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Quantum systems with time-dependent boundaries

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We present here a set of lecture notes on quantum systems with time-dependent boundaries. In particular, we analyze the dynamics of a non-relativistic particle in a bounded domain of physical space, when the boundaries are moving or changing. In all cases, unitarity is preserved and the change of boundaries does not introduce any decoherence in the system.

Keywords: Quantum boundary conditions; time-dependent Hamiltonians; product formulae.

Mathematics Subject Classification 2010: 81Q10, 46N50, 35J57

1. Introduction

We present here the notes of three lectures given by one of us at the International Workshop on Mathematical Structures in Quantum Physics, held in February 2014 in Bangalore at the Center for High Energy Physics, Indian Institute of Science. The course considers some aspects of quantum systems with time-dependent boundaries, a very active area both from the mathematical point of view, see for instance the works of Yajima [1, 2], Dell'Antonio *et al.* [3] and Posilicano *et al.* [4, 5], and from a physical perspective. Notable applications arise in different fields ranging from atoms in cavities [6, 7] to ions and atoms in magnetic traps [8], to superconducting quantum interference devices (SQUID) [9], to the dynamical Casimir effect

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2.1. *Hard walls*

Let us concentrate now on the textbook case of a particle confined in an infinitely deep well, Fig. 1. The appropriate boundary conditions are Dirichlet's: $\psi(a) = \psi(b) = 0$. The dynamics of the particle is described by the Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2}. \tag{17}$$

A separation of variables, $\psi(x,t) = u(x) \exp(-\mathrm{i}Et/\hbar)$, reduces the problem to the solution of the spatial part of the differential equation, that means to find eigenvectors and eigenvalues of the operator T:

$$-\frac{\hbar^2}{2m} u''(x) = E\, u(x). \tag{18}$$

The general solution is

$$u(x) = c_1\, \mathrm{e}^{+\mathrm{i}kx} + c_2\, \mathrm{e}^{-\mathrm{i}kx}, \tag{19}$$

with $k = \sqrt{2mE}/\hbar$ (in principle k can be imaginary, but see below), and c_1 and c_2 are arbitrary constants that can be fixed (up to a common phase) by imposing the Dirichlet boundary conditions,

$$u(a) = c_1\, \mathrm{e}^{\mathrm{i}ka} + c_2\, \mathrm{e}^{-\mathrm{i}ka} = 0, \tag{20}$$

$$u(b) = c_1\, \mathrm{e}^{\mathrm{i}kb} + c_2\, \mathrm{e}^{-\mathrm{i}kb} = 0, \tag{21}$$

and normalization

$$\langle u | u \rangle = 1. \tag{22}$$

Exercise 5. Prove that the normalized eigenfunctions of T, with the Dirichlet boundary conditions, are

$$u_n(x) = \sqrt{\frac{2}{l}} \sin\Big(\frac{n\pi}{l}(x-a)\Big), \tag{23}$$

where $l = b - a$, and that the eigenvalues, giving the permitted energy levels are

$$E_n = \frac{\hbar^2}{2m} \frac{n^2 \pi^2}{l^2}, \tag{24}$$

for $n = 1, 2, \ldots$. See Fig. 4.

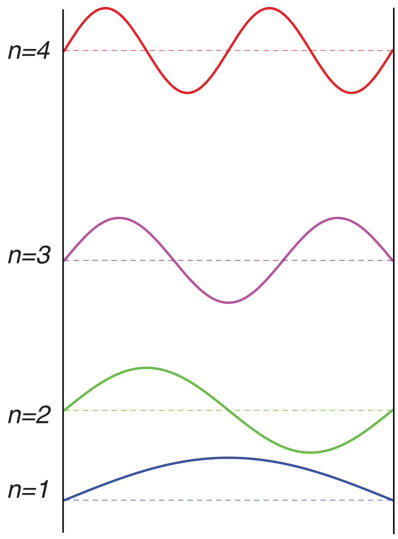

Fig. 4. The eigenfunctions (solid lines) of the operator T in the box at different levels of energy (dashed lines).

Remark 1. Equation (24) tells us two important things on the bound states of the particle:

(1) the energies are quantized;
(2) the energy is always strictly positive.

The strictly positivity of the energy is a property of the Dirichlet boundary conditions. Indeed, with the Neumann ones the energy of the ground state is 0, and, more surprisingly, it is even *negative* with Robin's boundary conditions!

Exercise 6. Prove that the ground state of T, with the Neumann boundary conditions is

$$v_0(x) = \sqrt{\frac{1}{l}}, \tag{25}$$

and has zero energy, $E_0 = 0$. Then, look at the eigenvalue problem with Robin's boundary conditions (8).

2.2. *Fractals in a box*

The textbook exercise of the quantum particle in a box inevitably ends with the evaluation of the eigenvalues (24) and the eigenfunctions (23). The result is so simple and intelligible that we all felt a profound satisfaction when we derived it in our first course of quantum mechanics. The simplicity of the spectrum is deceptive and leads us to think that we fully understand the physical problem. In particular, we are convinced that the dynamics, which is the solution to the Schrödinger equation (17), must surely be as much simpler. In fact, this belief is false, as showed by Berry [13]: the dynamics is instead very intricate.

Let us assume at time $t = 0$ that $\psi(x,0) = v_0(x)$, with v_0 given by (25). This is the simplest conceivable initial condition, corresponding to a flat probability in the box $[a,b]$, with $l = b - a$. We are interested in the time evolution of this initial wave function. Its L^2-expansion in terms of the eigenfunctions (23) of T reads

$$v_0(x) = \sum_{n=1}^{\infty} c_n u_n(x), \tag{26}$$

where $c_n = \langle u_n | v_0 \rangle$.

Exercise 7. Show that

$$c_n = \frac{\sqrt{2}}{n\pi}\,[1 - (-1)^n], \tag{27}$$

and, in particular, $c_{2n} = 0$, for all $n = 1, 2, \ldots$.

In the same way the quantum evolution, described by the action of the unitary operator $U(t) = \mathrm{e}^{-\mathrm{i}Tt/\hbar}$, can be written as an L^2-convergent series

$$\psi(x,t) = \left(\mathrm{e}^{-\mathrm{i}Tt/\hbar} v_0\right)(x) = \sum_{n=1}^{+\infty} c_n\ \mathrm{e}^{-\mathrm{i}E_n t/\hbar} u_n(x). \tag{28}$$

We can now use the explicit expressions (23)–(24) and obtain

$$\psi(x,t) = \sqrt{\frac{2}{l}}\ \sum_{n=1}^{+\infty} c_n \sin\!\left(\frac{n\pi}{l}(x-a)\right) \exp\!\left(-\frac{\mathrm{i}\hbar}{2m}\frac{n^2\pi^2 t}{l^2}\right). \tag{29}$$

In terms of the dimensionless variables $\xi = l^{-1}(x - (a+b)/2) \in [-1/2, 1/2]$, and $\tau = 2\pi\, t\, \hbar / m l^2 \in \mathbb{R}$, it reads

$$\vartheta(\xi,\tau) = \sqrt{\frac{2}{l}}\ \sum_{k=0}^{+\infty} c_{2k+1} \sin\left[2\pi\left(\xi + \frac{1}{2}\right)\left(k + \frac{1}{2}\right)\right] \exp\left[-\mathrm{i}\pi\tau\left(k + \frac{1}{2}\right)^2\right]. \tag{30}$$

By writing the sine as the sum of exponentials and by making use of the expression (27), we finally get

$$\vartheta(\xi,\tau) = \sum_{n=-\infty}^{+\infty} d_n \mathrm{e}^{\mathrm{i}2\pi\xi\left(n+\frac{1}{2}\right) - \mathrm{i}\pi\tau\left(n+\frac{1}{2}\right)^2}, \quad \xi \in \left[-\frac{1}{2}, \frac{1}{2}\right], \tag{31}$$

(notice that now the sum runs over all $n \in \mathbb{Z}$).

Exercise 8. Derive Eq. (31) and show that

$$d_n = \frac{1}{\pi\sqrt{l}} \frac{(-1)^n}{n + \frac{1}{2}}, \quad n \in \mathbb{Z}. \tag{32}$$

If we take a closer look at the expression (31) we notice that it is a Fourier series with quadratic phases. This series is the boundary value of a Jacobi theta function [18], which is defined in the lower complex half-plane of τ, and it has a very rich structure investigated at length by mathematicians. For a full immersion in its deep arithmetic properties see the charming "Tata Lectures on Theta" by Mumford [19]. A simple property is its quasi-periodicity in the rescaled time τ (check it!):

$$\vartheta(\xi, \tau + 1) = \mathrm{e}^{-\mathrm{i}\pi/4}\, \vartheta(\xi, \tau). \tag{33}$$

Thus at integer times τ the wave function comes back (up to a phase) to its initial flat form (25): these are the *quantum revivals.* More generally, at rational values of τ the graph of $|\vartheta(\xi, \tau)|^2$ is piecewise constant and there is a partial reconstruction of the initial wave function [20], see Fig. 5. On the other hand, at irrational times, the wave function is a fractal, with Hausdorff dimension $D_H = 3/2$, as shown in

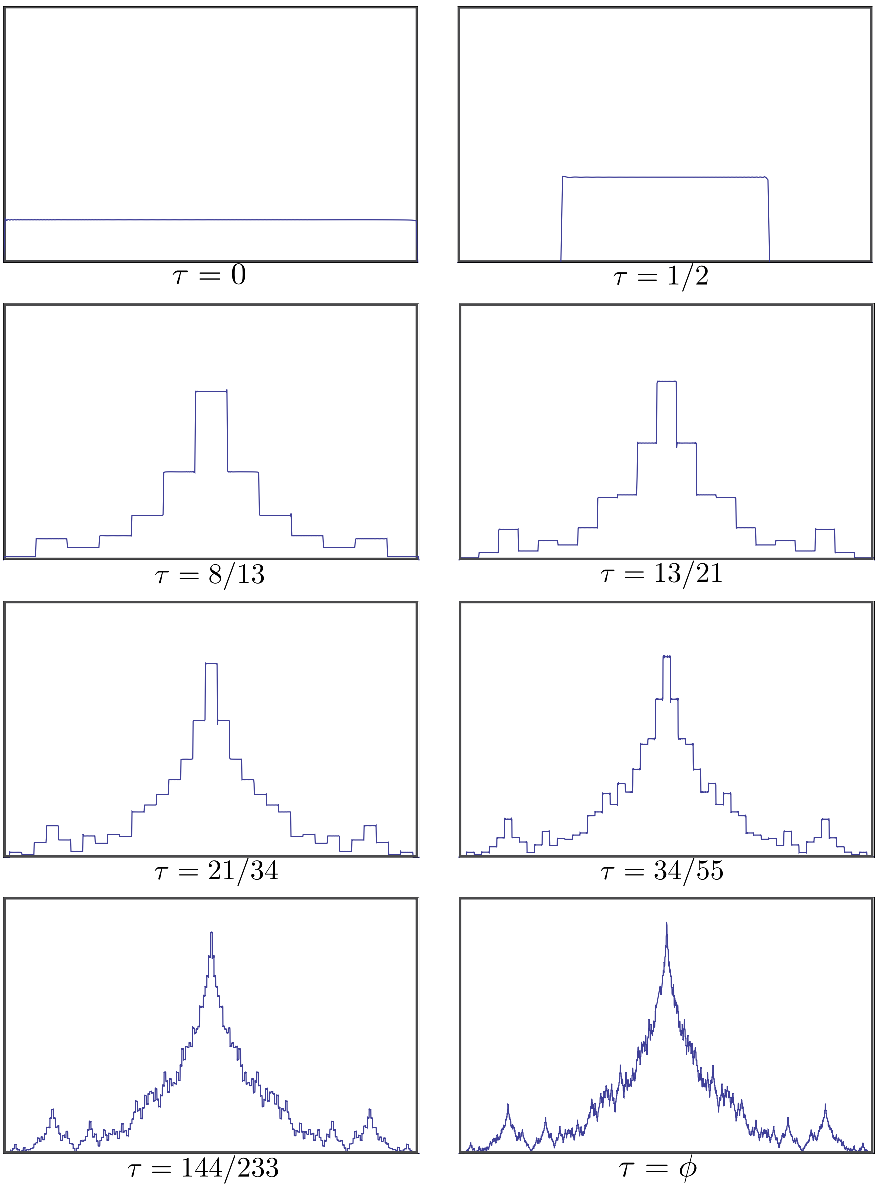

Fig. 5. Graphs of $|\vartheta(\xi, \tau)|^2$ vs. ξ at different rational times τ along the Fibonacci sequence tending to the golden mean, $\phi = (1 + \sqrt{5})/2$. See the emergence of a fractal structure.

the last panel of Fig. 5. In fact, $\vartheta(\xi, \tau)$ can be proved to be a fractal function in space *and* time, and to form a beautifully intricate *quantum carpet*, with different Hausdorff dimensions along different space-time directions [21].

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