Normalization of states for a quantum magnetic circular billiard

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An analytical expression is given for the normalization of wave functions of a charge particle inside a circular billiard in presence of an external magnetic field. The physical meaning of this normalizing factor is related to the derivative of the energy eigenvalue with respect to the radius of the billiard. A classical estimate of this factor gives another analytical expression which is in good numerical agreement with the quantum analytical result.

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I. INTRODUCTION

A charged particle confined inside a circle in the presence of an external magnetic field is a system usually called a magnetic circular billiard. The quantum spectrum of this two-dimensional system is well known (see, e.g., [1]). For a study of the relations between classical periodic orbit theory and quantum results for this system, see [2]. This system is a crude but useful model for complex systems called artificial atoms or quantum dots. For introductory papers on these complex systems, see, e.g., [3,4] and for a review paper, see, e.g., [5].

Since the eigenfunctions of the Hamiltonian for a quantum magnetic circular billiard can be expressed in terms of Whittaker functions, normalization can simply be done by numerical integration. This is the procedure proposed in [6]. As shown in the present Brief Report, there exists however an analytical expression for this normalization factor. This analytical expression illuminates the physical meaning of the normalization factor: its squared modulus is simply proportional to the derivative of the energy eigenvalue with respect to the confining radius. This interpretation leads to a classical estimate for the normalization factor (an estimation based on classical mechanics). This classical estimate in turn yields an approximate mathematical relation concerning partial derivatives of Whittaker functions at zero points.

II. GREEN'S FUNCTION FOR LANDAU STATES

We consider the uniform magnetic field $\mathbf{B}$ chosen as z axis, and the potential vector $\mathbf{A}=\frac{1}{2}\mathbf{B}\times\mathbf{r}$ (cylindrical gauge). Our study concerns the two-dimensional motion in the plane of Cartesian coordinates x, y and polar coordinates r, φ where the radial coordinate is $r=\sqrt{x^2+y^2}$. In the x, y plane, with the unit vector $\mathbf{e}_\varphi$, $\mathbf{A}=\frac{Br}{2}\mathbf{e}_\varphi$. Thus the uniform classical motion along the z axis is not considered. Moreover, spin is not taken into account and we use units such that the reduced Planck constant $\hbar$ is unity. Introducing the angular frequency $\omega\equiv\frac{eB}{Mc}$, the Lagrangian [7] $L=\frac{Mv^2}{2}+\frac{e}{c}\mathbf{A}\cdot\mathbf{v}$ can be expressed as $L=\frac{M}{2}\{(\dot{r}^2+r^2\dot{\varphi}^2)+\omega r^2\dot{\varphi}\}$. Note that according to the definition of ω, ω is negative for an electron and positive for a positron. The general definition of the momentum p_i associated with coordinate q_i, namely, $p_i=\frac{\partial L}{\partial \dot{q}_i}$ gives $p_r=M\dot{r}$ and $p_\varphi=Mr^2(\dot{\varphi}+\frac{\omega}{2})$. The Lagrange equations give $\ddot{r}=r\dot{\varphi}(\dot{\varphi}+\omega)$ and $p_\varphi=m$, with m as a constant of motion. In quantum mechanics, one needs the Hamiltonian H and, according to the general relation $H=\Sigma_i p_i\dot{q}_i-L$, one obtains after some calculations

$$H=\frac{p_r^2}{2M}+\frac{Mr^2}{2}\left(\frac{m}{Mr^2}-\frac{\omega}{2}\right)^2. \qquad (1)$$

Equation (1) makes clear that the energy cannot be negative.

Let the state $|a,m\rangle$ be a generalized eigenvector of the radial position operator r, with eigenvalue a and an eigenvector of the operator xp_y-yp_x with eigenvalue m. The expression generalized vector means a normalization with a Dirac distribution for the radial variable $\langle r'm'|r,m\rangle=\delta_{m'm}\frac{\delta(r'-r)}{r}$. The relation between the state $|a,m\rangle$ and the more familiar state $|\mathbf{r}\rangle$ corresponding to a particle ideally localized at point $\mathbf{r}$ is $\langle\mathbf{r}|a,m\rangle=\frac{\delta(r-a)}{a}\frac{\exp(im\varphi)}{\sqrt{2\pi}}$. Let $G(z)=(z-H)^{-1}$ denotes the resolvent of Hamiltonian (1). The matrix element $\langle r,m|G(z)|r_1,m_1\rangle$ corresponds to the radial Green's function of a charged particle in two-dimensional space in the presence of a magnetic field. This function can be calculated exactly [8],

$$\langle r,m|G(z)|r_1,m_1\rangle=-\delta_{mm_1}M\frac{\Gamma\left(\frac{1+|m|}{2}-\kappa\right)}{\Gamma(1+|m|)} \times\frac{M_{\kappa,|m|/2}(\zeta_<)}{\sqrt{\zeta_<}}\frac{W_{\kappa,|m|/2}(\zeta_>)}{\sqrt{\zeta_>}} \qquad (2)$$

with

$$\zeta=\frac{|e|B}{2c}r^2=\frac{M|\omega|}{2}r^2, \qquad (3)$$

$$\kappa=Mz\frac{c}{|e|B}+\frac{e}{|e|}\frac{m}{2}=\frac{z}{|\omega|}+\frac{e}{|e|}\frac{m}{2}. \qquad (4)$$

In Eq. (3) $\zeta_<$ indicates that the smallest values among r and r_1 must appear in the right-hand side and $\zeta_>$ indicates that the greatest one must appear in the right-hand side. The definitions for the gamma function Γ, the Whittaker functions $M_{\kappa,|m|/2}$, $W_{\kappa,|m|/2}$ in Eq. (2), are the standard one, as defined, for example, in [9]. Let us recall some properties of these functions [9,10]. The gamma function has no zeros; the only singularities of the gamma function are simple poles at the negative integers. The function $M_{\kappa,|m|/2}$ is regular at the origin, and the function $W_{\kappa,|m|/2}$ decreases exponentially at infinity. The radial Green's function (2) satisfies the radial differential Schrödinger equation for the Hamiltonian H [Eq. (1)] with respect either the variable r or r_1 for $r \neq r_1$. The poles of the resolvent G according to Eq. (2) are given by the poles of $\Gamma(\frac{1+|m|}{2}-\kappa)$, i.e., $\frac{1+|m|}{2}-\kappa=-n$ with n being positive integers, and one obtains the Landau spectrum [11].

III. ANALYTICAL EXPRESSION FOR THE NORMALIZATION CONSTANT

Let a be the radius of the circular billiard whose center is at the origin of the coordinate system discussed above. The eigenstates of the Hamiltonian must have a vanishing wave function for $r \geq a$ and therefore must be proportional to $|\psi\rangle = G(E)|a,m\rangle$, with the energies E determined as the roots of $M_{\kappa,|m|/2}(\frac{M|\omega|}{2}a^2)$ with respect to the variable z [see Eq. (4)]. A real normalizing factor N_{Em}, is then given by $N_{Em}=\{\langle a,m|[G(E)]^2|a,m\rangle\}^{-1/2}$. The total normalized wave function is

$$\psi(\mathbf{r}) = N_{Em}\langle \mathbf{r}|G(E)|a,m\rangle,$$

$$\psi(\mathbf{r}) = N_{Em}\frac{\exp(im\varphi)}{\sqrt{2\pi}}\langle r,m|G(E)|a,m\rangle. \quad (5)$$

It remains to compute the normalization factor N_{Em}. This is easily done from the relation

$$\langle r,m|[G(z)]^2|r_1,m_1\rangle = -\frac{\partial\langle r,m|G(z)|r_1,m_1\rangle}{\partial z} \quad (6)$$

with $\langle r,m|G(z)|r_1,m_1\rangle$ given by Eq. (2),

$$N_{Em}^{-2} = -\frac{\partial\langle a,m|G(E)|a,m\rangle}{\partial z},$$

$$N_{Em}^{-2} = \frac{2}{\Gamma(1+|m|)\omega^2a^2}\frac{\partial}{\partial\kappa}\left\{\Gamma\left(\frac{1+|m|}{2} - \kappa\right)M_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right)W_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right)\right\}, \quad (7)$$

where the value of the derivative has to be computed at $\kappa=\frac{E}{|\omega|}+\frac{e}{|e|}\frac{m}{2}$ with E as the eigenvalue of H. Taking into account the simplification induced by the boundary condition $M_{\kappa,|m|/2}(\frac{M|\omega|}{2}a^2)=0$,

$$N_{Em}^{-2} = \frac{2}{\Gamma(1+|m|)\omega^2a^2}\Gamma\left(\frac{1+|m|}{2} - \kappa\right)\times W_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right)\frac{\partial}{\partial\kappa}\left\{M_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right)\right\}. \quad (8)$$

For the classical interpretation to be discussed in Sec. IV, still another expression will now be given. The Wronskian relation [10]

$$W_{\kappa,\mu}(z)\frac{dM_{\kappa,\mu}(z)}{dz} - \left(\frac{dW_{\kappa,\mu}(z)}{dz}\right)M_{\kappa,\mu}(z) = \frac{\Gamma(1+\mu)}{\Gamma\left(\frac{1+\mu}{2}-\kappa\right)}$$

and the boundary condition $M_{\kappa,|m|/2}(\frac{M|\omega|}{2}a^2)=0$ yield

$$N_{Em}^{-2} = \frac{2}{\omega^2a^2}\left\{\frac{\left.\frac{\partial M_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right)}{\partial\kappa}\right|_{\kappa=E/|\omega|+e/|e|m/2}}{\left.\frac{\partial M_{\kappa,|m|/2}(x)}{\partial x}\right|_{x=(M|\omega|/2a^2)}}\right\}. \quad (9)$$

Let us recapitulate the global procedure. First determine the roots E of $M_{\kappa,|m|/2}(\frac{M|\omega|}{2}a^2)$ with respect to the variable z which appears only in κ [see Eq. (4)]. Then each root E is an eigenvalue of H, and the corresponding eigenstate is given by

$$\psi_{Em}(\mathbf{r}) = \frac{\exp(im\varphi)}{\sqrt{2\pi}}R_{Em}(r),$$

$$R_{Em}(r) = -2N_{Em}\frac{\Gamma\left(\frac{1+|m|}{2}-\kappa\right)}{\Gamma(1+|m|)a|\omega|r}W_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}r_>^2\right)\times M_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}r_<^2\right) \quad (10)$$

with $r_>=\max(r,a)$, $r_<=\min(r,a)$ and with N_{Em} defined by Eq. (7) and (8), or (9). It is then clear from Eq. (10) that the radial wave function $R_{Em}(r)$ is regular at origin and satisfies $R_{Em}(r)=0$ if $r \geq a$. The orthonormalization relations is (with $\delta_{E'E}$ the Kronecker symbol) $\int_0^a dr r R_{E'm}(r)R_{Em}(r)=\delta_{E'E}$.

IV. PHYSICAL INTERPRETATION OF THE NORMALIZATION FACTOR

We now consider $\frac{\partial E}{\partial a}$, i.e., the behavior of energies with respect to the billiard radius a. If z is a root of $M_{\kappa,|m|/2}(\frac{M|\omega|}{2}a^2)$, it can be viewed as a function of a and

$$0 = dM_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right) = \frac{\partial M_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right)}{\partial z}dz + \frac{\partial M_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right)}{\partial a}da,$$

$$\frac{\partial E}{\partial a} = -M\omega^2 a\left[\left.\frac{\partial M_{\kappa,|m|/2}(x)}{\partial x}\right|_{x=(M|\omega|/2a^2)}\right]\times\left[\left.\frac{\partial M_{\kappa,|m|/2}\left(\frac{M|\omega|}{2}a^2\right)}{\partial\kappa}\right|_{\kappa=E/|\omega|+e/|e|m/2}\right]^{-1}. \quad (11)$$

The comparison of this expression with Eq. (9) gives the physical interpretation in term of the partial derivative of the energy eigenvalue with respect to the radius of the billiard,

$$N_{Em}^2 = -\frac{a}{2M}\frac{\partial E}{\partial a}. \quad (12)$$

V. CLASSICAL ESTIMATE OF THE NORMALIZATION FACTOR

Let us calculate the change in momentum due to a collision on the circular billiard. The center O of the circular

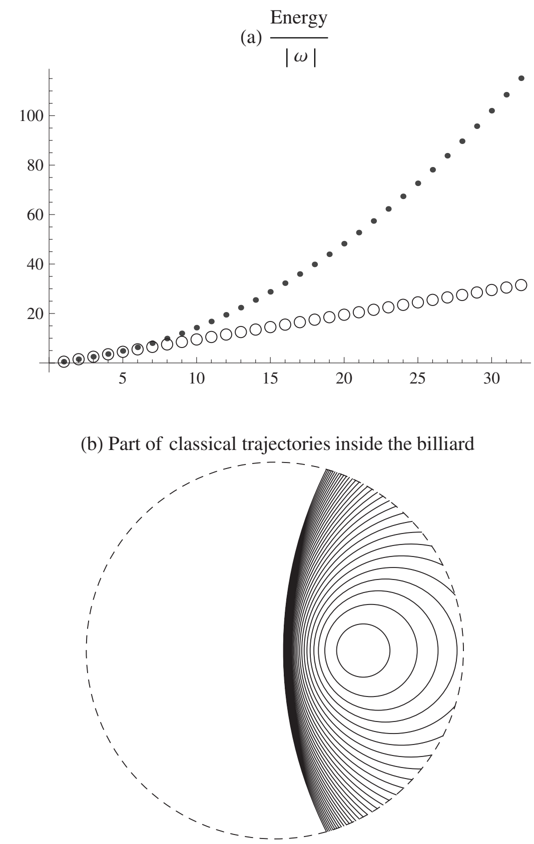

FIG. 1. (a) The dots are the quantum energies in units of $|\omega|$ for the first 32 levels. The small circles are the corresponding energies $\frac{1}{2}+i$, $i=1,\ldots,32$, of Landau levels. (b) For each energy, part of a corresponding classical trajectory inside the circular billiard whose boundary is represented by a dashed circle.

billiard is the origin of coordinates, C denotes the center of the circular trajectory $\mathbf{r}(t)$ of radius R, and r_c denotes the distance between O and C. Then classical mechanics yields (see, e.g., [12]) $E=M\omega^2R^2/2$, $r_c^2=2\frac{E+m\omega}{M\omega^2}$, and

$$r(t)=r_c\sqrt{1+\left(\frac{R}{r_c}\right)^2+2\frac{R}{r_c}\cos(\omega t)}. \tag{13}$$

Classically, if $r(t)<a$ all the times, the circular trajectory does not collide with the billiard. Collisions with the billiard occur only for $r=a$, and it is clear from Eq. (13) that collisions can occur only for

$$r_c+R=\frac{1}{|\omega|}\sqrt{\frac{2}{M}}(\sqrt{E+m\omega}+\sqrt{E})>a, \tag{14}$$

a condition that is now assumed.

Figure 1(a) represents some quantum energy levels in order of increasing energy, and Fig. 1(b) shows corresponding possible classical trajectories inside the billiard. The data of this figure are for $M=1$, $\omega=2$, $a=5$, and $m=5$. It is seen on Fig. 1(b) that the four firsts trajectories do not collide the billiard. It is also seen in Fig. 1(a) that the energies of these four first levels are very close to the Landau energy levels, as expected.

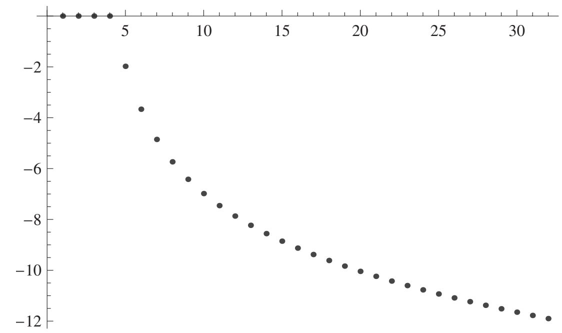

FIG. 2. For the same conditions as those of Fig. 1 (see text), the natural logarithm of the relative error of the classical estimate with respect to the quantum result is plotted in order of increasing energy levels (see text).

Let P be a point of collision and $\angle OPC$ be the angle at P determined by the lines PO and PC. Then $\cos(\angle OPC)=\frac{a^2+R^2-r_c^2}{2aR}$. The angle α of the circular trajectory with the normal to the circular billiard at the point of collision P satisfies $\alpha=\frac{\pi}{2}-\angle OPC$, and therefore $\cos(\alpha)=\sqrt{1-\cos^2(\angle OPC)}$.

A collision yields a change in momentum $\delta p=2\sqrt{2ME}\cos(\alpha)$. The time interval T between two successive collisions is the difference between the time $\frac{2\pi}{|\omega|}$ for a full circular trajectory (in absence of the billiard) and the time $2\frac{(\pi-\angle OCP)}{|\omega|}$ of a fictitious trajectory outside the circular billiard. The ratio $\delta p/T$ is the mean force exerted by the particle on the billiard due to collisions and therefore is the classical equivalent to $\frac{\partial E}{\partial a}$, to be denoted $(\frac{\partial E}{\partial a})_c$. It remains to collect all results in terms of basic variables of the problem. If Eq. (14) is satisfied one obtains

$$\left(\frac{\partial E}{\partial a}\right)_c=-|\omega|\frac{\sqrt{8a^2EM-(a^2M\omega-2m)^2}}{2a\left[\arccos\left(\frac{4E+\omega(2m-a^2M\omega)}{4\sqrt{E(E+m\omega)}}\right)\right]} \tag{15}$$

and the classical estimate for the normalization factor is $N_{Em}^2=-\frac{a}{2M}(\frac{\partial E}{\partial a})_c$. Condition (14) ensures that the particle collides with the billiard. If this condition is not satisfied, the particle does not interact with the billiard and $(\frac{\partial E}{\partial a})_c=0$.

Although the derivation of Eq. (15) relies completely on classical mechanics, it is stressed that the energy E in its right-hand side is computed quantum mechanically, and the values of m are quantified (integers).

For the same conditions as for Fig. 1, Fig. 2 reports the natural logarithm of the relative error $[(\frac{\partial E}{\partial a})-(\frac{\partial E}{\partial a})_c]/(\frac{\partial E}{\partial a})$ for the 32 first energy levels. For the four first energy levels whose classical trajectory does not encounter the billiard, $(\frac{\partial E}{\partial a})_c=0$, and the relative error is maximal, i.e., unity, giving zero for the logarithm. For the following energy levels, the agreement between the exact results [Eq. (11)] and the classical result [Eq. (15)] is seen to be very good and the accuracy of the classical estimate increases with energy. The relative error is only 6.78×10^{-6} for the last energy level.

VI. CONCLUDING REMARKS

The present method can be applied to other problems. Consider, for example, the magnetic hard disk, where the particle is now confined *outside* a circle in the plane. The essential change is that $W_{\kappa,|m|/2}$ should be used in place of $M_{\kappa,|m|/2}$ for the determination of energy eigenvalues and in Eq. (9). The expression for the classical estimate of the derivative of the energy with respect to the radius a of the hard disk can also be shown to be

$$\left(\frac{\partial E}{\partial a}\right)_c = |\omega| \frac{\sqrt{8a^2EM - (a^2M\omega - 2m)^2}}{2a\left[\pi - \arccos\left(\frac{4E + \omega(2m - a^2M\omega)}{4\sqrt{E(E+m\omega)}}\right)\right]}$$

to be compared with Eq. (15). The generalization to the magnetic annulus billiard (a charged particle confined between two concentric circles) is a little more complicated but presents no basic difficulties. Other generalizations concern two- or three-dimensional systems for which the Green's function is analytically known, such as free or Coulombic billiard systems.

Semiclassical approaches such as the Jeffreys, Wentzel, Kramers, Brillouin (JWKB) method have not been discussed in this Brief Report because they are well known, but it is clear that they are well suitable [1] to all the problems considered here.

It is worth interesting to note that comparison of the right-hand sides of Eqs. (11) and (15) provides a purely mathematical approximate relation for partial derivatives of Whittaker functions at some zeros of these functions. This approximate mathematical relation has been obtained by comparison between a quantum and a classical approach to the same physical problem.

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