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1996 J. Phys. A: Math. Gen. 29 1497

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Quantum mechanics in multiply-connected spaces

Vu B Ho and Michael J Morgan

Department of Physics, Monash University, Clayton Victoria 3168, Australia

Received 2 June 1995, in final form 12 October 1995

Abstract. This paper analyses quantum mechanics in multiply-connected spaces. It is shown that the multiple connectedness of the configuration space of a physical system can determine the quantum nature of physical observables, such as the angular momentum. In particular, quantum mechanics in compactified Kaluza–Klein spaces is examined. These compactified spaces give rise to an additional angular momentum which can adopt half-integer values and therefore, may be identified with the intrinsic spin of a quantum particle.

1. Introduction

Quantum mechanics conventionally deals with the evolution of a particle in a simply connected configuration space, whose topology is Euclidean \mathbb{R}^n . The Euclidean space \mathbb{R}^n has a simple topology in the sense that paths in this space are contractible to a point, and so the fundamental homotopy group is trivial, i.e. $\pi_1(\mathbb{R}^n) \cong \{0\}$. However, novel features can arise from configuration spaces that exhibit a non-trivial topology [1, 2]. In a multiply-connected space, the nature of the Schrödinger wavefunction may depend on the topological structure of the configuration space. On the other hand, multiply-connected configurational spaces have also been shown to play an important role in field theory and particle physics, where stable solutions to field equations can exist for appropriate topologies of the configuration spaces [3, 4].

In this paper we analyse quantum mechanics in multiply-connected configuration spaces. It is assumed that a physical system is described by a complex wavefunction Ψ defined on a configuration space M , and the time evolution of the system is determined by the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \quad (1)$$

where H is the Hamiltonian of the system. According to the orthodox interpretation of the wavefunction in quantum mechanics, all of the physical information is contained in the square of the modulus of the wavefunction; therefore, all complex wavefunctions that differ from one another by a phase can be used to describe the same quantum state of the physical system. Consequently, the absolute phase is regarded as unobservable and the phase of a wavefunction can be defined globally as a $U(1)$ -valued function on the configuration space M , when M is simply-connected. In terms of a fibre bundle structure, this result can be seen as an admission of a global section of a principal fibre bundle, since nonrelativistic quantum mechanics can be associated with the trivial complex line bundle $M \times C$ and the wavefunction is simply a global section of the line bundle. The quantum state of a physical system is regarded as an equivalence class $\{e^{i\alpha}\psi\}$ of normalized wavefunctions defined on

the principal $U(1)$ -bundle $M \times S^1$ on M . Because physical observables correspond only to the squared modulus of a wavefunction, wavefunctions on the $U(1)$ -bundle must satisfy the condition $\psi(x, e^{i(\alpha+\beta)}) = \psi(x, e^{i\alpha})e^{i\beta}$ [3, 5, 6].

When the topological structure of the configuration space is non-trivial, ambiguities may arise when attempts are made to specify a value for the phase of a wavefunction for the whole configuration space. In this case the fibre bundle representation of the system is not trivial and so it does not admit a global section. However, since physical observables related to $\psi^*\psi$ are considered as functions on the configuration space, wavefunctions which are functions on a fibre bundle over the configuration space are allowed, provided they satisfy the requirement $\psi(xe^{i\alpha}) = \psi(x)e^{in\alpha}$. This problem is related to the problem of formulating quantum mechanics on the universal covering space of a multiply-connected configuration space. This paper is organized as follows. In section 2 a brief review of quantum mechanics on universal covering spaces is given. Section 3 discusses the quantization of angular momentum. Section 4 discusses quantum mechanics on multiply-connected spaces. In particular, we show that quantum mechanics in compactified Kaluza–Klein spaces gives rise to an additional angular momentum which adopts half-integer values, and therefore may be identified with the intrinsic spin of a particle.

2. Quantum mechanics on universal covering spaces

Consider the case where the configuration space M of a physical system is a topological space which may be multiply-connected, so that its fundamental homotopy group $\pi_1(M) \neq \{0\}$. If the space M satisfies the conditions of arcwise and local connectedness, then it is possible to construct a covering space \tilde{M} which is simply connected with the property $\pi_1(\tilde{M}) = \{0\}$. The covering space \tilde{M} is called a universal covering space of M . The space \tilde{M} is a bundle space over the space M with a covering projection $\pi: \tilde{M} \rightarrow M$, so that the homotopy group of the bundle space \tilde{M} is a factor group of the fundamental homotopy group of the base space M [7–9]. Although it is always possible to construct a conventional quantum mechanics on the universal covering space \tilde{M} , because it is simply-connected, the question of how to relate the quantum mechanics on \tilde{M} to quantum mechanics on the multiply-connected space M does not have an obvious answer. Consider a single-valued wavefunction $\tilde{\psi}(\tilde{x})$ on \tilde{M} . If the point $x = \pi(\tilde{x})$ on M is taken around a loop γ , then when the loop γ lifts to a curve $\tilde{\gamma}$ in the space \tilde{M} , with the initial point \tilde{x} , the wavefunction $\tilde{\psi}$ will take its value at the end point \tilde{x}' of the curve $\tilde{\gamma}$, obtained from the point \tilde{x} by the action of the homotopy class $[\gamma]$, that is, $\tilde{\psi}(\tilde{x}') = \tilde{\psi}([\gamma]\tilde{x})$. Therefore, if quantum mechanics on the bundle space \tilde{M} is projectable to quantum mechanics on the multiply-connected space M , in the sense that the squared modulus of the wavefunction $\tilde{\psi}$ on \tilde{M} depends only on $x = \pi(\tilde{x})$, then the wavefunction $\tilde{\psi}$ must satisfy the boundary conditions

$$\tilde{\psi}([\gamma]\tilde{x}) = a([\gamma])\tilde{\psi}(\tilde{x}) \quad (2)$$

$$|a([\gamma])| = 1 \quad (3)$$

for all $\tilde{x} \in \tilde{M}$ and all homotopy classes $[\gamma] \in \pi_1(M)$. Furthermore, because the wavefunction $\tilde{\psi}$, being defined on a simply-connected space, is single-valued, the phase $a([\gamma])$ must also satisfy the condition $a([\gamma])a([\gamma']) = a([\gamma][\gamma'])$. The conditions imposed on the phase $a([\gamma])$ show that the map $a: \pi_1(M) \rightarrow U(1)$ defined by $[\gamma] \rightarrow a([\gamma])$ is a one-dimensional unitary representation of the fundamental homotopy group $\pi_1(M)$ [5].

To illustrate how quantum mechanics on a multiply-connected space can be realized in physics, let us consider the quantum dynamics of a particle moving in a one-dimensional lattice with a periodic potential $V(x + nd) = V(x)$. Assume the dynamics is governed

by a Hamiltonian of the form $H = p^2/2m + V(x)$, where m and p are the mass and the momentum of the particle, respectively. The system in this case has translational symmetry, since the Hamiltonian is invariant under the transformation $x \rightarrow x + nd$. Let $T(n)$ be an operator that corresponds to this transformation in the vector space of physical states of the system, then it can be shown that the set $\{t_n(\theta) = e^{-in\theta}; -\pi \leq \theta < \pi\}$, forms a one-dimensional unitary representation of the translation group $T(n)$. It follows that the Schrödinger wavefunctions of the particle, known as Bloch functions, must satisfy the boundary condition $\psi_{nk}(x + d) = \exp(ikd)\psi_{nk}(x)$. Now if the endpoints of a unit cell of the lattice are identified, so that the cell has the topology of a circle S^1 , which has the fundamental homotopy group isomorphic to Z , then it is seen that the characters are $a([\gamma]) = \exp(ikd)$, $-\pi \leq kd < \pi$. Another illustration of quantum mechanics on multiply-connected spaces is that of the hydrogen atom in the Euclidean plane \mathbb{R}^2 . The time-independent wavefunction for the system is written in the form $\psi(r, \phi) = \exp(im\phi)R(r)$, where $R(r)$ is the radial solution. When the configuration space of the system is simply-connected, the wavefunction ψ must be single-valued, which imposes the requirement that the quantity m must be an integer. However, if the electron of the system cannot penetrate the nucleus, it is reasonable to reduce the space to $\mathbb{R}^2 \setminus \{0\}$, which is now multiply-connected, and whose fundamental homotopy group is isomorphic to $\pi_1(S^1)$. Therefore, the wavefunction on the original space \mathbb{R}^2 is projectable even if the quantity m takes half-integer values; in this case the wavefunction satisfies the boundary condition $\psi(r, [\gamma]\phi) = \psi(r, n\phi) = \exp(in\pi)\exp(im\phi)R(r)$ and hence $a([\gamma]) = a(n) = \exp(in\pi)$. This problem will be discussed in more detail in the next section.

Having shown how to construct a projectable quantum mechanics on a universal covering space \tilde{M} of a multiply-connected configuration space M , there still remains the question: what is the nature of the wavefunctions on M ? The universal covering space \tilde{M} is the union of fundamental domains, each of which is isomorphic to the configuration space M . If quantum mechanics on the universal covering space \tilde{M} is restricted to that of a particular domain, then the wavefunction $\tilde{\psi}$ can be projected down to a well-defined wavefunction ψ on the space M . However, since a point $x \in M$ corresponds to many different points $\tilde{x} = \pi^{-1}(x) \in \tilde{M}$, which are connected by the action of the fundamental homotopy group $\pi_1(M)$ on \tilde{M} , the projection of the wavefunction $\tilde{\psi}$ on \tilde{M} to a wavefunction ψ on M will make the wavefunction ψ multivalued. The construction of a projectable quantum mechanics on universal covering spaces requires that the multiple-valuedness of a wavefunction on the original configuration space (obtained by the projection of a wavefunction on a universal covering space) is not arbitrary, but is limited to multiplication by the characters of the fundamental homotopy group of the original configuration space [3, 5].

3. On the quantization of angular momentum

As mentioned earlier the quantum mechanics of a hydrogen atom in the configuration space $\mathbb{R}^2 \setminus \{0\}$ can be considered in terms of a multiply-connected space whose first fundamental homotopy group is isomorphic to $\pi_1(S^1)$. In this case, wavefunctions on the space $\mathbb{R}^2 \setminus \{0\}$ are allowed to be multivalued [13]. Here we examine the relationship between the multiple-valuedness of the wavefunction and the quantization of angular momentum. Consider the eigenvalue equation of a generalized hydrogen-like atom consisting of a single electron of

charge $-e$ and a nucleus of charge Ze [10–12]:

$$-\frac{\hbar^2}{2\mu} \nabla_N^2 \psi(\mathbf{r}) - \frac{Ze^2}{r} \psi(\mathbf{r}) = E \psi(\mathbf{r}) \quad (4)$$

where μ is the reduced mass, $r = \sqrt{g_{\mu\nu} x^\mu x^\nu}$ and $\nabla_N^2 = g^{\mu\nu} \partial_\mu \partial_\nu$, where $g_{\mu\nu}$ is the N -dimensional Euclidean metric. In an N -dimensional Euclidean space, spherical polar coordinates are defined in terms of the coordinates θ_i , $1 \leq i \leq N-1$, i.e.

$$\begin{aligned} x_1 &= r \cos \theta_1 \prod_{i=2}^{N-1} \sin \theta_i \\ x_2 &= r \prod_{i=1}^{N-1} \sin \theta_i \\ x_i &= r \cos \theta_{i-1} \prod_{j=i}^{N-1} \sin \theta_j \quad i = 3, \dots, N \end{aligned} \quad (5)$$

where the range of the variables is $0 \leq r < \infty$, $0 \leq \theta_1 \leq 2\pi$ and $0 \leq \theta_i \leq \pi$ for $i = 2, \dots, N-1$. It is straightforward to verify that the Laplacian ∇_N^2 expressed in terms of the N -dimensional polar coordinates takes the form

$$\nabla_N^2 = \frac{1}{r^{N-1}} \frac{\partial}{\partial r} r^{N-1} \frac{\partial}{\partial r} - \frac{L_{N-1}^2}{\hbar^2 r^2} \quad (6)$$

where the generalized angular momentum operators are defined by the recursion relation

$$L_{i-1}^2 = -\hbar^2 \left\{ \frac{1}{\sin^{i-2} \theta_{i-1}} \frac{\partial}{\partial \theta_{i-1}} \sin^{i-2} \theta_{i-1} \frac{\partial}{\partial \theta_{i-1}} - \frac{L_{i-2}^2}{\hbar^2 \sin^2 \theta_{i-1}} \right\}. \quad (7)$$

The generalized spherical harmonics $Y(l_{(N-1)}, \dots, l_1)$ are defined as the simultaneous eigenfunctions of the set of operators $\{L_k^2\}$

$$L_k^2 Y(l_{(N-1)}, \dots, l_1) = l_k(l_k + k - 1) \hbar^2 Y(l_{(N-1)}, \dots, l_1) \quad (8)$$

where $1 \leq k \leq N-1$. Imposing the requirement of single-valuedness, the quantum number l_i with $1 \leq i \leq N-1$ must be an integer. On the other hand, integer values of the quantum number l are required for consistency of the group representation [14, 20]. When the eigenfunction of the generalized hydrogen atom is written as

$$\psi_{nl}(l, l_{N-2}, \dots, l_1) = R_{nl} Y(l, l_{N-2}, \dots, l_1) \quad (9)$$

with $l = l_{N-1}$, then the radial equation for the function R_{nl} , for the case of bound states with $E < 0$, becomes

$$\frac{d^2 R_{nl}}{d\rho^2} + \frac{N-1}{\rho} \frac{dR_{nl}}{d\rho} - \left[\frac{l(l+N-2)}{\rho^2} + \frac{\lambda}{\rho} - \frac{1}{4} \right] R_{nl} = 0 \quad (10)$$

where ρ and λ are defined by

$$\rho = \left[\frac{8\mu(-E)}{\hbar^2} \right]^{1/2} r \quad \lambda = \left[\frac{Z^2 e^4 \mu}{2\hbar^2(-E)} \right]^{1/2}. \quad (11)$$

We seek solutions for R_{nl} of the form

$$R_{nl} = \exp(-\rho/2) \rho^l S(\rho). \quad (12)$$

By substitution into the equation for R_{nl} the following differential equation for $S(\rho)$ is obtained, i.e.

$$\frac{d^2 S}{d\rho^2} + \left(\frac{2l + N - 1}{\rho} - 1 \right) \frac{dS}{d\rho} + \frac{\lambda - (N - 1)/2 - l}{\rho} S = 0. \quad (13)$$

This equation can be solved by a series expansion of $S(\rho)$

$$S(\rho) = \sum_{n=0}^{\infty} a_n \rho^n \quad (14)$$

with the coefficients a_n satisfying the recursion relation

$$a_{n+1} = \frac{n + l + (N - 1)/2 - \lambda}{(n + 1)(n + 2l + N - 1)} a_n. \quad (15)$$

The bound-state energy spectrum is given by

$$E_n = -\frac{Ze^4 \mu}{2\hbar^2} \frac{1}{[n + l + (N - 1)/2]^2}. \quad (16)$$

This result shows that for spaces of odd dimension the quantum number l must be an integer for the energy E_n to have the same form as that of the Bohr model. On the other hand, for spaces of even dimension, the Bohr spectrum is obtained only when the quantum number l is half-integer. However, in quantum mechanics the quantum number l must always be an integer by the requirement of single-valuedness of the Schrödinger wavefunction, irrespective of the dimension of the configuration space. We now discuss this problem from the perspective of quantum mechanics on multiply-connected spaces, showing the important relationship between the topology of the system and the multiply-connected configuration space of the atom. In two-dimensional space, the Schrödinger equation in planar polar coordinates takes the form

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right] \psi(r, \phi) - \frac{Ze^2}{r} \psi(r, \phi) = E \psi(r, \phi) \quad (17)$$

where it is assumed that the Coulomb potential has the r^{-1} form. This equation admits solutions of the form $\psi(r, \phi) = R(r) \exp(im\phi)$, where m is identified with the angular momentum of the system. We normally require the angular momentum m to take integer values so that the single-valuedness condition is satisfied. However, the requirement that m be an integer is not compatible with assumption that an observer in a two-dimensional space must obtain an energy spectrum identical to the Bohr model, because the energy spectrum in this case can be written explicitly in the form

$$E = -\frac{Z^2 e^4 \mu}{2\hbar^2 (n + m + \frac{1}{2})^2}. \quad (18)$$

Hence, if the hydrogen-like atom is viewed as a two-dimensional physical system, and if the energy is observed to have the same spectrum as that of the Bohr model then the angular momentum m must take half-integer values. These half-integer values are allowable provided the configuration space is not simply-connected. This will be the case for a hydrogen-like atom viewed as a planar system, in which the atomic electron cannot penetrate the nucleus. In this situation the single-valuedness condition is no longer a sufficient requirement to ensure that the angular momentum adopts integer values. However, it can be verified that integer values for the angular momentum m can be retained if we add to the Coulomb potential a quantity $-(\hbar\sqrt{E/2\mu})/r$, when the hydrogen-like atom is viewed as a two-dimensional physical system.

In the above example it is seen that topological structure of a configuration space can determine the quantum nature of an observable. This result is not unexpected in quantum mechanics. If the electron in a hydrogen-like atom is constrained to move in a plane, then the orbital angular momentum of the electron must take half-integer values in order to reproduce the same energy spectrum as the Bohr model. As a consequence, it may be possible to invoke topological constraints to explain the Stern–Gerlach experiment, without the necessity of introducing spin into non-relativistic quantum theory in an *ad hoc* manner. In the following sections we address these issues in more detail.

4. Quantum mechanics in compactified Kaluza–Klein spaces

The topological structure of a physical system can determine the nature of an observable of a quantum system, such as angular momentum. In the case of a hydrogen-like atom, the non-trivial topological structure of the system can only be revealed when the electron is constrained to move in a plane, so that the fundamental homotopy group, $\pi_1(\mathbb{R}^2 \setminus \{0\})$, is non-trivial. This results in the angular momentum adopting half-integer values, since the wavefunction in this case is allowed to be multivalued. However, there remains the problem of how to incorporate topological constraints into the dynamics of the electron in three-dimensional space. One possible approach is to use path integral methods in multiply-connected spaces, where spin can be incorporated by specifying an appropriate space, e.g. $SO(3)$. In this manner, continuous classical mechanics, when defined and quantized, can provide a framework for incorporating spin [15, 16]. However, in the present work it is desired that the topological description should only involve spacetime structures. Consider the quantum mechanics of a generalized N -dimensional hydrogen atom whose bound-state spectrum is given by $E_n = -\mu e^4 / (2\hbar^2 [n + (N - 3)/2]^2)$. It is noted that for spaces of even dimensions the Bohr energy spectrum is retained only if the angular momentum adopts half-integer values. This energy spectrum is derived for a hydrogen atom in the simply-connected N -dimensional Euclidean space \mathbb{R}^N whose fundamental homotopy group is trivial, i.e. $\pi_1(\mathbb{R}^N) \cong \{0\}$. In the simply-connected Euclidean space \mathbb{R}^N , the wavefunction must be single-valued, and as a consequence, the angular momentum must be integer. However, for quantum mechanics in multiply-connected spaces, the Euclidean space \mathbb{R}^N may be considered as a universal covering space of some multiply-connected space in which a wavefunction of the Schrödinger equation can be multivalued. It is known that the Euclidean space \mathbb{R}^N is a universal covering space of the space $\mathbb{R}^{N-1} \times S^1$ [6, 8]. The space $\mathbb{R}^{N-1} \times S^1$ has a non-trivial topological structure because its fundamental homotopy group is isomorphic to \mathbb{Z} , i.e. $\pi_1(\mathbb{R}^{N-1} \times S^1) \cong \pi_1(\mathbb{R}^{N-1}) \oplus \pi_1(S^1) \cong \{0\} \oplus \mathbb{Z} \cong \mathbb{Z}$. The multiply-connected space $\mathbb{R}^{N-1} \times S^1$ has the structure of a Kaluza–Klein space, because, according to modern perspectives a Kaluza–Klein space is not considered as an M^N manifold whose symmetries are the N -dimensional Poincaré symmetries, but rather a compactified manifold of the form $M^4 \times S^d$. Here M^4 is four-dimensional Minkowski spacetime and S^d is some compact manifold whose size is much smaller than any length that has ever been measured [17, 18]. In the following sections we consider nonrelativistic quantum mechanics in a compactified Kaluza–Klein space $\mathbb{R}^{N-1} \times S^1$ consisting of the direct product of an $(N - 1)$ -dimensional Euclidean space \mathbb{R}^{N-1} with the compact circle S^1 . We assume quantum mechanics is valid in these compactified spaces. The introduction of the compact circle makes it possible to incorporate spin into the nonrelativistic Schrödinger wave equation. Since the topological structure of the configuration space of a physical system depends on the dimension of the space of the system, we discuss two-, three- and four-dimensional compactified spaces separately.

4.1. Quantum mechanics in a two-dimensional space $\mathbb{R}^1 \times S^1$

Let us consider first the case of quantum mechanics in a two-dimensional Kaluza–Klein space $\mathbb{R}^1 \times S^1$, where the compact space S^1 is a circle of radius ρ and \mathbb{R}^1 is a one-dimensional Euclidean space. This space has the form of a cylinder of radius ρ embedded in the three-dimensional Euclidean space \mathbb{R}^3 . The time-independent Schrödinger wave equation for a free particle moving in this space can be written as

$$-\frac{\hbar^2}{2\mu} \left(\frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \right) \psi(z, \phi) = E\psi(z, \phi). \tag{19}$$

When the wavefunction is written in the separable form $\psi(z, \phi) = Z(z)\Phi(\phi)$, the above Schrödinger equation is reduced to the following system of differential equations

$$\frac{d^2\Phi}{d\phi^2} + s^2\Phi = 0 \tag{20}$$

$$\frac{\hbar^2}{2\mu} \frac{d^2Z}{dz^2} + \left(E - \frac{\hbar^2 s^2}{2\mu\rho^2} \right) Z = 0 \tag{21}$$

where the quantity s may be identified with the angular momentum of the system. The solution for function Φ is of the form $\Phi(\phi) = \exp(is\phi)$. In order to obtain non-trivial solutions, the energy of the particle must satisfy the condition $E \geq s^2\hbar^2/2\mu\rho^2$. In this case, the solution is of the form $Z(z) = \exp(ikz)$, where k is a real number defined via the relation

$$E = \left(k^2 + \frac{s^2}{\rho^2} \right) \frac{\hbar^2}{2\mu}. \tag{22}$$

It is interesting to note that free particles in this compactified Kaluza–Klein space can possess an angular momentum s which can adopt half-integer values, since the space $\mathbb{R}^1 \times S^1$ is multiply-connected. This result allows an interpretation of the spin of a particle as a manifestation of the topological structure of spacetime at the quantum level. It is also noted that the ground-state energy $E = s^2\hbar^2/2\mu\rho^2$ of a free particle in this space is very large if the size of the compact space S^1 is very small. However, if the size of the compact space is not measurable then this energy is unobservable because it is associated only with the compact space.

Now consider a particle under the influence of a Coulomb-like potential which depends only on distance. Let the nucleus of positive charge e of a hydrogen-like atom be at the origin of the space $\mathbb{R}^1 \times S^1$; the distance from the nucleus to the atomic electron is $r = \sqrt{z^2 + (\rho\phi)^2}$. In this case the Schrödinger equation takes the form

$$-\frac{\hbar^2}{2\mu} \left(\frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \right) \psi - \frac{e^2}{r} \psi = E\psi. \tag{23}$$

We assume that the size of the compact manifold is small so that the condition $\rho \ll z$ can be imposed. This allows us to expand the Coulomb potential and use perturbation theory to calculate the first-order correction to the energy spectrum. Consider the electron confined to the region $z > 0$, which is equivalent to a potential of the form [12]

$$V(z) = \begin{cases} -\frac{e^2}{z} + \frac{e^2\rho^2\phi^2}{2r^3} - \frac{3e^2\rho^4\phi^4}{8r^5} + \dots & \text{for } z > 0 \\ +\infty & \text{for } z \leq 0. \end{cases} \tag{24}$$

The terms involving $\rho\phi$ are treated as a perturbation. The unperturbed Schrödinger equation takes the form

$$\frac{d^2\Phi}{d\phi^2} + s^2\Phi = 0 \quad (25)$$

$$\frac{\hbar^2}{2\mu} \frac{d^2Z}{dz^2} + \left[\frac{e^2}{z} + \left(E - \frac{\hbar^2 s^2}{2\mu\rho^2} \right) \right] Z = 0. \quad (26)$$

The solution to equation (25) is $\Phi(\phi) = \exp(is\phi)$. On the other hand, equation (26) represents the time-independent Schrödinger equation for a one-dimensional hydrogen atom. The solution is given by

$$\psi_n(z) = \left[\frac{(n-1)!}{2n(n!)^3} \right]^{1/2} e^{-u/2} u L_n^1(u) \quad (27)$$

where $L_n^1(u)$ is the associated Laguerre polynomial and $u = 2\mu e^2 z / \hbar^2 n$. The bound-state energy spectrum in this case is given by

$$E_n = -\frac{\mu e^4}{2\hbar^2 n^2} + \frac{\hbar^2 s^2}{2\mu\rho^2}. \quad (28)$$

It is seen that the energy levels are shifted by the amount $\hbar^2 s^2 / 2\mu\rho^2$ which is identical to that predicted by equation (22), so the hydrogen atom in the compactified Kaluza–Klein space $\mathbb{R}^1 \times S^1$ has the same energy spectrum as that of a hydrogen atom in a one-dimensional Euclidean space. However, if the length of the compact manifold S^1 is measurable then the energy levels would be different, because in such a situation the condition $\rho \ll z$ could not be imposed. In that case it would be possible to detect the difference by a measurement of the frequency spectrum. Perturbative corrections to the energy spectrum can be calculated using the generating function for Laguerre polynomials. In this case the generating function is [19, 21]

$$-t \exp\left(-\frac{ut}{1-t}\right) = (1-t)^2 \sum_{n=1}^{\infty} \frac{L_n^1(u)}{n!} t^n. \quad (29)$$

The first-order correction, ΔE_n , using the term $e^2 \rho^2 \phi^2 / (2r^3)$ as a perturbation, is given by

$$\begin{aligned} \Delta E_n &= \int_0^{2\pi} \int_{z>0}^{\infty} \psi_{ns}^*(z, \phi) \left(\frac{e^2 \rho^2}{2z^3} \right) \psi_{ns}(z, \phi) dz d\phi \\ &= \frac{\mu^2 e^6 \rho^2 (n-1)!}{\hbar^4 n^3 (n!)^3} \int_{u>0}^{\infty} e^{-u} u^{-1} [L_n^1(u)]^2 du \\ &= \frac{\mu^2 e^6 \rho^2 \phi^2}{\hbar^4 n^2} Ei(u) \end{aligned} \quad (30)$$

where $Ei(u)$ is the exponential-integral defined by

$$Ei(u) = \int_{u>0}^{\infty} \frac{e^{-y}}{y} dy. \quad (31)$$

This result shows that perturbative corrections to the unperturbed energy spectrum can only be carried out for $z > 0$. If the hydrogen atom in this case is measurable only for $z \gg \rho$, then the correction term is negligible. Higher order perturbative terms can also be calculated and in general they depend on the quantum number n and integrals of the form $\int_{u>0}^{\infty} e^{-y} y^{-2k-1} dy$, where $k = 1, 2, \dots$

4.2. Quantum mechanics in a three-dimensional space $\mathbb{R}^2 \times S^1$

The time-independent Schrödinger equation for a free particle in a three-dimensional compactified Kaluza–Klein space $\mathbb{R}^2 \times S^1$ can be written in the form

$$-\frac{\hbar^2}{2\mu} \left(\nabla^2 + \frac{1}{\rho^2} \frac{\partial^2}{\partial \Omega^2} \right) \psi = E \psi \tag{32}$$

where ρ is the radius of the compact circle S^1 parametrized by the angle Ω , and ∇^2 is the Laplacian in two-dimensional Euclidean space. If the two-dimensional wavefunction ψ is written in the form $\psi = \omega(\Omega)\Phi(\phi)\mathcal{R}(r)$, where (r, ϕ) are the polar coordinates in the space \mathbb{R}^2 , then the above Schrödinger equation reduces to the system of equations

$$\frac{d^2\omega}{d\Omega^2} + s^2\omega = 0 \tag{33}$$

$$\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0 \tag{34}$$

$$\frac{d^2\mathcal{R}}{dr^2} + \frac{1}{r} \frac{d\mathcal{R}}{dr} - \frac{m^2}{r^2} \mathcal{R} + \frac{2\mu}{\hbar^2} \left(E - \frac{\hbar^2 s^2}{2\mu\rho^2} \right) \mathcal{R} = 0. \tag{35}$$

It is seen that a free particle moving in a three-dimensional compactified Kaluza–Klein space $\mathbb{R}^2 \times S^1$ possesses an angular momentum s associated with the third compactified dimension, in addition to the angular momentum associated with two-dimensional Euclidean space. An important feature of this extra angular momentum is that it can take on half-integer values, because the configuration space is multiply-connected and so multivalued wavefunctions are allowed. On the other hand, although the solution for the function Φ is of the form $\Phi(\phi) = \exp(im\phi)$, the angular momentum m can only adopt integer values, since in this case the quantity m is associated with the simply-connected Euclidean space \mathbb{R}^2 . To reiterate, the quantum dynamics of an electron in a hydrogen atom whose configuration space is $(\mathbb{R} \setminus \{0\}) \times S^1$ allows for the angular momentum m to have half-integer values. The Schrödinger equation for the stationary states of an hydrogen atom in a three-dimensional compactified Kaluza–Klein space, $\mathbb{R}^2 \times S^1$, is

$$-\frac{\hbar^2}{2\mu} \left(\nabla^2 + \frac{1}{\rho^2} \frac{\partial^2}{\partial \Omega^2} \right) \psi - \frac{e^2}{r_3} \psi = E \psi \tag{36}$$

where $r_3 = \sqrt{r^2 + \rho^2\Omega^2}$, with $r = \sqrt{x^2 + y^2}$. As in the case of a hydrogen atom in a two-dimensional compactified Kaluza–Klein space, $\mathbb{R}^2 \times S^1$, the condition $\rho \ll r$ can be imposed, since the size of the compact space is assumed to be small. The potential can be expanded as a binomial series and terms (other than e^2/r) may be regarded as a perturbation. The energy corrections are calculated using the Laguerre polynomials. Since the calculation is similar to that carried out in the next section, we postpone a discussion until later. The unperturbed Schrödinger equation for the hydrogen atom reduces to the system of differential equations

$$\frac{d^2\omega}{d\Omega^2} + s^2\omega = 0 \tag{37}$$

$$\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0 \tag{38}$$

$$\frac{d^2\mathcal{R}}{dr^2} + \frac{1}{r} \frac{d\mathcal{R}}{dr} - \frac{m^2}{r^2} \mathcal{R} + \frac{2\mu}{\hbar^2} \left(\frac{e^2}{r} + E - \frac{\hbar^2 s^2}{2\mu\rho^2} \right) \mathcal{R} = 0. \tag{39}$$

The quantities s and m can take half-integer values, since both are associated with multiply-connected spaces. The fundamental homotopy group of the space $\mathbb{R}^2 \setminus \{0\}$ is isomorphic to $\pi_1(S^1)$, and the fundamental homotopy group of the space $(\mathbb{R}^2 \setminus \{0\}) \times S^1$ is isomorphic to the fundamental homotopy group of the space $S^1 \times S^1$, which is just the two-dimensional torus T^2 , i.e. $\pi_1((\mathbb{R}^2 \setminus \{0\}) \times S^1) \cong \pi_1(S^1 \times S^1) \cong \pi_1(S^1) \oplus \pi_1(S^1) \cong \mathbb{Z} \oplus \mathbb{Z}$. Therefore, the fundamental group $\pi_1((\mathbb{R}^2 \setminus \{0\}) \times S^1)$ has a unitary representation $a: \pi_1((\mathbb{R}^2 \setminus \{0\}) \times S^1) \rightarrow U(1) \times U(1)$ defined by the characters $a(n, m) = \exp(in\pi) \exp(im\pi)$, where $n, m \in \mathbb{Z}$. It is seen that the use of multivalued wavefunctions in this case is permitted, since the multivalued wavefunctions are determined by the characters of the fundamental homotopy group of the configuration space.

For a comparison, let us consider quantum mechanics constructed on a multiply-connected configuration space whose fundamental homotopy group is nonabelian; such an example is that of the planar hydrogen molecular ion H_2^+ , with the assumption that the electron of the system can not penetrate either nucleus. The general multiply-connected configuration space of this kind has the form $\mathbb{R}^2 \setminus \{x_1, \dots, x_n\}$, where x_1, \dots, x_n are n distinct points in the plane \mathbb{R}^2 . The fundamental homotopy group π_1 of the space $\mathbb{R}^2 \setminus \{x_1, \dots, x_n\}$ is an infinite nonabelian group for $n \geq 2$. This is a free group of n generators which can be constructed by the homotopy classes $[\gamma_i]$ of closed curves γ_i each of which encloses the corresponding point x_i but none of the remaining points. However, the generators are not determined uniquely, and when specified, they give rise to a representation of the group. Hence, the fundamental homotopy group of the configuration space of the hydrogen molecular ion H_2^+ has two generators which can be identified with two independent loops. It is known that all higher homotopy groups of $\mathbb{R}^2 \setminus \{x_1, \dots, x_n\}$ vanish [8, 9]. However, in the case where the atomic electron of the hydrogen molecular ion, H_2^+ , is not constrained to the two-dimensional plane $\mathbb{R}^2 \setminus \{x_1, \dots, x_n\}$, all loops are contractible; in other words, the configuration space of the system is simply-connected. In this case, the wavefunctions that describe the quantum electronic motion must be single-valued, and as a consequence, the angular momentum takes on integer values. Let the origin of the polar coordinates be at the midpoint of two nuclei which are separated by a distance d , then the Schrödinger equation for the stationary states of the electronic motion is written as

$$-\frac{\hbar^2}{2\mu} \nabla^2 \psi - \left(\frac{e^2}{r_1} + \frac{e^2}{r_2} - \frac{e^2}{d} \right) \psi = E\psi \quad (40)$$

where r_1 and r_2 are the position vectors of the electron with respect to the two protons of the molecule. Using elliptic coordinates (ξ, η, ϕ) , where ϕ is the azimuthal angle with the z -axis being the line joining the two protons, $\xi = (r_1 + r_2)/d$ and $\eta = (r_1 - r_2)/d$, the Laplacian operator expressed in terms of these coordinates takes the form [20, 21]

$$\nabla^2 = \frac{4}{d^2(\xi^2 - \eta^2)} \left\{ \frac{\partial}{\partial \xi} (\xi^2 - 1) \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} + \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2}{\partial \phi^2} \right\}. \quad (41)$$

When the wavefunction is written as a product $\psi = \Phi(\phi)F(\xi)G(\eta)$, the Schrödinger equation reduces to the system of equations, in atomic units $\mu = e = \hbar = a_0 = 1$,

$$\frac{d^2 \Phi}{d\phi^2} + m^2 \Phi = 0 \quad (42)$$

$$\frac{d}{d\xi} (\xi^2 - 1) \frac{dF}{d\xi} + \left(\frac{d^2}{2} \left(E - \frac{1}{d} \right) \xi^2 + 2d\xi - \frac{m^2}{\xi^2 - 1} + \lambda \right) F(\xi) = 0 \quad (43)$$

$$\frac{d}{d\eta} (1 - \eta^2) \frac{dG}{d\eta} - \left(\frac{d^2}{2} \left(E - \frac{1}{d} \right) \eta^2 + \frac{m^2}{1 - \eta^2} + \lambda \right) G(\eta) = 0 \quad (44)$$

where m and λ are separation constants. The solution to equation (42) is of the form $\Phi = \exp(im\phi)$ and in this case m must take integer values because the fundamental group of the configuration space vanishes.

4.3. Quantum mechanics in a four-dimensional space $\mathbb{R}^3 \times S^1$

The time-independent Schrödinger equation for a free particle in a four-dimensional compactified Kaluza–Klein space $\mathbb{R}^3 \times S^1$ can be written in the form

$$-\frac{\hbar^2}{2\mu} \left(\nabla^2 + \frac{1}{\rho^2} \frac{\partial^2}{\partial \Omega^2} \right) \psi_4 = E \psi_4 \tag{45}$$

where ρ is the radius of the compact circle S^1 parametrized by the angle Ω , and ∇^2 is the Laplacian in three-dimensional Euclidean space. If the four-dimensional wavefunction ψ_4 is written in the form $\psi_4 = \omega(\Omega)\psi(r, \theta, \phi)$, where (r, θ, ϕ) are the three-dimensional spherical coordinates, then the above Schrödinger equation reduces to the system of equations

$$\frac{d^2\omega}{d\Omega^2} + s^2\omega = 0 \tag{46}$$

$$\frac{\hbar^2}{2\mu} \nabla^2 \psi + k^2 \psi = 0 \tag{47}$$

where k is defined by $E = \hbar^2 k^2 / 2\mu - \hbar^2 s^2 / 2\mu \rho^2$. As in the case of a free particle in a three-dimensional compactified Kaluza–Klein space, $\mathbb{R}^2 \times S^1$, the Schrödinger equation gives rise to an angular momentum s which can take on half-integer values. The energy spectrum is also shifted by an amount $\hbar^2 s^2 / 2\mu \rho^2$. Therefore, free particle eigenfunctions in a four-dimensional compactified Kaluza–Klein space $\mathbb{R}^3 \times S^1$ can be classified by the continuous energy eigenvalues E and three discrete indices s , l and m , where the quantum numbers l and m result from the three-dimensional free-particle solutions $\psi_{Elm}(\mathbf{r}) = j_{El}(kr)Y_{lm}(\theta, \phi)$. Both of the quantum numbers l and m are integers since they are associated only with the simply-connected Euclidean space \mathbb{R}^3 .

The Schrödinger equation for the stationary states of an hydrogen atom in a four-dimensional compactified Kaluza–Klein space, $\mathbb{R}^3 \times S^1$ can be written in the form

$$-\frac{\hbar^2}{2\mu} \left(\nabla^2 + \frac{1}{\rho^2} \frac{\partial^2}{\partial \Omega^2} \right) \psi_4 - \frac{e^2}{r_4} \psi_4 = E \psi_4 \tag{48}$$

where $r_4 = \sqrt{r^2 + \rho^2 \Omega^2}$ with $r = \sqrt{x^2 + y^2 + z^2}$. As in the case of a hydrogen atom in a two-dimensional compactified Kaluza–Klein space, the condition $\rho \ll r$ is imposed, since the size of the compact space is assumed to be small. The potential is expanded in a binomial series as

$$V = \frac{e^2}{r} \left[1 - \frac{1}{2} \left(\frac{\rho\Omega}{r} \right)^2 + \frac{3}{8} \left(\frac{\rho\Omega}{r} \right)^4 - \frac{5}{16} \left(\frac{\rho\Omega}{r} \right)^6 + \dots \right]. \tag{49}$$

If the terms that contain the quantity $\rho\Omega$ are treated as a perturbation, then the unperturbed Schrödinger equation for the hydrogen atom reduces to the system of differential equations

$$\frac{d^2\omega}{d\Omega^2} + s^2\omega = 0 \tag{50}$$

$$\frac{\hbar^2}{2\mu} \left(\nabla^2 + \frac{e^2}{r} + k^2 \right) \psi = 0. \tag{51}$$

The behaviour of an hydrogen atom in a four-dimensional compactified Kaluza–Klein space is therefore identical to that of a hydrogen atom in three-dimensional Euclidean space, since the ground-state energy $\hbar^2 s^2 / 2\mu\rho^2$ is unobservable. However, unlike the situation in three-dimensional Euclidean space, the Schrödinger equation in a four-dimensional compactified Kaluza–Klein space gives rise to an angular momentum that can take on half-integer values, which hints at a possible topological origin of the spin of the electron. It should be emphasized again that the half-integer values of the angular momentum s are possible because the background space $\mathbb{R}^3 \times S^1$ is multiply-connected.

If the terms in the binomial series of the potential, that contain the quantity $\rho\Omega$, are treated perturbatively then their correction to the energy spectrum can be calculated from

$$\begin{aligned} \langle r^s \rangle_{nlm} &= \int \psi_{nlm}^*(\mathbf{r}) r^s \psi_{nlm}(\mathbf{r}) d\mathbf{r} \\ &= \int_0^\infty r^{2+s} |R_{nl}(r)|^2 dr \end{aligned} \quad (52)$$

where the radial wavefunctions $R_{nl}(r)$ are defined by

$$R_{nl}(r) = - \left\{ \left(\frac{2}{na_0} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right\}^{1/2} e^{-\rho/2} \rho^l L_{n+l}^{2l+1}(\rho) \quad (53)$$

with L_{n+l}^{2l+1} being the associated Laguerre polynomials and

$$\rho = \frac{2}{na_0} r \quad a_0 = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}. \quad (54)$$

Here a_0 denotes the Bohr radius and μ is the reduced mass of the system.

For the case $s = -1$ and $s = -2$, using a generating function for the associated Laguerre polynomials $L_q^p(\rho)$

$$\begin{aligned} G_p(\rho, s) &= \frac{(-s)^p \exp[-\rho s / (1-s)]}{(1-s)^{p+1}} \\ &= \sum_{q=p}^{\infty} \frac{L_q^p(\rho)}{q!} s^q \end{aligned} \quad (55)$$

it can be shown that [19, 21]

$$\left\langle \frac{1}{r} \right\rangle_{nlm} = \frac{1}{a_0 n^2} \quad (56)$$

$$\left\langle \frac{1}{r^2} \right\rangle_{nlm} = \frac{1}{a_0^2 n^3 (l + \frac{1}{2})}. \quad (57)$$

However for $s \leq -3$ the following recursion relation can be used [22]:

$$\frac{s+1}{n^2} \langle r^s \rangle - (2s+1)a_0 \langle r^{s-1} \rangle + \frac{s}{4} [(2l+1)^2 - s^2] a_0^2 \langle r^{s-2} \rangle = 0 \quad (58)$$

with the condition $s > -2l - 1$. In this case it is found, for example, that

$$\left\langle \frac{e^2 \rho^2 \Omega^2}{2} \frac{1}{r^3} \right\rangle_{nlm} = \frac{e^2 \rho^2 \Omega^2}{2a_0^3 n^3 l(l + \frac{1}{2})(l+1)}. \quad (59)$$

Because these corrections involve the quantity ρ , the above results show that the corrections only become significant when the compact dimension is measurable. When the size of the compact space is unmeasurable all energy corrections can be ignored and the hydrogen atom in this case behaves like a hydrogen atom in ordinary three-dimensional Euclidean space.

5. Conclusion

We have analysed quantum mechanics in multiply-connected spaces emphasizing the role which topology may play in determining the nature of a quantum observable. Based on the fact that the configuration space of physical systems, such as the planar hydrogen atom, is multiply-connected, it has been argued that the angular momentum of those physical systems can adopt half-integer values, which hints at a topological origin of the spin of the electron. In order to incorporate topological constraints into the dynamics of the electron in three-dimensional space we have considered nonrelativistic quantum mechanics in a compactified Kaluza–Klein space consisting of the direct product of an $(N - 1)$ -dimensional Euclidean space with the compact circle S^1 . The configuration space in this form, whose universal covering space is the simply-connected Euclidean space \mathbb{R}^N , allows the introduction of the intrinsic spin into the nonrelativistic Schrödinger wave equation in a simple manner. Furthermore, the hydrogen atom in the background space of compactified Kaluza–Klein space has an energy spectrum that differs from that in the background Euclidean space. If the size of the compactified space is unmeasurable then the two energy spectra are not distinguishable, which is shown by carrying out a simple perturbation calculation. However, this result does not exclude the possibility that spin is a manifestation of the compact dimension of the spacetime manifold.

Acknowledgments

We would like to thank the referees for their constructive comments. We would also like to thank C R Hagen for a private communication on the two-dimensional hydrogen atom and references related to this problem. One of us (VBH) acknowledges the financial support of an APA Research Award.

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