The restricted rotor: the effect of topology on quantum mechanics

1990 J. Phys. A: Math. Gen. 23 2939

(http://iopscience.iop.org/0305-4470/23/13/030)

J. Phys. A: Math. Gen. **23** (1990) 2939–2944. Printed in the UK

The restricted rotor: the effect of topology on quantum mechanics

Sami M Al-Jaber and Walter C Henneberger

Department of Physics and Molecular Science Program, Southern Illinois University, Carbondale, IL 62901, USA

Received 8 March 1990

Abstract. We consider the case of a limited rigid rotor, controlled by passive mechanical devices on a circle located at $\theta = 0$ and $\theta = \pi$. The devices have the effect of restricting the particle motion to the interval $(0, 3\pi)$. This system, which cannot be described by a Hamiltonian on $(0, 2\pi)$, is compared with a Hamiltonian system having delta function barriers at $\theta = 0$ and $\theta = \pi$. Many of the wavefunctions of the system having systematic reflections are the same as those of the Hamiltonian system with a reflection probability of $\frac{1}{4}$. Finally, the effect of a whisker of flux at the origin (Aharonov–Bohm effect) is discussed in the case of the non-Hamiltonian system.

1. The limited rigid rotor

Topological considerations are becoming increasingly important in the discussion of interference questions. This is true, in particular, for problems involving the Feynman path integral method [1, 2]. One obtains a solution of the Schrödinger equation on a covering space, as proposed long ago by Schulman [3]. There have been several discussions of applications of the path integral method to problems involving multiple paths around the origin [2, 4, 5].

The purpose of this work is to consider the consequences of a rather straightforward problem, for which the solution on the covering space can be written down. The path integral method necessarily yields the same solutions as those given here.

We consider a particle of mass m constrained to move on a ring of radius a, but limited to motion such that the coordinate θ lies between 0 and 3π. The ring is provided with a passive mechanical device permitting the particle to pass the points 0 and π only once, moving in a given direction, before being reflected. Such a device is simple to design. It may be considered part of the system, not connected with any observation. The motion of the wavepacket is then given by $\tilde{\psi}(\theta)$ on the covering space $(0, 3\pi)$. The Hamiltonian for the rigid rotor is

$$H = \frac{-h^2}{2ma^2}\frac{\partial^2}{\partial\theta^2} \tag{1.1}$$

and the stationary states corresponding to the vanishing of $\tilde{\psi}(\theta)$ at $\theta = 0$ and $\theta = 3\pi$ are

$$\tilde{\psi}(\theta) = A \sin\frac{N}{3}\theta \tag{1.2}$$

where N is a positive integer and A is a normalisation factor. The superposition principle then induces a solution $\psi(\theta)$ on the physical space $0 \leqslant \theta \leqslant 2\pi$ given by

$$\psi_N(\theta) = K_N \begin{cases} \sin \frac{N}{3}\theta + \sin \frac{N}{3}(\theta + 2\pi) & 0 < \theta < \pi \\ \sin \frac{N}{3}\theta & \pi < \theta < 2\pi. \end{cases} \tag{1.3}$$

The normalisation factor K_N that normalises $\psi(\theta)$ on $(0, 2\pi)$ is

$$K_N = \begin{cases} \sqrt{2}(5\pi)^{-1/2} & \text{for } N = \text{multiple of } 3 \\ \sqrt{2}\left(2\pi \pm \frac{3\sqrt{3}}{N}\right)^{-1/2} & \begin{array}{l} + \text{ for } N = 1 \bmod 3 \\ - \text{ for } N = 2 \bmod 3. \end{array} \end{cases} \tag{1.4}$$

2. The double delta function potential

In the limited rotor problem of section 1, the particle experiences infinite forces at $\theta = 0$ and $\theta = \pi$ according to a well defined rule. Since the forces are not random, the system is not, strictly speaking, a Hamiltonian one, although a Hamiltonian describes the motion in the covering space. Measurements are made in the space $0 < \theta < 2\pi$, unless definite information concerning the winding number is also given. In the absence of such information, one must superpose the wavefunction on $(0, \pi)$ with the wavefunction on $(2\pi, 3\pi)$. The reader may compare the result for double-slit diffraction with the case in which one has definite information concerning which slit the particle has passed through [6, 7].

In this section we consider the Hamiltonian system that most closely approximates the non-Hamiltonian one of the previous section.

We consider a particle of mass m moving in a double delta function potential defined on the interval $(-\pi, \pi)$ as

$$V(\theta) = V_0[\delta(\theta) + \delta(\theta - \pi)] \tag{2.1}$$

where V_0 is the strength of the potential. Symmetric solutions are

$$\psi(\theta) = A_q \begin{cases} \cos(q\theta + \delta_1) & 0 < \theta < \pi \\ \cos(q\theta + \delta_2) & -\pi < \theta < 0 \end{cases} \tag{2.2}$$

where A_q is a normalisation factor, q is a quantum number, and δ_1 and δ_2 are phase shifts. The conditions $\psi(\theta) = \psi(-\theta)$ and $\psi(0^+) = \psi(0^-)$ give $\delta_2 = -\delta_1$, so if we let $\delta = \delta_1 = -\delta_2$, then

$$\psi(\theta) = A_q \begin{cases} \cos(q\theta + \delta) & 0 < \theta < \pi \\ \cos(q\theta - \delta) & -\pi < \theta < 0. \end{cases} \tag{2.3}$$

The time-independent Schrödinger equation for this problem is

$$\left[\frac{-\hbar^2}{2ma^2}\frac{\partial^2}{\partial\theta^2} + V_0(\delta(\theta) + \delta(\theta - \pi))\right]\psi(\theta) = E\psi(\theta). \tag{2.4}$$

Integrating both sides of (2.4) from $-\varepsilon$ to $+\varepsilon$, where ε is infinitesimal, we find

$$\tan \delta = -\frac{c}{q} \tag{2.5}$$

with $c = mV_0a^2/\hbar^2$.

To find the allowed values of q, we integrate (2.4) from π^- to π^+ and use (2.5) to get

$$\cot(q\pi) = \frac{q2 - c^2}{2cq}. \tag{2.6}$$

The normalisation factor A_q in (2.2) is given by

$$A_q = \sqrt{2}\left[2\pi + \frac{1}{q}(\sin 2(q\pi + \delta) - \sin 2\delta)\right]^{-1/2}. \tag{2.7}$$

We define the reflection coefficient of the delta potential in the usual way. A plane wave incident on one side of the potential will be partially reflected and partially transmitted. In the incident region

$$\psi_{\mathrm{I}} = \mathrm{e}^{\mathrm{i}q\theta} + D\,\mathrm{e}^{-\mathrm{i}q\theta}$$

and in the transmitted region

$$\psi_{\mathrm{II}} = B\,\mathrm{e}^{\mathrm{i}q\theta}.$$

Matching the boundary conditions

$$\psi_{\mathrm{I}}(0) = \psi_{\mathrm{II}}(0) \qquad \text{and} \qquad \left.\frac{\partial \psi_{\mathrm{II}}}{\partial \theta}\right|_{\theta=0} - \left.\frac{\partial \psi_{\mathrm{I}}}{\partial \theta}\right|_{\theta=0} = \frac{2ma^2 V_0}{\hbar^2}\psi(0)$$

gives $D = -\mathrm{i}c/(q - \mathrm{i}c)$, where $C = mV_0 a^2/\hbar^2$. The reflection coefficient is $R = |D|^2$; therefore

$$R = \frac{c^2}{q^2 + c^2}. \tag{2.8}$$

If we define $\lambda > 1$ such that $R = 1/\lambda$ then from (2.8)

$$q = \pm c\sqrt{\lambda - 1} \tag{2.9}$$

and (2.5) and (2.6) yield

$$\tan\delta = \mp\frac{1}{\sqrt{\lambda - 1}} \tag{2.10}$$

and

$$q = \mp\frac{1}{\pi}\tan^{-1}\left(\frac{2\sqrt{\lambda - 1}}{\lambda - 2}\right) + n. \tag{2.11}$$

Since q is an angular momentum eigenvalue, the $-q$ is also, because of the symmetry of the problem. We therefore need to consider only positive q. Hence, in (2.11), n is a non-negative integer for the + sign and a positive integer for the − sign. Note that, for a given λ, each value of q corresponds to a different Hamiltonian since $H = H(V_0)$. Hence, the symmetric solutions in (2.3) become

$$\psi(\theta) = \frac{A_n}{\sqrt{\lambda}}\begin{cases}\sqrt{\lambda - 1}\cos(q\theta) \mp \sin(q\theta) & 0 < \theta > \pi \\ \sqrt{\lambda - 1}\cos(q\theta) \mp \sin(q\theta) & -\pi < \theta < 0\end{cases} \tag{2.12}$$

where the lower sign corresponds to negative δ and the upper sign corresponds to positive δ.

To find $\psi(\theta)$ on the $(0, 2\pi)$ space, we map $\psi(\theta)$ on the $(-\pi, 0)$ space to the $(\pi, 2\pi)$ space by letting $\theta \to 2\pi - \theta$. Therefore;

$$\psi(\theta) = \frac{An}{\sqrt{\lambda}} \begin{cases} \sqrt{\lambda - 1}\cos(q\theta) \mp \sin(q\theta) & 0 < \theta < \pi \\ \sqrt{\lambda - 1}\cos q(2\pi - \theta) \pm \sin q(2\pi - \theta) & \pi < \theta < 2\pi. \end{cases} \tag{2.13}$$

We wish to compare the result of (2.13) with the result of section 1. One might argue that the appropriate reflection coefficient R should be $\frac{1}{4}$. Consider the device that allows the particle to pass the point $\theta = 0$. The device always allows the particle to pass in the counter-clockwise direction. When the particle approaches $\theta = 0$ in the clockwise direction, it is reflected half the time. We therefore expect that the Hamiltonian system that approximates the non-Hamiltonian one of section 1 has barriers at $\theta = 0$ and $\theta = \pi$ that give a reflection coefficient of $R = \frac{1}{4}$. This implies that $\lambda = 4$ in (2.13).

Substitute $\lambda = 4$ in equations (2.7) and (2.11) to yield

$$q = n \mp \tfrac{1}{3} \tag{2.14}$$

and

$$A_n = \sqrt{2}\left(2\pi \mp \frac{\sqrt{3}}{n \mp \frac{1}{3}}\right)^{-1/2}. \tag{2.15}$$

Therefore, the symmetric stationary states become

$$\psi(\theta) = \frac{A_n}{2} \begin{cases} \sqrt{3}\cos(n \mp \frac{1}{3})\theta \mp \sin(n \mp \frac{1}{3})\theta & 0 < \theta < \pi \\ \sqrt{3}\cos[(n \mp \frac{1}{3})(2\pi \mp \theta)] \pm \sin[(n \mp \frac{1}{3})(2\pi \mp \theta)] & \pi < \theta < 2\pi \end{cases} \tag{2.16}$$

where the lower sign corresponds to negative δ and the upper sign corresponds to positive δ.

It is interesting to compare (2.15) and (2.16) with (1.3) and (1.4) of the previous section. If we set $N = 3n \mp 1$ in equations (2.15) and (2.16), we get

$$A_N = \sqrt{2}\left(2\pi \mp \frac{3\sqrt{3}}{N}\right)^{-1/2} \tag{2.17}$$

and, with some algebraic manipulation,

$$\psi_N(\theta) = \mp A_N \begin{cases} \sin\frac{N}{3}\theta + \sin\frac{N}{3}(\theta + 2\pi) & 0 < \theta < \pi \\ \sin\frac{N}{3}\theta & \pi < \theta < 2\pi. \end{cases} \tag{2.18}$$

It is remarkable that the delta function system gives exactly the same wavefunctions as the non-Hamiltonian case. In this section, the reflection coefficient is energy dependent, while in section 1 it is not. The equivalence found here is valid only for a barrier strength appropriate to the particle energy. We note that, for any barrier height, the wavefunctions for which N is a multiple of 3 have the same functional form in the Hamiltonian case as in the non-Hamiltonian one. However, the amplitudes are different on different sides of the barrier in the non-Hamiltonian case.

3. The Aharonov–Bohm effect

It is a natural extension of the considerations of section 1 to consider (1.1) modified

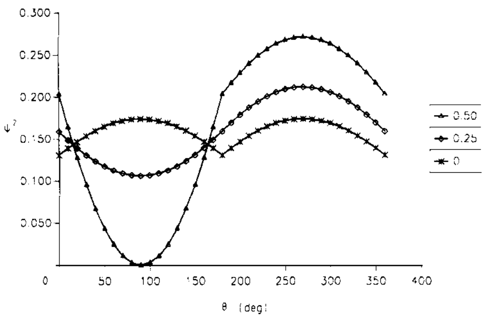

Figure 1. ψ^2 plotted against θ: $N = 1$, $M = 3$.

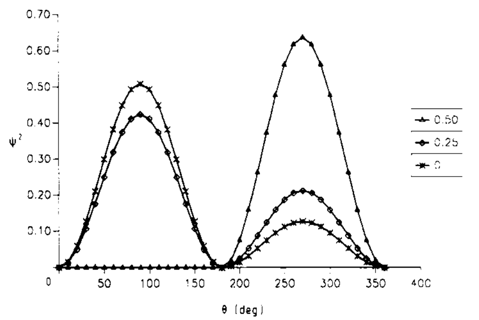

Figure 2. ψ^2 plotted against θ: $N = 3$, $M = 3$.

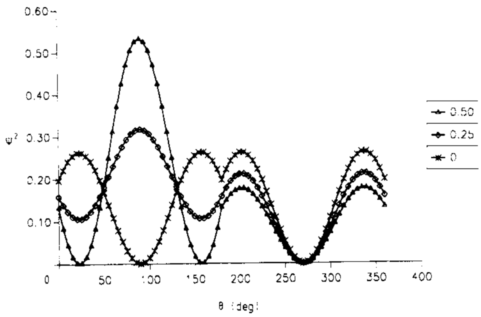

Figure 3. ψ^2 plotted against θ: $N = 4$, $M = 3$.

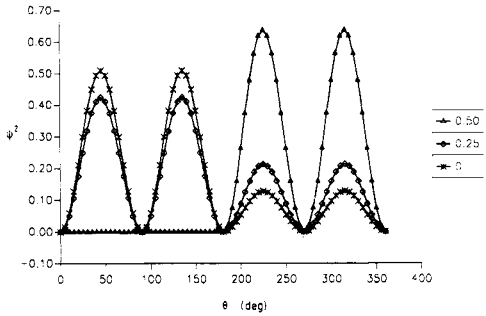

Figure 4. ψ^2 plotted against θ: $N = 6$, $M = 3$.

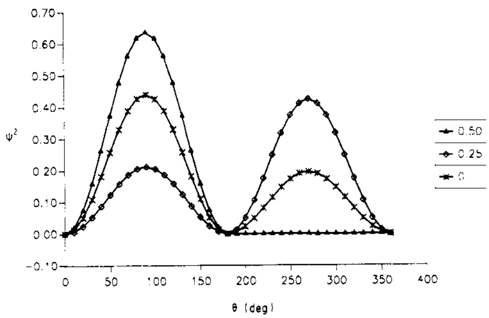

Figure 5. ψ^2 plotted against θ: $N = 5$, $M = 5$.

by a vector potential

$$A(r, \theta) = \hat{\theta} \frac{\Phi}{2\pi r}. \tag{3.1}$$

If, using Aharonov and Bohm [8], we define $\alpha = -e\Phi / ch$, where Φ is the flux contained in a whisker along the z axis and h is Planck's constant, then the minimal coupling leads to

$$\frac{-\hbar^2}{2ma^2} \left(\frac{\partial}{\partial \theta} + \mathrm{i}\alpha \right)^2 \tilde{\psi}(\theta) = E\tilde{\psi}(\theta) \tag{3.2}$$

for stationary states. The solutions of (3.2) are well known [9] to be $\tilde{\psi}(\theta) = \tilde{\psi}_0(\theta)\, \mathrm{e}^{-\mathrm{i}\alpha\theta}$, where $\tilde{\psi}_0(\theta)$ is the solution corresponding to zero flux. The $\tilde{\psi}_N(\theta)$ defined on $(0, 2\pi)$

have a flux-dependent norm. These functions differ considerably from the zero flux solutions, and in some cases are localised in the interval $(\pi, 2\pi)$ by the flux. Examples of the effect of flux, and of the 'Aharonov–Bohm localisation' are given in figures 1–5. It is straightforward to generalise the theory to the case of $\tilde{\psi}(\theta)$ limited to the interval $(0, M\pi)$. In all figures, M is the multiple of π through which the particle travels before it is reflected, N is the quantum number, and the curves are for different values of the parameter $\alpha = 0$ (*), 0.25 (◇), 0.50 (△). So, for the general case:

$$\tilde{\psi}(\theta) = A_M \sin\frac{N}{M}\theta\, \mathrm{e}^{-\mathrm{i}\alpha\theta}. \tag{3.3}$$

4. Discussion

The limited rigid rotor and the double delta function potential discussed here are one-dimensional problems. In these, and similar problems, the wavefunction overlaps itself in the physical space, with contributions coming from different winding numbers. In the case of the limited rigid rotor, the wavefunction in the $(0, 2\pi)$ physical space is determined by the wavefunctions on the $(0, 3\pi)$ space. We find that the 1 mod 3 and the 2 mod 3 quantum states of the limited rigid rotor coincide with the symmetric solutions of the double delta function potential when the reflection coefficient of the potential is $\frac{1}{4}$.

A magnetic flux along the z axis has no other effect on the wavefunction in the covering space than to modify it by a phase factor. However, the wavefunction is profoundly affected by the flux on the physical space $(0, 2\pi)$. The wavefunction on the physical space must be used to predict the outcome of a position measurement in the absence of information concerning the winding number. If the winding number is known with certainty, the flux-dependent phase factor has no observable consequences. Again, the reader may compare the double-slit diffraction with and without information concerning which slit the particle has passed through.

The flux-dependent results are illustrated in figures 1–5; in particular, figures 2, 4 and 5 show Aharonov–Bohm localisation in the case $\alpha = 0.5$. In all figures, N is the quantum number of (2.2) and M defines the domain of the covering space $0 \leqslant \theta \leqslant M\pi$.

References

[1] Feynman R P 1948 *Rev. Mod. Phys.* **20** 267
[2] Ohnuki Y 1987 *Proc. 2nd Int. Symp. on Foundations of Quantum Mechanics* (Tokyo: Physical Society of Japan) p 117
[3] Schulman L S 1971 *J. Math. Phys.* **12** 304
[4] Inomata A 1987 *Proc. 2nd Int. Symp. on Foundations of Quantum Mechanics* (Tokyo: Physical Society of Japan) p 127
[5] Gerry C C and Inomata A 1986 *Fundamental Questions in Quantum Mechanics* ed L M Roth and A Inomato (New York: Gordon and Breach) p 199
[6] Feynman R P 1965 *Feynman Lectures on Physics V* vol 3 (Reading, MA: Addison-Wesley) 3rd edn pp 1–3
[7] Henneberger W C and Zitter R N 1983 *Am. J. Phys.* **51** 464
[8] Aharonov Y and Bohm D 1959 *Phys. Rev.* **115** 485
[9] Dirac P A M 1931 *Proc. R. Soc.* A **133** 60