}\frac{\cosh(\omega_c s/2)}{\sinh^2(\omega_c s/2)}\ . \tag{32}$$

It is the contribution to the s integral from the isolated second-order poles at $s_n=2\pi i n/\omega_c$ which yields the temperature-dependent dHvA oscillatory part of $C_s^{(B)}$ in the form

$$C_{s(\text{dHvA})}^{(B)}=-\frac{m\omega_c^2}{16}\sum_n f'(s_n)\ , \tag{33a}$$

where

$$(\omega_c/2)^2 f'(s)=(-1)^n e^{s\zeta}\left\{\frac{k_B\zeta}{\sin(\pi s k_B T)}-\pi k_B^2 Ts\zeta\frac{\cos(\pi s/\beta)}{\sin^2(\pi s/\beta)}-2\pi k_B^2 T\frac{\cos(\pi s/\beta)}{\sin^2(\pi s/\beta)}+s\pi^2 k_B^3 T^2\frac{\cos^2(\pi s/\beta)}{\sin^3(\pi s/\beta)}+s\pi^2 k_B^3 T^2\csc^3(\pi s/\beta)\right\}\ . \tag{33b}$$

This dHvA oscillatory result for the surface specific heat $C_s^{(B)}$ is illustrated in Fig. 3, where $TC_s^{(B)}$ is plotted as a function of $\zeta/\hbar\omega_c$ for density $\rho = 10^{16}$ cm^3, $m = 0.0665 m_e$.

IV. DISCUSSION AND CONCLUSIONS

We have presented a comprehensive determination of the surface statistical thermodynamic functions and magnetic susceptibility of a semi-infinite Landau-quantized electron gas subject to the boundary condition of specular reflection at its surface. In this, we found useful closed-form representations for the surface contributions to the grand potential W_s, internal energy E_s, magnetization M_s, and specific heat C_s. Our work was focused on employing the analytic relation for the surface contribution to number N_s [Eq. (5)]

$$N_s = -\tfrac{1}{4}\rho(2\text{D}) ,$$

in terms of the 2D density expression $\rho(2\text{D})$ as a function of the actual bulk chemical potential: This has enabled us to bring to bear extensive earlier analysis of $\rho(2\text{D})$ upon the evaluation of N_s. It is to be noted that the negative sign in Eq. (5) for N_s reflects the expulsion of electron density from the surface region by the boundary condition requiring that the wave function vanish at $z=0$. This feature permeates all of the surface thermodynamic functions for the specular reflection boundary condition, and one may expect moderation of it only as the perfect specularity requirement is relaxed.

The brief historical survey in the Introduction points up much important earlier work on the subject. Nonetheless, our closed-form analytic evaluations offer some new, useful representations for W_s, E_s, M_s, and C_s, as well as N_s. We have examined nondegenerate quantum magnetic field effects in all these quantities, presenting explicit results. The Bohr–Van Leeuwen theorem is seen to be satisfied by $M_s \rightarrow 0$ in the classical limit for magnetic field normal to the surface, with the vanishing of the quantum magnetic field parameters. Our investigation of surface thermodynamics below the degeneracy temperature includes surface de Haas–van Alphen oscillatory phenomena for low–intermediate magnetic fields, along with monotonic magnetic field effects. Furthermore, we have treated the quantum strong-field limit in which only the lowest Landau state is occupied. In this case, quantum effects are large, with Landau-level separation exceeding Fermi energy. Moreover, we have also discussed finite-temperature effects below the degeneracy temperature, as well as above. In all cases, our analysis yields explicit results in terms of the closed-form expressions presented above for W_s, E_s, M_s, and C_s, as well as N_s. Finally, we have presented numerical results that illustrate the utility of these highly tractable expressions in Fig. 3, illustrating the dHvA oscillatory structure of the surface specific heat $C_{s(\text{dHvA})}^{(B)}$ (denoted by $C_s^{(B)}$ in Fig. 3) in its dependence on $\zeta/\hbar\omega_c$.

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