Thermodynamics in a complete description of Landau diamagnetism

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In the present study we analyze some consequences that come from revised measures as the Wehrl entropy and the Fisher information for the problem of a particle in a magnetic field starting from a complete description of the Husimi function. We discuss in the most complete form (three dimensions) some results related to measures in contrast with the incomplete form (two dimensions) shown in previous contributions. Some limiting cases as high and low temperatures are discussed. From the present reasoning, it is suggested that the formulation in two dimensions is sufficient unto itself to explain the problem whenever the length of the cylindrical geometry of the system is large enough. Otherwise, it is not possible to work in all finite temperatures, a natural lower temperature bound emerges from the analysis when three dimensions are considered.

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I. INTRODUCTION

Diamagnetism was a problem first appointed by Landau who showed the discreteness of energy levels for a charged particle in a magnetic field [1]. By the observation of the diverse scenarios in the framework provided by the Landau diamagnetism we can study some relevant physical properties [2–4] as thermodynamic limit, role of boundaries, decoherence induced by the environment. The main motivation for several specialists work even today it is to make an accurate description of its theoretical and practical consequences.

In the past the appropriate partition function for this problem was calculated by Feldman and Kahn appealing to the concept of Glauber's coherent states as a set of basis states [5]. This formulation allows the use of classical concepts to describe electron orbits, even containing all quantum effects [5]. In a previous effort, this approach was used to obtain the Wehrl entropy [6,7] and Fisher information [8] with the purpose of studying the thermodynamics of the Landau diamagnetism problem, namely, a free spinless electron in a uniform magnetic field [9]. In such contribution the authors focused only in the transverse motion of a particle. For this reason, it was necessary to normalize the Husimi distribution in order to arrive to a consistent expression for semiclassical measures [9–11].

Certainly, because the relevant effects seem to come only from the transverse motion, several efforts are made to describe this problem in two dimensions [3,4,9–13]. Furthermore, since the discovery of interesting phenomena, as the quantum Hall effect, there has been much interest in understanding the dynamics of electrons confined to move in two dimensions in the presence of a magnetic field perpendicular to the motion plane [13]. The confinement is possible at the *interface* between two materials, typically a semiconductor and an insulator, where a quantum well that traps the particles is formed, forbidding their motion in the direction perpendicular to the interface plane at low energies.

However, we propose here to discuss this problem in the most complete form (three dimensions), some results related to the behavior of the Wehrl entropy in contrast with the incomplete form (two dimensions). From the present line of reasoning, it is concluded that the two-dimensional formulation is sufficient unto itself to explain the problem whenever the length of the cylindrical geometry of the system is large enough. Nevertheless, as suggested before, electronic devices are based in interfaces. Thus, this fact theoretically imposes a natural lower temperature bound that emerges from the analysis when three dimensions are considered.

The main goal of this paper is to illustrate how to obtain new properties concerning this problem when the complete motion of the particle is considered, i.e., the free motion along the z axis (in the magnetic field direction), and the transverse motion. Thus, we can supply the exact Wehrl entropy and Fisher information starting from a revised version of calculations. From this kind of analysis, a likely range of validity of the present formulation is derived.

We will start our present endeavor defining the Hamiltonian $\hat{H}=\hat{H}_t+\hat{H}_l$ for a particle of mass m and charge q in a magnetic field H, where $\hat{H}_t=\hbar\Omega(\hat{N}+1/2)$ describes the transverse motion, being $\Omega=qH/mc$ the cyclotron frequency [5] and $\hat{N}$ the number operator. In addition, the Hamiltonian $\hat{H}_l=\hat{p}_z^2/2m$ represents a longitudinal one-dimensional free motion. After constructing a coherent state basis, a possible way to define the Husimi function η, for the complete motion, is given by

$$\eta(x,p_x;y,p_y;p_z)=\langle\alpha,\xi,k_z|\hat{\rho}|\alpha,\xi,k_z\rangle, \tag{1}$$

where $\hat{\rho}$ is the thermal density operator and the set $\{|\alpha,\xi,k_z\rangle\}$ represents the coherent states for the motion in three dimensions. Taking the direct product $|\alpha,\xi,k_z\rangle\equiv|\alpha,\xi\rangle\otimes|k_z\rangle$, the set $\{|\alpha,\xi\rangle\}$ corresponds to the coherent states of the transverse motion and $\{|k_z\rangle\}$ to the longitudinal motion. Therefore, the thermal density operator is given by

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$$\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H}_l + \hat{H}_t)}, \tag{2}$$

where $\beta = 1/k_B T$, k_B the Boltzmann constant and T the temperature. Besides, Z is the partition function for the particle total motion. If Z is separated in a similar way as other physical properties are separated, it is possible to assure that $Z = Z_l Z_t$, where Z_t is the contribution for the transverse motion and Z_l the contribution for the one-dimensional free motion. Thus, the Husimi function [14] is written as

$$\eta = \frac{e^{-\beta p_z^2/2m}}{Z_l Z_t} \sum_{n,m} e^{-\beta\hbar\Omega(n+1/2)} |\langle n,m|\alpha,\xi\rangle|^2. \tag{3}$$

where $Z_t = Am\Omega/[4\pi\hbar \sinh(\beta\hbar\Omega/2)]$, being L the length, $A = \pi R^2$ the area for cylindrical geometry [5], and $Z_l = (L/h)(2\pi m k_B T)^{1/2}$ [5]. In addition, the matrix element $|\langle n,m|\alpha,\xi\rangle|^2$ represents the probability of finding the electron in the coherent state $|\alpha,\xi\rangle$ and we can find its expression as defined previously [15].

It should be noticed that the distribution η can be written as follows:

$$\eta = \eta_l(p_z)\,\eta_t(x,p_x;y,p_y), \tag{4}$$

where η has been separated as a function of two distributions, namely, $\eta_l = \eta_l(p_z)$ and $\eta_t = \eta_t(x,p_x;y,p_y)$. The dependence on the variable z has been missed due to the explicit form of the Hamiltonian $\hat{H}_l$. Accordingly, after summing in Eq. (3) we find

$$\eta_l = \frac{e^{-\beta p_z^2/2m}}{Z_l}, \tag{5}$$

$$\eta_t = \frac{2\pi\hbar}{Am\Omega}(1 - e^{-\beta\hbar\Omega}) e^{-(1-e^{-\beta\hbar\Omega})|\alpha|^2/2\ell_{\mathrm{H}}^2}, \tag{6}$$

where the length $\ell_H = (\hbar c/qH)^{1/2}$ is the classical radius of the ground-state Landau orbit [5]. From expressions (5) and (6), we emphasize again that $\eta_l(p_z)$ describes the free motion of the particle in the magnetic field direction and $\eta_t(x,p_x;y,p_y)$ the Landau levels due to the circular motion in a transverse plane to the magnetic field. Consequently Eqs. (4)–(6) together contain the complete description of the system. We noticed both distributions are naturally normalized in a standard form, i.e.,

$$\int \frac{dz dp_z}{h} \eta_l(p_z) = 1, \tag{7}$$

and

$$\int \frac{d^2\alpha d^2\xi}{4\pi^2 \ell_{\mathrm{H}}^4} \eta_t(x,p_x;y,p_y) = 1. \tag{8}$$

In consequence, both Eqs. (5) and (6), under conditions (7) and (8), bring a promising way to get the exact form of the Wehrl entropy. Furthermore, using the additivity as the most basic property of the entropy, we can state $W_{\mathrm{total}} = W_l + W_t$. Hence,

$$W_l = -\int \frac{dz dp_z}{h} \eta_l(p_z) \ln\, \eta_l(p_z), \tag{9}$$

$$W_t = -\int \frac{d^2\alpha d^2\xi}{4\pi^2 \ell_{\mathrm{H}}^4} \eta_t(x,p_x;y,p_y) \ln\, \eta_t(x,p_x;y,p_y), \tag{10}$$

where, as before, the subindex l stands for the longitudinal motion and t the transverse.

After evaluating the respective integrals in Eqs. (9) and (10), it is feasible to identify the two particular entropies

$$W_l = \frac{1}{2} + \ln\left(\frac{L}{\lambda}\right), \tag{11}$$

$$W_t = 1 - \ln(1 - e^{-\beta\hbar\Omega}) + \ln(g), \tag{12}$$

where $\lambda = h/(2\pi m k_B T)^{1/2}$ is the mean thermal wavelength of the particle and $g = A/2\pi\ell_{\mathrm{H}}^2$ stands for the degeneracy of a Landau level [16]. Indeed, Eq. (11) coincides with the classical entropy for a free particle in one dimension. Equation (12) is the exact result [9] for the transverse motion and possesses a form for the Wehrl entropy close to the harmonic oscillator entropy, with the exception of a term associated with the degeneracy.

II. DISCUSSION OF RESULTS

Although the total Wehrl entropy is expressed simply as follows:

$$W_{\mathrm{total}} = \frac{3}{2} - \ln(1 - e^{-\beta\hbar\Omega}) + \ln(g) + \ln\left(\frac{L}{\lambda}\right), \tag{13}$$

we notice that some of its properties are directly derived from Eqs. (11) and (12). First, as we commented before, W_l coincides with the classical entropy for the free motion in one dimension. From this glance, we can add that W_l has to be nonnegative, $W_l \geq 0$ at all temperatures. This last condition imposes a minimum temperature, given by

$$T_0 = \frac{h^2}{2\pi m e k_B L^2}, \tag{14}$$

where $e = 2.718\,281\,828$. The standard behavior of W_l obligates the system to take high values of temperature, wherever the temperature T ought to be greater than T_0, in such case the conduct of the system is classical. This is equivalent to assert that, if $T/T_0 \geq 1$, the length of a thermal wave λ lower than the average of the spacing among particles and quantum considerations are not relevant [17]. In addition, T_0 only depends on the size of the system and does not depend on other external or internal physical parameters such as transverse area, external magnetic field, charge of the particle, etc. If the system is large then the minimum temperature is low. However, modern electronic systems has junctions where L is practically zero. In such case the required minimum temperature to make applicable our description is numerically high enough [18].

Nevertheless, the entropy associated with transverse motion satisfies $W_t \geq 1 + \ln(g)$ for all temperatures in the system of a particle in a magnetic field where the symmetry is polar, which is almost the Lieb condition for systems in one dimension [19] with an additional term associated with the degeneracy g. Roughly speaking, the transverse motion is bidimensional, but in the Landau approach the quantum motion of the particle in a magnetic field is reduced to a degenerate spectrum in one dimension. This degeneracy essentially recovers the physics of the missing dimension. Resuming the discussion of the behavior of the Wehrl entropy, it is not plausible to adventure any conclusion about the applicability of the present treatment because the Lieb condition is always satisfied. This is the main problem stems from the restricted vision presented in other contributions over this topic which only put its emphasis on the transverse motion [5,9–11] and represent the main difference from the vision obtained in that other contributions that discuss this topic. From the combined reasoning of both motions we conclude that the present description, this is the calculation of W_t, has sense when the imposition over the temperature is satisfied. Under T_0 the behavior is intrinsically anomalous and the present proposal is not applicable.

A. High temperature approximation

If we consider $k_B T \gg \hbar\Omega$, we can apply the first order of approximation as $\ln[g/(1-e^{-\beta\hbar\Omega})] \approx \ln(AT/T_0 L^2)$. Indeed, taking into account that the thermal wavelength can be rewritten in terms of the temperature T_0 this way $\lambda = L(eT_0/T)^{1/2}$, the expression (13) after a bit of algebra reduces to

$$W_{\text{total}}^{(1)} \approx \frac{3}{2}\ln\left(\frac{T}{T_0}\right) + \ln\left(\frac{A}{L^2}\right). \tag{15}$$

Considering that $V = AL$ in Eq. (15), the total Wehrl entropy can be expressed as follows:

$$W_{\text{total}}^{(1)} = \frac{3}{2} + \ln\left(\frac{V}{\lambda^3}\right). \tag{16}$$

This is a particular expression for the entropy of a free particle in three dimensions related to the motion of a charged particle into a region of the magnetic field making mention of some geometrical properties of the system.

In second order of approximation for high temperatures, considering the special condition $A \sim L^2$, Wehrl entropy is expressed as follows:

$$W_{\text{total}}^{(2)} \approx \frac{T_0}{T}g + \frac{3}{2} + \frac{3}{2}\ln\left(\frac{T}{T_0}\right) = \frac{T_0}{T}g + W_{\text{total}}^{(1)}. \tag{17}$$

In Fig. 1, according to current approach, the trend of the Wehrl entropy is depicted as a function of certain values of $T/T_0 \geq 1$ and $H/H_0 \geq 1$. As explained before, the Wehrl entropy takes values that are permitted by the Lieb condition, namely, $W \geq 1$. This fact is shown in Fig. 1(a) and 1(b). Particularly, in Fig. 1(b), the linear dependence of the total Wehrl entropy on the magnetic field at fixed temperature is evident. According to Eq. (16) the slope decreases as temperature increases, which is graphically shown for $T/T_0 = 15$ and 20. This fact illustrates why the disorder slowly

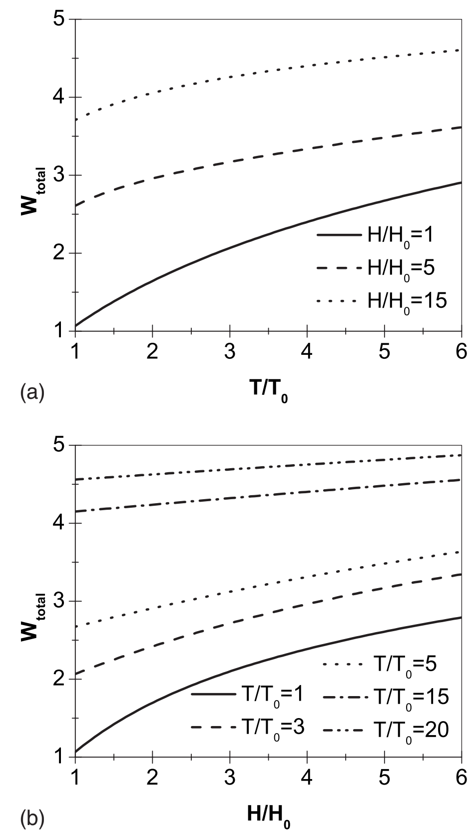

FIG. 1. *The total Wehrl entropy is depicted as a function of* (a) the temperature and (b) the magnetic field. It is emphasized that the total Wehrl entropy is shown in (a) at different values of the magnetic field greater than H_0 and in (b) at several fixed values of temperature greater than T_0. Besides, it is shown in (a) a natural bound for the temperature when we force W_{total} to satisfy the Lieb bound and in (b) the linear behavior of the Wehrl entropy for high values of temperature.

increases as the magnetic field increases too. Consequently, at extremely high temperatures as expected, the slope of the present linear dependence tends to zero apparently taking a constant value close to the corresponding classical entropy of the free particle in three dimensions.

B. Low temperature approximation

The lower bound of temperature is related to $T/T_0 \to 1^+$, because this approach does not consider temperature values under T_0. The total Wehrl entropy is reduced to logarithm behavior of the magnetic field. This tendency is shown in Fig. 1 through a solid line.

To study what occurs close to zero temperature, in accordance with Eq. (14), we need to take systems with $L \to \infty$ and after this consideration the transverse entropy of Eq. (12) can be seen as follows:

$$W_t^{T\to 0^+} = 1 + \ln(g). \tag{18}$$

As we discussed before, this Wehrl entropy is also a kind of harmonic oscillator entropy and the lower bound complies with being greater than a bound limiting value of the temperature, which has been suggested by Wehrl and shown by Lieb, $W \geq 1$ [19]. Starting from this condition it must arrive to the following inequality for the magnetic field

$$g \geq 1, \tag{19}$$

where $g = qAH/hc$ also accounts for the ratio between the flux of the magnetic field HA and the quantum of the magnetic flux given by $hc/q = 4.14 \times 10^{-7}$ [gauss/cm^2] [22]. Then the inequality (19) adopts the form

$$H \geq \frac{1}{A}\frac{hc}{q} = H_0. \tag{20}$$

Therefore, the quantity $H_0 = hc/Aq$ becomes a bound limiting field that represents the minimum value for the external magnetic field. To study what occurs close to zero magnetic field we need to take systems with $A \to \infty$.

For finite values of A and H lower than H_0 is manifested the Haas–van Alphen effect, which describes oscillations in the magnetization because at temperatures low enough the particles will tend to occupy the lowest energy states. Whereas if the value of the magnetic field decreases a less number of particles can be in the lowest state due to degeneracy is directly proportional to H [16]. Then, the transverse Wehrl entropy W_t is well defined for values of the magnetic field over H_0, this is $H/H_0 \geq 1$ and/or $g \to 1^+$.

We can assert that this description of the system is not quantum, we say that it is semiclassical; for instance, it does not contain the Haas–van Alphen effect, the same condition marks the beginning of one description and the ending of the other.

Other relevant effect that emerges from the Landau quantization [20] is the quantum Hall effect [21] which is a quantum-mechanical version of the Hall effect [13], observed in two-dimensional electron systems subjected to low temperatures and strong magnetic fields. The degeneracy is given by [22]

$$\phi = \nu\phi_0, \tag{21}$$

where $\phi_0 = hc/q$ is the quantum of the magnetic flux. The factor ν is related to the "filling factor" that takes integer values ($\nu = 1, 2, 3, \ldots$). The discovery of the fractional quantum Hall effect [12] extend these values to rational fractions ($\nu = 1/3, 1/5, 5/2, 12/5, \ldots$). The integer quantum Hall effect is simply explained in terms of the conductivity quantization $\sigma = \nu q^2/h$. However, the fractional quantum Hall effect relies on other phenomena related to interactions. Consistently, we see that the degeneracy is equal to ν, which must be greater than 1 due to the inequality (19) obtaining an infinite family of Wehrl entropies

$$W_t = 1 - \ln(1 - e^{\beta\hbar\Omega}) + \ln \nu. \tag{22}$$

Again, Eq. (19) provides the limiting value of ν and, as before, the transverse entropy always satisfies the Lieb bound for all temperatures and large enough systems when the quantum Hall effect is manifested at least for the integer quantum Hall effect. Conversely, fractional values of ν less than 1 are left out the present approach.

III. FISHER INFORMATION MEASURE VERSUS DEGENERACY

Here is proposed a compact expression for the transverse Fisher information measure. We take into account a special way, as formerly developed [23], a form given by

$$I_t = \int \frac{d^2\alpha d^2\xi}{4\pi^2\ell_{\mathrm{H}}^4}\eta_t(\alpha)\left(\frac{\partial \ln \eta_t(\alpha)}{\partial\alpha}\right)^2. \tag{23}$$

After introducing the known expression for η_t, we arrive to

$$I_t = \frac{2}{\ell_{\mathrm{H}}^2}(1 - e^{-\beta\hbar\Omega}). \tag{24}$$

We notice this measure has a space dimension $(L)^{-2}$. Thus, I_t quantifies the ability for estimating the parameter α [5], which represents the radio of the circular orbit of the coherent states. Indeed, Eq. (24) shows a linear dependence that the parameter I_t exhibits with the magnetic field through the constant ℓ_{H}^2 at low temperature. Then, combining Eqs. (24) and (21) with the definition of ℓ_{H} we obtain

$$I_t = \frac{4\pi\nu}{A}(1 - e^{-\beta\hbar\Omega}), \tag{25}$$

which represents the quantization of the Fisher information measure. From Eq. (25), we can see that Fisher information exponentially decreases as temperature increases. Beside, the growth of the starting value directly depends on the factor ν. The larger is ν, the higher is the Fisher information at all temperatures. This gain of the ability for estimating the parameter α is due to the degeneracy via the factor ν. Thus

$$\frac{4\pi\nu}{A} \leq I_t < 0. \tag{26}$$

In addition, with the purpose to describe the complete motion, we consider now the Fisher information measure for the longitudinal movement, this is

$$I_l = \int \frac{dz dp_z}{h}\eta_l(p_z)\left(\frac{\partial \ln \eta_l(p_z)}{\partial p_z}\right)^2, \tag{27}$$

where p_z is the parameter to be considered and previously ignored [9]. Writing η_l into the above equation, we get

$$I_l = \frac{\beta}{m}. \tag{28}$$

This particular result coincides with the one-dimensional Fisher measure for the classical free particle [24]. Finally, it is emphasized that the total Fisher measure is constructed multiplying Eq. (25) by Eq. (28).

IV. CONCLUDING REMARKS

In the present contribution, we have widely discussed the behavior of several thermodynamical quantities whereas a complete vision in phase space is adopted. When only the transverse motion is considered, diverse difficulties appear in the corresponding interpretation of results, specifically, a non-normalized Husimi distribution [9] is obtained. In the present work we solve the problem by considering the complete motion of the particle. As a consequence we obtain a normalized Husimi distribution in a natural way and all thermodynamic quantities are well defined. In this instance, we have calculated the semiclassical total Wehrl entropy as a sum of two terms, one for the transverse motion and the other for the longitudinal motion. Indeed, the total Wehrl entropy has been expressed in terms of the cyclotron frequency, the mean thermal wavelength and, the degeneracy of the Landau levels [Eq. (13)]. We have analyzed two limit cases. At high temperatures, we have associated the semiclassical entropy with the geometrical properties of the system and with the temperature T_0 such that this approach has sense [Eq. (15)]. At low temperatures, we have found the minimum value of the external magnetic field that depends on the transversal area. Moreover, from the quantization of the quantum Hall effect, we have obtained a family of quantized Wehrl entropies [Eq. (22)]. Also, we have given a quantized version [Eq. (25)] of the transverse Fisher information, which is inverse to the area. Furthermore, we have found the longitudinal Fisher information [Eq. (28)] inverse to the temperature.

Finally, we assert that our semiclassical description constitutes a useful framework to illustrate problems related to size effects, role of boundaries and other typical anomalies derived from the size of the system, which are refereed to two parameters as A and L and they explicitly appear in the form of the T_0, H_0, etc. In addition, the zero temperature can be achieved only if the length of the system L is large enough, otherwise physical properties strongly depend on the size of the system.

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