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The particle in a Möbius wire and half-integer orbital angular momentum

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Restricting one particle on the rim of a Möbius strip (Möbius wire), its wavefunctions are explicitly calculated through the non-relativistic quantum theory. Demanding the wavefunction to be single-valued, it is proven that in the case of a narrow strip the orbital angular momentum of the particle takes both integer and half-integer values of \hbar . In addition, the energy values of two chiral Möbius wires are proven to be equal.

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I. INTRODUCTION

The angular momentum operator in the quantum mechanics domain is defined as any vectorial operator $\hat{\vec{J}} = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$, whose components obey to the well known commutation relations $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$, $[\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y$, and $[\hat{J}_y, \hat{J}_z] = i\hbar\hat{J}_x$. Out of these relations, someone can extract any property of these operators, or even study the angular momentum coupling between different sources (e.g. the total spin angular momentum of a two electrons system, or the spin and orbital angular momentum of an electron in a Coulombic field).[1] It's noteworthy that the explicit form of \hat{J}_x , \hat{J}_y , and \hat{J}_z is not necessary.

It can be proved, for instance, that \hat{J}^2 and one of its components, say \hat{J}_z , share the same eigenfunctions $|j, m\rangle$. [1]

$$\begin{aligned}\hat{J}^2 |j, m\rangle &= j(j+1)\hbar^2 |j, m\rangle \\ \hat{J}_z |j, m\rangle &= m\hbar |j, m\rangle\end{aligned}\tag{1}$$

The eigenvalues of the \hat{J}^2 and \hat{J}_z operators are $j(j+1)\hbar^2$ and $m\hbar$, respectively. In addition m is allowed to take values from $-j$ to j in step of one, i.e. $m = -j, -j+1, \dots, j-1, j$. Of course, this implies that j and m can only be either integer or half-integer numbers, otherwise $-j$ can never reach j , adding several times the unit. Ignoring angular momenta coupling, it is well established that orbital angular momentum is related only to integer m values, whereas spin to all possible values of m .

Usually, in the textbooks the whole story starts with the particle confined in a ring of radius R . If μ is the mass of the particle, and ϕ the rotation angle, then the Hamiltonian operator of the system is

$$\hat{H} = -\frac{\hbar^2}{2\mu R^2} \frac{d^2}{d\phi^2}\tag{2}$$

and the solution of the Schrödinger equation $\hat{H}\Phi_m = E_m\Phi_m$ gives $E_m = \hbar^2 m^2 / 2\mu R^2$ and $\Phi_m = c_1 e^{im\phi} + c_2 e^{-im\phi}$. The choice of the exact values of c_1 , c_2 , and m is not straightforward. The Hamiltonian operator commutes with both the angular momentum operator $\hat{L}_z = -i\hbar\partial/\partial\phi$, and the parity operator $\hat{\Pi}_\phi (\phi \rightarrow -\phi)$, but the latter operators do not commute to each other. The eigenfunctions of \hat{L}_z are $N_\pm e^{\pm im\phi}$, whereas those of $\hat{\Pi}_\phi$ are $N_\pm (e^{im\phi} \pm e^{-im\phi})$. So, someone should choose what kind of solutions they need. The former notation is appropriate for the next step, the particle on a sphere, and the latter is suitable for drawing the wavefunctions on a sheet of paper.

To obtain the values of m , we have to apply the boundary conditions. But what are the boundary conditions? Someone could say that the wavefunction must be single-valued at any (x, y) point, or that the density must be single-valued. In the first case only integer m values are allowed, while in the second case both integer and half-integer values are obtained, independently of the c_1 and c_2 values. Of course, the single-valuedness of a wavefunction constitutes a *sine qua non* postulate of quantum mechanics, but it turns out that it can be rationalized. Merzbacher stated that "It may even be said that the strange double-valued eigenfunctions of angular momentum have appeared only because we have changed from *Cartesian* coordinates, which are adapted to the homogeneity and isotropy of ordinary space, to *polar* coordinates, which are singular at the coordinate origin and distinguish a particular direction in space".[2] Moreover, Henneberger and Opatrný reported that "In bound states, the superposition principle by itself guarantees single-valuedness".[3] Nevertheless, the particle on a ring has only integer m values. Providing the $N_\pm e^{\pm im\phi}$ wavefunctions are selected, then \hat{L}_z has eigenvalues $0\hbar, \pm 1\hbar, \pm 2\hbar, \dots$

Next, moving to the particle on a sphere we introduce the angle θ , and the conclusions we can infer are similar. The wavefunctions are the spherical harmonics $Y_{j,m}(\phi, \theta)$, and the fact that j , and thus m , takes only integer values can be substantiated in several ways.[4] It seems that half-integer orbital angular momentum in the three-dimensional space can not exist, and that spherical harmonics with half-integer j values do not describe an angular momentum eigenfunction.[4]

In the present study, we present a one particle system in the three dimensional space, with the eigenvalue of \hat{L}_z taking both integer and half-integer values towards some limit (*vide infra*), while the eigenfunction of the system can be characterized as pseudo double valued. This system is the Möbius wire.

II. THE PARTICLE IN A MÖBIUS WIRE

The Möbius surface was first introduced by A. F. Möbius and J. B. Listing, and practically it can be constructed using a strip of paper, twisting one narrow edge by 180 degrees, and attaching it to the other. Alternatively, it is

the surface created by a stick, which rotates around a circle of radius R , and at the same time around itself with the half angular velocity (see Fig. 1 and ref. 5). Depending on the direction (clock-wise or counter-clockwise) of the self-rotation, we get two different Möbius strips, which are mirror images to each other (chirality).[5] The Möbius wire is defined as the rim of a Möbius surface. Beginning from any point of this curve and moving on it, someone will arrive at the same point after a 4π rotation. The Cartesian coordinates of such a shape as a function of the rotation angle ϕ are[5]

$$\begin{aligned} x &= (R + s \cdot \cos(\pm\phi/2)) \cdot \cos \phi \\ y &= (R + s \cdot \cos(\pm\phi/2)) \cdot \sin \phi \\ z &= s \cdot \sin(\pm\phi/2) \end{aligned} \quad (3)$$

where R , and s are parameters of the Möbius wire (see Fig.1), and the plus or minus sign covers both chirals. Note that if $s \ll R$ then the Möbius wire tends to become a “double” circle. Observe, also, that for given x and y values, the angle ϕ is fully determined. Using the first two equations, we get

$$\phi = \arctan(y/x) \quad (4)$$

Consequently, the z coordinate depends on x and y , $z = z(x, y)$. So, even if we wrote $\phi = \phi(x, y, z)$, then we would result in $\phi = \phi(x, y, z(x, y)) = \phi(x, y)$. The necessity of the third dimension (z coordinate) will become clear later. Finally, the partial derivatives of ϕ relative to x , y , and z , are

$$\begin{aligned} \frac{\partial \phi}{\partial x} &= -\frac{\sin \phi}{r}, \quad \frac{\partial \phi}{\partial y} = \frac{\cos \phi}{r}, \quad \frac{\partial \phi}{\partial z} = 0 \\ \text{with } r &= R + s \cdot \cos(\phi/2) \end{aligned} \quad (5)$$

so that $\partial/\partial x = -\sin \phi/r \partial/\partial \phi$, $\partial/\partial y = \cos \phi/r \partial/\partial \phi$, while $\partial/\partial z$ vanishes, and the Hamiltonian operator for both chiral systems in terms of ϕ is

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{2\mu} \nabla^2 = -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{\partial}{\partial \phi} \frac{1}{r} \frac{\partial}{\partial \phi} \\ \text{or } \hat{H} &= -\frac{\hbar^2}{2\mu} \left(\frac{1}{r} \frac{\partial}{\partial \phi} \right)^2 \end{aligned} \quad (6)$$

Now, r is rewritten as $r = R(1 + \lambda \cos(\phi/2)) = R\rho(\phi)$, where $\lambda = s/R$, and the Hamiltonian reads

$$\hat{H} = -\frac{\hbar^2}{2\mu R^2} \left(\frac{1}{\rho} \frac{\partial}{\partial \phi} \right)^2 \quad (7)$$

Markedly, the Schrödinger equation $\hat{H}\Phi_m = E_m\Phi_m$ is solved explicitly and gives $E_m = \hbar^2 m^2 / 2\mu R^2$ with $\Phi_m = c_1 e^{im\phi} e^{2im\lambda \sin(\phi/2)} + c_2 e^{-im\phi} e^{-2im\lambda \sin(\phi/2)}$. The choice of c_1 and c_2 is matter of our will; if we want to exploit the commutation of \hat{H} with $\hat{M} = -i\hbar/\rho \partial/\partial \phi$ the eigenfunctions become $\Phi_m = N_{\pm} e^{\pm im\phi} e^{\pm 2im\lambda \sin(\phi/2)}$, or the commutation of \hat{H} with the parity operator $\hat{\Pi}_{\phi}$, and then Φ_m is either $N_c \cos[m(\phi + \lambda \sin(\phi/2))]$ or $N_s \sin[m(\phi + \lambda \sin(\phi/2))]$. In order to find the allowed m values, we impose $\Phi_m(\phi + 4\pi) = \Phi_m(\phi)$, which yields $m = 0, \pm 1/2, \pm 1, \pm 3/2, \pm 2, \dots$. If the z -coordinate were absent, then the curve in question would have a crossing, and thus breaking down the proposed boundary conditions.

In Fig. 2 the wavefunctions of cases $m = 1/2$ and 1 with $\lambda = 0.3$ are shown. For reason of comparison the wavefunctions of the particle on a ring are also included ($\lambda = 0$). Notice that the eigenfunctions at angles ϕ and $\phi + 2\pi$, in general, have completely different values, i.e. they are not related by equality or a sign inversion.

Observe, now, that the operator \hat{M} has eigenvalues equal to $m\hbar$, and towards the limit $s \ll R$, it transforms to \hat{L}_z . Indeed, in this case the Möbius wire looks like two circles of radius R almost attached to each other, and the eigenfunctions adopt the form $\Phi_m = N_{\pm} e^{\pm im\phi}$ ($\lambda \rightarrow 0$). Hence, after a rotation of 2π radians the wavefunction may have the same value (integer m value) or exactly the opposite (half-integer m value). The following question is in order: “in the case of half-integer m value, what is the value of the eigenfunction at a specific ϕ , minus or plus something?” The answer is that it depends on “which” circle the particle is. Thus the eigenfunction is characterized as pseudo double valued.

III. SUMMARY AND CONCLUSIONS

Studying the one-particle system confined in a Möbius wire through the non-relativistic quantum mechanical principles, we prove that in the three dimensional space we may have half-integer projections (on an axis) of *orbital* angular

momentum, retaining the single-valuedness property of the wavefunction. Of course, half-integer values of the total angular momentum quantum number j have already been ruled out in the literature.[4] The reason for that may be ascribed to the fact that we can not construct a “single-sided” 3d-volume (introducing two angles, ϕ and θ); we need the fourth dimension. In addition, we prove that the two chiral conformations of the Möbius wire have the same Hamiltonian, and thus exactly the same energy values, although it might seem obvious.

ACKNOWLEDGEMENTS

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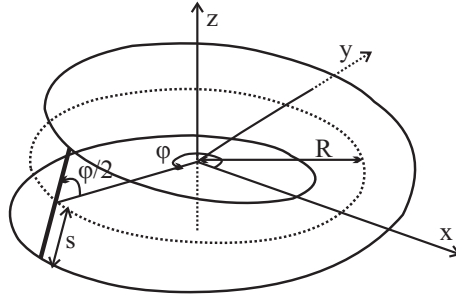


FIG. 1. A stick of length $2s$ rotates around the circle of radius R (dashed line), and simultaneously around itself. The former rotation occurs twice faster than the latter, so that the stick after $\phi = \phi + 2\pi$ rotation will have the same position, but opposite orientation. The orbit of the two edges of the stick constitutes the Möbius wire.

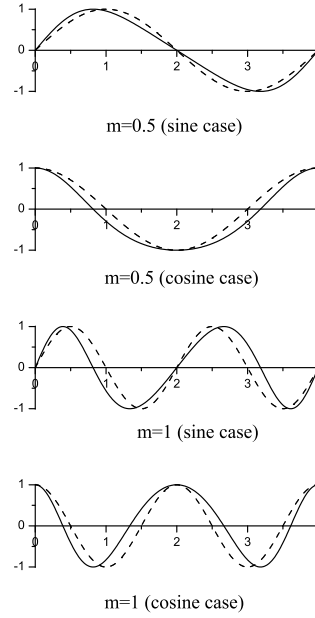


FIG. 2. Plots of the eigenfunctions of the Möbius wire (solid lines) as compared to those of the ring model (dashed lines) for $m = 1/2$ and $m = 1$, and for both sine and cosine cases. The eigenfunctions are normalized so that their maximum is at 1.0. The ϕ values are counted in π radians.