Analytical thermodynamical properties of a two-dimensional electron gas in a magnetic field*

Chen Jin-Wang(陈金望) and Pan Xiao-Yin(潘孝胤)†

Department of Physics, Ningbo University, Ningbo 315211, *China*

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Analytical expressions for the thermodynamical properties of a two-dimensional electron gas in a perpendicular magnetic field are derived. This is accomplished by first deriving the general expression for the thermodynamical potential, and then employing this result to obtain the corresponding expression for the two-dimensional gas. The chemical potential and magnetization are studied as a function of temperature and magnetic field, and shown to be in agreement with prior work. It is also shown that the results are close to those obtained by assuming a Gaussian density of states for the Landau levels.

Keywords: thermodynamical potential, magnetization, de Hass–van Alphen effect, density of states

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1. Introduction

The explanation of the quantum oscillations of the magnetization[1] in the de Haas–vanAlphen (dHvA) effect in metals[2,3] is mainly due to Lifshitz and Kosevich (LK) formula.[4] The dHvA effect is a powerful experimental method for the determination of the Fermi surface of metals. However, the LK theory cannot be quantitatively applied to two-dimensional (2D) systems as many approximations that are made in its derivation break down. The theory of 2D dHvA effect was initiated by Peierls[5] many years ago, which showed that the zero-temperature limit ($T = 0$) of the magnetization in an ideal two-dimensional electron gas (2DEG) has a sharp, saw-tooth form. Since the early 1980s, the growing experimental progress of 2D conductors[6–15] has driven new theoretical investigations of the 2D dHvA effect. For example, Vagner and co-workers[16,17] obtained an analytical expression for the chemical potential and magnetization as functions of the magnetic field at finite temperature in the limit of sharp Landau levels.[18] Zawadski and co-workers[19–21] have studied numerically the magnetization and thermodynamics of 2D electron gases. Shoenberg[22] investigated the finite-temperature 2D theory in certain limiting approximations. Wang and O'Connell[23] investigated the magnetization of an ideal 2DEG in the strong magnetic field limit and at non-zero temperature. They also obtained a new exact expression for the free energy at low but finite temperature.[24] Champel and Mineev[25,26] developed an analytical theory of dHvA effect for two- and quasi-two-dimensional metals in normal and superconducting mixed states under the condition of $\mu/\omega_c \gg 1$ (μ is the chemical potential and ω_c the cyclotron frequency).

The above-mentioned studies are all based on the model of a 2D free electron gas (non-interacting fermions) trapped in a perpendicular magnetic field. The thermodynamical potential (or the free energy) is the crucial property in these theories. The difference in the above-mentioned methods lies in the approximate expressions employed for the thermodynamical potential since the exact analytical expression has never been obtained. Usually, the expression for the free energy of a 2DEG can be written as a sum of infinite Fourier series[22,23,27,28] by the Poisson summation formula[2] or the Euler–Maclaurin formula,[18] or the expression obtained[24] using the Sondheimer–Wilson technique.[29] Then, various approximations such as low temperature and strong or weak magnetic field limit are made. Another approach is to express the thermodynamical potential as an integral in terms of the density of states (DOS), then the approximations are made in the calculation of the DOS. It is well known that the DOS of free electron gas in a perpendicular magnetic field consists of a series of discrete Landau levels, but in the real 2D electron systems found in various experiments the Landau levels are broadened by impurities.[6,30] Nevertheless, the model of an ideal 2DEG in a magnetic field has intrinsic value from a purely theoretical point of view, and can improve the physical description. It is also the basis for other further studies that include many-body effects[31,32] and impurity scattering.[25,26]

In this paper, using the contour integration we present an exact analytical formula for the thermodynamical potential Ω as an integral in terms of the partition function. The formula is then applied to an ideal 2DEG in a magnetic field. The exact analytical expression for the thermodynamical potential Ω is obtained as a function of the temperature T, magnetic field B, and chemical potential μ. This expression then allows one

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†Corresponding author. E-mail: panxiaoyin@nbu.edu.cn

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to derive the equation for other thermodynamical properties such as magnetization, magnetic susceptibility, and the heat capacity.

2. Calculation of the thermodynamical potential

The system under consideration is a 2D electron gas in the $x-y$ plane subjected to a perpendicular magnetic field B along the z direction. The energy levels are the Landau levels (LL)

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega_{\rm c}, \quad n=0,1,\ldots, \tag{1}$$

where $\omega_{\rm c}=eB/(m^*c)$ is the cyclotron frequency, and m^* is the effective mass of the electron. The level degeneracy per unit area is $N_{\rm L}(B)=eB/(\pi\hbar)$. The partition function per unit area is

$$Z(\beta)=D{\rm Tr}({\rm e}^{-\beta\hat{H}})=D\sum_{n=0}^{\infty}{\rm e}^{-\beta E_n}=\frac{D}{2\sinh(\beta\hbar\omega_{\rm c}/2)}, \tag{2}$$

where $\hat{H}$ is the Hamiltonian, $\beta=1/(k_{\rm B}T)$ with $k_{\rm B}$ being the Boltzmann constant, and $D=N_{\rm L}(B)$. The DOS is determined by the inverse Laplace trasform[33]

$$g(\varepsilon)=D\sum_n\delta(\varepsilon-E_n)=\frac{1}{2\pi{\rm i}}\int_{\alpha-{\rm i}\infty}^{\alpha+{\rm i}\infty}Z(\beta){\rm e}^{\varepsilon\beta}\,{\rm d}\beta, \tag{3}$$

where $\alpha>0$ is a real constant. It is evident that the partition function has simple poles at $\beta_n=2n\pi{\rm i}/(\hbar\omega_{\rm c})$ $(n=0,\pm1,\pm2,\ldots)$, and these poles are located on the imaginary axis. Since $\varepsilon>0$, the contour can be closed on the left-hand side of the complex β plane, as shown in Fig. 1. Applying the residue theorem, we obtain

$$g(\varepsilon)=\frac{D}{\hbar\omega_{\rm c}}\left[1+2\sum_{n=1}^{\infty}(-1)^n\cos\left(\frac{2\pi n\varepsilon}{\hbar\omega_{\rm c}}\right)\right]. \tag{4}$$

The Helmholtz free energy $\mathscr{F}$ is defined as

$$\mathscr{F}=N\mu+\Omega, \tag{5}$$

where μ is the chemical potential, N is the particle number, and Ω is the thermodynamical potential. Under experimental conditions, it is often the number of electrons N rather than the chemical potential μ that is a constant. We shall work in the canonical ensemble (i.e., for fixed particle number). Thus, we have

$$N=D\sum_n f(E_n)=\int\frac{g(\varepsilon)}{{\rm e}^{(\varepsilon-\mu)\beta}+1}\,{\rm d}\varepsilon, \tag{6}$$

where $f(\varepsilon)=1/({\rm e}^{(\varepsilon-\mu)\beta}+1)$ is the Fermi–Dirac distribution. The thermodynamical potential Ω is given by

$$\Omega = -\frac{D}{\beta}\sum_n\ln(1+{\rm e}^{-\beta(E_n-\mu)}) = \int g(\varepsilon)\ln({\rm e}^{(\varepsilon-\mu)\beta}+1)\,{\rm d}\varepsilon. \tag{7}$$

The magnetization M is calculated by taking the derivative of $\mathscr{F}$ with respect to the magnetic field B

$$M=-\frac{\partial\mathscr{F}}{\partial B}|_{N,T}. \tag{8}$$

It is clear that the chemical potential μ depends upon the particle number N, the strength of the magnetic field B, and the temperature T, i.e., $\mu=\mu(N,B,T)$. Thus, the problem of magnetization is reduced to solving the combination of Eqs. (6) and (8). In spite of its simple appearance, the analytical expression for M is not easily obtainable.

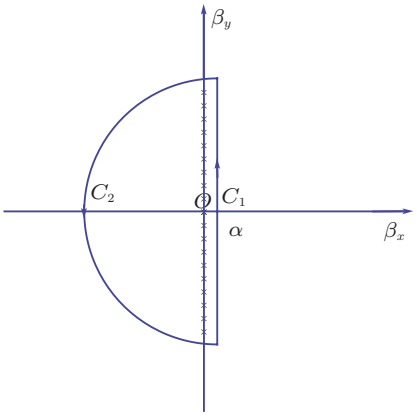


Fig. 1. The contour of integration in the complex plane of β for calculating the integral in Eq. (3).

Prior to determining the analytical expression for M, we focus on obtaining an exact expression for the thermodynamical potential Ω. Making use of the following identity:[34]

$$f(\varepsilon_i)=\frac{1}{1+{\rm e}^{\beta(\varepsilon_i-\mu)}}=\frac{1}{2\pi{\rm i}}\int_{\alpha-{\rm i}\infty}^{\alpha+{\rm i}\infty}\frac{\pi{\rm e}^{k(\mu-\varepsilon_i)}}{\sin(\pi k/\beta)}\,{\rm d}k, \tag{9}$$

we have[35]

$$\ln(1+{\rm e}^{-\beta(\varepsilon_i-\mu)})=\frac{1}{2\pi{\rm i}}\int_{\alpha-{\rm i}\infty}^{\alpha+{\rm i}\infty}\frac{\pi{\rm e}^{k(\mu-\varepsilon_i)}}{\beta\sin(\pi k/\beta)(k)}\,{\rm d}k. \tag{10}$$

Note that in Eqs. (10) and (11), the contour is closed on the left-hand side of the complex plane of k if $\mu-\varepsilon_i>0$ and on the right-hand side if $\mu-\varepsilon_i<0$. Inserting Eq. (10) into Eq. (7), the thermodynamical potential Ω can be written formally as follows:

$$\Omega=\frac{1}{2\pi{\rm i}}\int_{\alpha-{\rm i}\infty}^{\alpha+{\rm i}\infty}\frac{\pi{\rm e}^{k\mu}Z(k)}{\beta\sin(\pi k/\beta)(-k)}\,{\rm d}k. \tag{11}$$

This equation is one of the key results of the paper. In principle, all other properties are expressible in terms of the partition function based on Eq. (11).

Now we apply the formula to an ideal 2DEG in a perpendicular field and determine the thermodynamical potential precisely. Substituting Eq. (2) into Eq. (11) yields

$$\Omega=-\frac{D\pi}{\beta}\frac{1}{2\pi{\rm i}}\int_{\alpha-{\rm i}\infty}^{\alpha+{\rm i}\infty}\frac{{\rm e}^{k(\mu-\hbar\omega_{\rm c}/2)}}{\sin(\pi k/\beta)k(1-{\rm e}^{-k\hbar\omega_{\rm c}})}\,{\rm d}k. \tag{12}$$

The above integral can be evaluated by employing the residue theorem when the integrand satisfies the Jordan lemma. Hence, one has to consider the following two cases: (a) $\mu - \hbar\omega_c/2 \geq 0$; (b) $\mu - \hbar\omega_c/2 \leq 0$. In case (a), the contour is closed on the left-hand side of the complex plane of k. It is clear that (i) $k_0 = 0$ is a triple pole, (ii) $k_n = n\beta$ $(n < 0, n \in Z)$, and (iii) $k_m = 2m\pi i/(\hbar\omega_c)$ $(m \in Z,\ m \neq 0)$ are simple poles. After straightforward calculations, we obtain

$$\Omega_a = \Omega_i + \Omega_{ii} + \Omega_{iii}, \tag{13}$$

where

$$\Omega_i = D\left(\frac{\hbar\omega_c}{24} - \frac{\pi^2}{6\beta^2\hbar\omega_c} - \frac{\mu^2}{2\hbar\omega_c}\right), \tag{14}$$

$$\Omega_{ii} = \frac{D}{2\beta}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\frac{e^{-n\beta\mu}}{\sinh(n\beta\hbar\omega_c/2)}, \tag{15}$$

$$\Omega_{iii} = \frac{D}{\beta}\sum_{m=1}^{\infty}\frac{\cos(2m\pi\mu/\hbar\omega_c)(-1)^m}{m\sinh(2m\pi^2/\beta\hbar\omega_c)}. \tag{16}$$

In case (b), the contour is closed on the right-hand side of the complex plane of k and involves only the simple poles (iv) $k_l = l\beta$ $(l > 0, l \in Z)$. Applying the residue theorem again, we obtain

$$\Omega_b = \frac{D}{2\beta}\sum_{l=1}^{\infty}\frac{(-1)^l}{l}\frac{e^{l\beta\mu}}{\sinh(l\beta\hbar\omega_c/2)}. \tag{17}$$

It should be pointed out that a result similar to Eq. (17) has appeared in Ref. [36], obtained by expanding the Fermi–Dirac distribution function as a power series. However, that method only works in the case when $\mu < \hbar\omega_c/2$.

3. Chemical potential

It is well accepted that the chemical potential oscillations play an important role in 2D systems,[37] while it is negligibly small in the 3D case. Next we shall exploit the expressions for the thermodynamical potential to obtain the equation to determine the chemical potential μ. Making use of Eq. (7), equation (6) can be rewritten as

$$N = -\frac{\partial\Omega}{\partial\mu}|_{B,T}. \tag{18}$$

Substituting Eqs. (13) and (17) into Eq. (18), one obtains for $\mu \geq \hbar\omega_c/2$ that

$$\frac{N}{C} = \mu + \sum_{m=1}^{\infty}(-1)^m\left[\frac{2\pi}{\beta}\frac{\sin(2m\pi\mu/\hbar\omega_c)}{\sinh(2m\pi^2/\beta\hbar\omega_c)} - \frac{(\hbar\omega_c)e^{-m\beta\mu}}{2\sinh(m\beta\hbar\omega_c/2)}\right], \tag{19}$$

and for $\mu \leq \hbar\omega_c/2$,

$$\frac{N}{C} = -\sum_{m=1}^{\infty}\frac{(-1)^m e^{m\beta\mu}}{2\sinh(m\beta\hbar\omega_c/2)}(\hbar\omega_c), \tag{20}$$

where $C = D/(\hbar\omega_c)$. The chemical potential μ as a function of the particle number N, the strength of the magnetic field B, and temperature T, i.e., $\mu = \mu(N,B,T)$ can thus be obtained from Eq. (19) or (20).

At zero temperature, the chemical potential $\mu(N,B,0)$ can be obtained by taking the limit $T \to 0$ $(\beta \to \infty)$ in Eq. (19),

$$\begin{aligned}\frac{N}{C} &= \mu(N,B,0) + \sum_{m=1}^{\infty}\left[\frac{(-1)^m\hbar\omega_c}{m\pi}\sin\left(\frac{2m\pi\mu(N,B,0)}{\hbar\omega_c}\right)\right] \\ &= \mu(N,B,0) - \frac{1}{2f}\mathrm{St}[f,\mu(N,B,0)],\end{aligned} \tag{21}$$

where

$$f = \frac{1}{\hbar\omega_c},$$

and

$$\mathrm{St}[f,t] = \frac{2}{\pi}\sum_{m=1}^{\infty}\left[\frac{(-1)^{m+1}}{m}\sin(2m\pi ft)\right]$$

is the sawtooth function.

We present the solutions to Eqs. (19)–(21) in Fig. 2. We can see that the chemical potential oscillates perfectly sawtoothlike at zero temperature. The result is in agreement with those in Ref. [19], where the zero temperature chemical potential was obtained numerically. As the temperature increases, the amplitudes of oscillations decrease. The amplitudes of oscillations decrease when the strength of the magnetic field decreases. However, the chemical potential always oscillates around its value for $B = 0$, irrespective of the change in temperature. Moreover, our results are very close to those in Ref. [38], although they are calculated by using a model DOS, assuming a Gaussian broadening of the Landau levels.

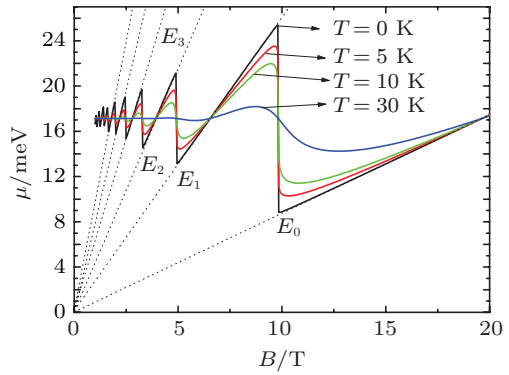


Fig. 2. (color online) Chemical potential μ as a function of B at different values of temperature ($T = 0, 5, 10, 30$ K). We set the particle number density $N/A = 4.75 \times 10^{15}$ m^{-2}. The dotted lines represent the Landau energies $E_j = (j + 1/2)\hbar\omega_c$.

When the strength of the magnetic field approaches zero, Eq. (19) becomes

$$\frac{N}{C} = \mu_0 + \frac{1}{\beta}\ln(1 + e^{-\beta\mu_0}), \tag{22}$$

where $\mu_0 = \mu(N,0,T)$. Equation (22) can be solved analytically and we obtain $\mu_0 = \ln(\mathrm{e}^{N\beta/C} - 1)/\beta$. When the particle number is very large ($N \gg 1$), it is clear that μ approaches the constant N/C in the limit of $B \to 0$ at non-zero temperature.

In Fig. 3, we plot the chemical potential μ as a function of particle number N at $B = 5$ T for several values of temperature. This displays discrete steps at a particle number $N = nD$ ($n = 1,2,\ldots$), where $D = Be/\pi\hbar = 2.414 \times 10^{15}$. The steps gradually smooth out as the temperature increases. The results are in agreement with those obtained in Ref. [22].

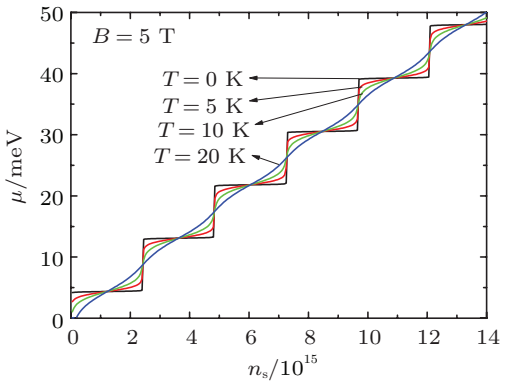


Fig. 3. (color online) Chemical potential μ as a function of the particle number N at several values of temperature $T = 0,5,10,20$ K.

4. Magnetization

Having studied the chemical potential, we next use the exact expression for the thermodynamical potential to investigate the magnetization of the system. Employing Eqs. (8), and (13)–(17) for the case of $\mu \geq \hbar\omega_c/2$, we obtain

$$M = \left(\frac{-e}{\pi\hbar}\right)\left\{\frac{\hbar\omega_c}{12} + \sum_{m=1}^{\infty}\frac{(-1)^m}{m\beta}\left[\frac{\cos(2m\pi\mu/\hbar\omega_c)}{\sinh(2m\pi^2/\hbar\omega_c\beta)} - \frac{1}{2}\frac{\mathrm{e}^{-m\beta\mu}}{\sinh(m\beta\hbar\omega_c/2)} + \frac{\sin(2m\pi\mu/\hbar\omega_c)}{\sinh(2m\pi^2/\hbar\omega_c\beta)}\left(\frac{2m\pi\mu}{\hbar\omega_c}\right) + \frac{\cos(2m\pi\mu/\hbar\omega_c)\cosh(2m\pi^2/\hbar\omega_c\beta)}{\sinh^2(2m\pi^2/\hbar\omega_c\beta)}\left(\frac{2m\pi^2}{\beta\hbar\omega_c}\right) + \frac{m\beta\hbar\omega_c}{4}\frac{\mathrm{e}^{-m\beta\mu}\cosh(m\beta\hbar\omega_c/2)}{\sinh^2(m\beta\hbar\omega_c/2)}\right]\right\}. \quad (23)$$

For the case of $\mu \leq \hbar\omega_c/2$,

$$M = \left(\frac{-e}{\pi\hbar}\right)\left\{\sum_{m=1}^{\infty}\frac{(-1)^m}{m\beta}\left[\frac{\mathrm{e}^{m\beta\mu}}{\sinh(m\beta\hbar\omega_c/2)} - \frac{m\beta\hbar\omega_c}{2}\frac{\mathrm{e}^{-m\beta\mu}\cosh(m\beta\hbar\omega_c/2)}{\sinh^2(m\beta\hbar\omega_c/2)}\right]\right\}. \quad (24)$$

We present the results of Eq. (23) in Fig. 4. It is evident that following closely the oscillation of the chemical potential, the magnetization oscillates as a function of magnetic field strength and tends to be zero at low field strength. A sawtoothlike dHvA oscillation occurs in the magnetization at low temperature. Our results confirm the results obtained numerically in Ref. [19].

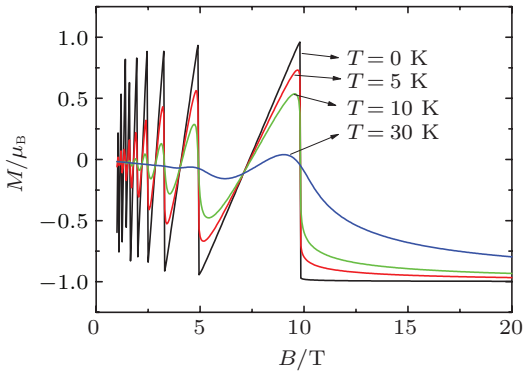


Fig. 4. (color online) Magnetization as a function of the strength of the magnetic field B at different temperatures $T = 0,5,10,30$ K. The particle number density $N/A = 4.75 \times 10^{15}$ m^{-2}.

5. Comparison with the results using the model DOS

In real systems, the LLs are broadened mostly by the electron–impurity scattering,[6,30] resulting in the deformation of the DOS. One commonly employed model of LL broadening is the Gaussian DOS, which assumes that each LL has a Gaussian-shaped broadening,

$$g(\varepsilon) = xD_0 + (1-x)N_L\sum_j \frac{1}{\sqrt{2\pi}\Gamma}\exp\left[-\frac{(\varepsilon - E_j)^2}{2\Gamma^2}\right], \quad (25)$$

where the first term is the background DOS, represented as a fraction x of the zero-field DOS $D_0 = m*/\pi\hbar^2$, and Γ is a broadening parameter. We compare our results with those calculated using this DOS since it describes the experimental results very well.[38] Comparison are made in Figs. 5 and 6. We can see that the chemical potential and magnetization from the Gaussian DOS are almost the same as those obtained from the DOS of Eq. (4). This is a remarkable result, which means that despite its simplicity, under certain conditions the model of an ideal 2DEG describes the real system strikingly well.

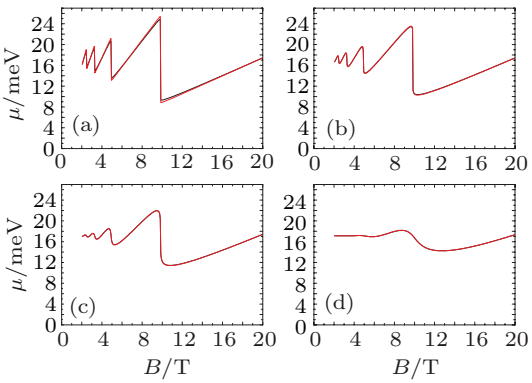


Fig. 5. (color online) Chemical potential μ as a function of B at (a) $T = 0$ K, (b) $T = 5$ K, (c) $T = 10$ K, and (d) $T = 30$ K, calculated using the model DOS of Eq. (23) (black line) with $\Gamma = 0.29$ and $x = 0$ and the exact DOS of Eq. (4) (red line).

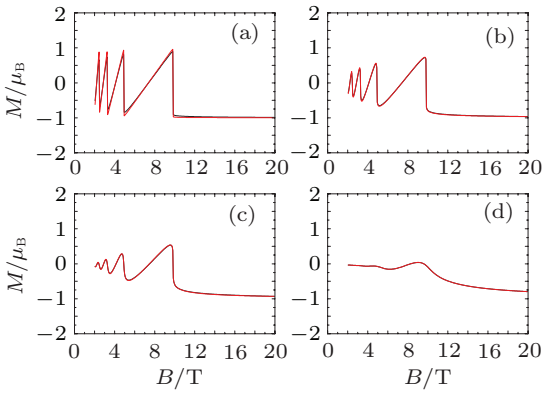


Fig. 6. (color online) Magnetization M as a function of B at (a) $T = 0$ K, (b) $T = 5$ K, (c) $T = 10$ K, and (d) $T = 30$ K, calculated using the model DOS of Eq. (23) (black line) with $\Gamma = 0.29$ and $x = 0$, and the exact DOS of Eq. (4) (red line).

6. Conclusions

In summary, using contour integration we have developed an exact formula for the thermodynamical potential. Employing this formula, we obtain the exact analytical expressions for the thermodynamical potential of an ideal 2DEG in a magnetic field. The chemical potential and the magnetization are then investigated. The results confirm earlier work. The results have been compared with the results obtained using the commonly employed model of LL broadening with the Gaussian DOS, and the comparison shows excellent agreement. Finally, we stress that the formula for thermodynamical potential is exact and general. It can be used to investigate many other problems such as the magnetization of the spin–orbit coupled systems,[39,40] and it also can be generalized to other dimensions and include spin splitting.

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