An extension of the particle in a one dimensional box model

Cristiano C. Bastos[1], Gerson S. Paiva[2], Eduardo S. G. Leandro[3], and Antonio C. Pavão[1]

[1]Departamento de Química Fundamental
Universidade Federal de Pernambuco
Recife 50670-901, Brazil.

[2]Centro Brasileiro de Pesquisas Físicas
Rio de Janeiro 22290-180, Brazil

[3]Departamento de Matemática
Universidade Federal de Pernambuco
Recife 50740-540, Brazil

(*Submitted* Dec 2012)

Abstract

Under the hypotheses commonly employed in textbooks, we calculated the spectrum of a particle in a one-dimensional regular curve embedded in 2D with a general smooth parameterization x = g(*t*) and y = h(*t*), where t is the curve parameter. The solution of the one-dimensional Schrödinger equation under the confined boundary conditions corresponding to our generalized particle in a box model shows that the linear box has the same energy spectrum as parabolas, cubics, exponentials, or any other open regular curves: $E = h^2n^2/8mL^2$, whereas the circular box has the same energy spectrum as ellipses, ovals, or any other closed regular curves: $E = h^2n^2/2mL^2$. There are many studies of quantum mechanics on curves using different theoretical approaches, however the present elementary approach and its conclusions are not found in the literature. We observe that the Schrödinger equation does not make sense when applied to spaces that are not manifolds.

1. The particle in a box problem

The particle in a box model (PIB model) is one of the most fundamental and versatile tools in the history of quantum mechanics [1-5]. Since Erwin Schrödinger's pioneering paper published in 1926 [1], the PIB model has emerged in a number of studies on diverse subjects such as: the spectrum of solids, the electronic absorption spectrum, nuclei, specific heat, optical rotation, NMR, PIB in the presence of an electric field, and the particle in a ring system. But the PIB model *is not so simple*, as evidenced by its applications in quantum mechanics propagators, Feynman path integrals, quark confinement and the Casimir effect, delta potential, two particles in two boxes, minimum Planck length, the PIB relativistic model, D-dimensional PIB, and quantum dots in nanotechnology [3-13]. In light of these different approaches, it is worth asking: how is the energy spectrum of the particle modified as a result of changes in the geometry of the curve? The answer to this question, that we were not able to find in the chemistry and physics literatures [9-15], could help to further expand the applicability of the PIB model. Let us start with the circular box problem (rotator with fixed axis), which was first solved by Schrödinger [1] using the eigenvalue equation:

$$H\Psi(\phi) = -\frac{\hbar^2}{2mr^2}\frac{d^2}{d\phi^2}\Psi(\phi) = E\Psi(\phi) \qquad (1)$$

where m is the rest-mass of the particle and r is the circumference radius. Using the boundary condition for the wave function $\Psi(\phi) = \Psi(\phi+2\pi)$, the particle energy is $E = (h^2n^2/2mL^2)$, where $L = 2\pi r$ is the length of the one-dimensional box [1,5,6]. The PIB model has since spread to classrooms and textbooks, and it has been revisited, directly or indirectly, in scientific and didactic papers [1-13]. As a result, the PIB model is now considered one of the fundamental problems in quantum mechanics. In this paper, we provide an extended PIB model taking into account a box with a smooth shape in order to calculate the spectrum of a particle in any one-dimensional regular curve embedded in 2D. We found two expressions for the energy spectrum: $E = h^2n^2/8mL^2$ for open curves and $E = h^2n^2/2mL^2$ for closed curves. This means that, once fixed the length, the linear box has the same energy spectrum as parabolas, cubics, exponentials or any other open regular curves. Also, the circular box has the same energy spectrum as ellipses, ovals, or any other closed regular curves possessing the same length.

2. The one-dimensional Laplacian operator

Let us consider the following parametrization of a smooth regular curve x = g(*t*) and y = h(*t*), where *t* is the parameter (*t* is not the time).

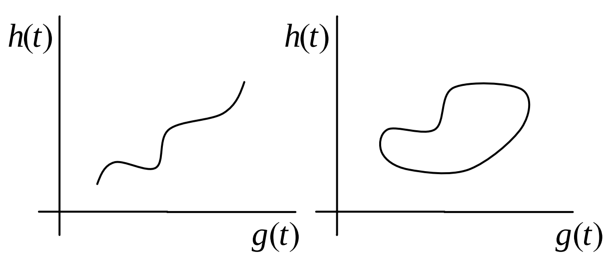

Figure 1. Open and closed regular curves.

We recall that a smooth curve is said to be regular if its velocity vector, α`(t) = (g`(t), h`(t)), is nowhere vanishing. Taking into account this parameterization, we obtain the one-dimensional Laplacian operator (Laplace-Beltrami) on the curve and rewrite it in the arc-length variable *s*:

$$\nabla^2 = g^{-1/2}\frac{\partial}{\partial q^i}\left(g^{1/2}g^{ik}\frac{\partial}{\partial q^k}\right) = g^{-1/2}\frac{d}{dt}\left(g^{-1/2}\frac{d}{dt}\right).$$

Since:

$$g^{1/2} = g_{11}{}^{1/2} = \sqrt{\left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2} = \frac{ds}{dt},$$

it follows that:

$$\nabla^2 = \frac{d^2}{ds^2}. \qquad (2)$$

Using expression 2., note that in the original case of equation 1. (using t as angle) we have x = r cost and y = r sint and find the Laplacian operator $\nabla^2 = d^2/dx^2 + d^2/dy^2 = (1/r^2)d^2/dt^2$ (the arc length depends on the angle and the radius).

Using the Laplacian operator 2., the Schrödinger equation 1. turns out to be in the well known case:

$$\frac{d^2}{ds^2}\Psi(s) = -\frac{2mE}{\hbar^2}\Psi(s) \qquad (3)$$

This is the usual one-dimensional harmonic oscillator equation, and from this point on the discussion of eigenvalues and eigenfunction follows the traditional steps. We can now solve the PIB model by using equation 3. and considering the two possible cases of boundary conditions. For the open curve (linear or not), the boundary conditions are $\Psi(s_o) = \Psi(s_1) = 0$, which are similar to those of the linear box [4]; for the closed curve, the boundary conditions are $\Psi(s_o) = \Psi(s_1)$ (univalued periodic wave function condition), which are similar to those of the circular box [1].

The general solution of 3. is $\Psi(s) = A\sin(ks) + B\cos(ks)$, with A and B real constants. The parameter k relates to the energy as follows:

$$k^2 = \frac{2mE}{\hbar^2}$$

The arc length relates to the box length L as indicated by the equation:

$$L = \int_{t_o}^{t_1} \sqrt{\left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2}\, dt = s(t_1) - s(t_o) \equiv s_1 - s_o$$

Using this result for the open curve, with the usual assumption $s_o = 0$, and the boundary condition requires $\Psi(s_o) = \Psi(s_1) = 0$, then $A\sin(ks_o) = A\sin(ks_1) = 0$, $ks_o = m\pi$ and, from the periodicity of the sine function, $ks_1 = m\pi + n\pi$, $ks_1 - ks_o = k(s_1 - s_o) = kL = n\pi$, where n is a natural number. In order to find a final expression for the energy, we have:

$$k^2 = \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$$

$$E = \frac{h^2 n^2}{8mL^2} \tag{4}$$

This relation describes the energy spectrum of any regular open curve, such as straight lines, parabolas, hyperbolas, cubics, sinusoidal curves, etc.

For a closed curve, let s_o be the initial arc length and let s_1 be the arc length after one turn around the curve $L = s_1 - s_o$. In order to find an expression for the energy, we impose the boundary condition $\Psi(s_o) = A\sin(ks_o) + B\cos(ks_o) = \Psi(s_1) = A\sin(ks_1) + B\cos(ks_1)$ and the periodicity condition $\Psi(s_o) = \Psi(s_o+L)$; from the periodicity of the sine function, $ks_1 = ks_o + (2\pi n)$, then $k = (2\pi n)/L$, where n is an integer number, we deduce:

$$k^2 = \frac{2mE}{\hbar^2} = \frac{4\pi^2 n^2}{L^2}$$

$$E = \frac{h^2 n^2}{2mL^2} \tag{5}$$

Relation 5. describes the energy spectrum for the conventional circular box with length L, and, as evidenced above, it actually describes the energy spectrum of any regular closed curve, for example ellipses, ovals, smoothed polygons, etc. The two expressions 4. and 5. show that, for regular curves of the same length L, the energy spectrum can be used to distinguish between open and closed curves. For the same n, we have $E_{closed} = 4E_{open}$. As far as we know, this result is not found in the literature [1-13]. It represents an explicit general solution for the PIB model of regular curves under the usual hypotheses found in textbooks [2, 9-12].

3. Mathematical note

It is well known in differential topology [16] that a smooth curve which is a manifold (locally, at each point, it looks like a line segment) can only be diffeomorphic to either a line segment or a circle. In this paper, we show that the energy spectrum of a smooth, regular curve of a fixed length is determined by this topological classification; the topology (open or closed) of such a curve, whose length is known, suffices to determine its spectrum, and conversely, given the length of the curve, the energy spectrum determines the topology of the curve. Although this is a criterion which mixes topology and geometry, a purely topological criterion can be obtained by noticing that, for all closed regular curves, the eigenfunctions come in pairs, sine and cosine, and zero is also an admissible eigenvalue. These properties are not shared by open regular curves.

The problem of understanding the topology of a manifold from its spectrum is currently of interest in Mathematics. In that sense, a classical reference to this problem is the famous paper “Can you hear the shape of a drum?’’ by Mark Kac [17]. In this paper, we show that you can “hear the topology” of a 1D drum, provided you know its length. Notice that smooth curves with self-intersections are not manifolds in general and thus cannot be treated in the same way as regular embedded curves. The Schrödinger equation actually does not make sense when applied to spaces that are not manifolds since the Laplacian is no longer globally defined.

4. Conclusions

We used the corresponding Laplacian operator for a smooth curve with a general parameterization in the Schrödinger equation and found the eigenfunctions $\Psi(s) = A\sin(ks) + B\cos(ks)$, where s is the arc length parameter, and energy spectrum E given by only two possible expressions: $E = h^2n^2/8mL^2$ for open curves, and $E = h^2n^2/2mL^2$ for closed curves. This result is a new contribution to the literature on the PIB model spectrum calculation of a particle constrained to a one-dimensional regular curve embedded in a 2D surface.

Acknowledgements

This work was supported by the Brazilian agencies CNPq and CAPES.

References:

[1] E. Schrödinger, Ann. Phys. **79**, 13 (1926).
[2] L. Pauling, *Introduction to Quantum Mechanics*, (Mc Graw-Hill, New York, 1935).
[3] F. E. Cummings, Am. J. Phys. **45**, 158 (1977).
[4] K. Volkamer and M. J. Lerom, J. Chem. Educ. **69**, 100 (1992).
[5] A. J. Vicent, J. Chem Educ. **73**, 1001 (1996).
[6] N. Bera, J. Bhattacharjee, S. Mitra and S. Khastgir, Eur. Phys. J. D **46**,41 (2008).
[7] W. Li and S. Blinder, Chem. Phys. Lett. **496**, 339 (2010).
[8] J. Gravesen and M. Willatzen, Physica B **371**, 112 (2006).
[9] C. Cohen-Tanoudji, B. Diu, F. Laloë, *Quantum Mechanics*, (John Wiley & Sons, New York, 2005).
[10] S. Gasiorowicz, *Quantum Physics*, (John Wiley & Sons, Inc., 1974).
[11] J. Griffits, *Introduction to Quantum Mechanics*, (Pearson Prentice Hall, 2005).
[12] P. W. Atkins and R. Friedman. *Molecular Quantum Mechanics*, (Oxford University Press Inc., New York, 2005).
[13] E. Miliordos, Phys. Rev. A **82**, 062118-1 (2010).
[14] R. Froese and I. Herbst, Israel J. Math. **170**, 337 (2009).
[15] E. M. Harrell II and M. Loss, Math. Phys. **195**, 643 (1998).
[16] J. Milnor, *Topology from the Differential Viewpoint*, (Princeton University Press, Princeton, NJ, 1965).
[17] M. Kac, Am. Math. Monthly, **73**, 1 (1966).