

# QUANTUM SYSTEMS WITH TIME-DEPENDENT BOUNDARIES

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A Thesis  
Presented to  
The Division of Mathematics and Natural Sciences  
Reed College

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In Partial Fulfillment  
of the Requirements for the Degree  
Bachelor of Arts

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May 2005



Approved for the Division  
(Physics)

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## **Abstract**

An infinite square well with one moving boundary is studied. Solving the time dependent Schrödinger equation for a linearly expanding or contracting well is shown to lead to a set of time dependent eigenfunctions. An exact propagator is derived by summing over all classical paths, as prescribed by Feynman. Spectral resolution of the propagator returns the time dependent eigenfunctions derived from the Schrödinger equation. Applying a perturbation to the propagator allows one to study the system numerically for cases when the wall velocity changes in time.



# 1

## Introduction

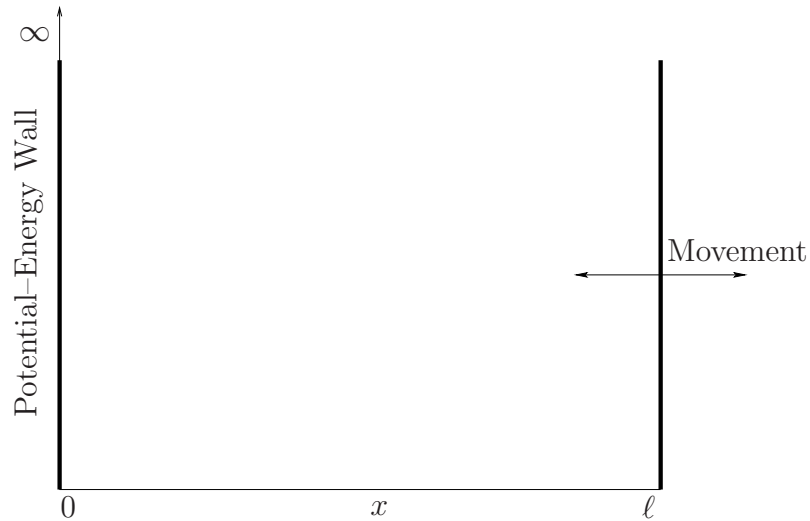
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It is no great secret that much of the discussion about quantum mechanics limits itself to time independent systems. Such is the foundation of the standard textbooks like Landau [1], Griffiths [2], or Schiff [3], and with good cause, too. The majority of systems the physicist is likely to encounter are independent of time for the simple reason that, generally in quantum mechanics, one deals only with conservative systems. This is to say, if some Hamiltonian describes a system in terms of kinetic and potential components, then chances are the potential field is temporally static, varying only with position<sup>1</sup>. Of course, this isn't to say nothing moves in these systems; particles interact and wavepackets bounce around, after all. In the same way, there isn't anything uninteresting or non-challenging about such systems either. Browsing through the table of contents of Griffiths, the reader encounters spin systems, Bell's theorem, the Hydrogen atom, harmonic oscillators, quantum tunneling, the Zeeman effect, and other equally rich topics. Real world applications continually present themselves for analysis by static-potential quantum mechanics, covering everything from electron microscopes to semiconductors. But for all the glory to be gained by studying those systems, one must wonder at some point, as I did, what happens when the system is shaken up a bit. Having gone through all the trouble to work out these static cases, it seems natural to start toying with time dependent situations. Herein we will busy ourselves with a small corner of the new, very large, world.

In fact, we will begin at the very place most physicists are first introduced to quantum mechanics. A perfect example of an oft-studied quantum system is the infinite square well. They don't actually exist in nature, are studied

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<sup>1</sup>See Chapter 1 of Griffiths, [2]. The notable exception to this are magnetic forces.



**Figure 1.1:** *The infinite-potential squarewell with one moving wall. This paper considers primarily linear movement.*

by every budding physicist, there is a great deal written about them, and the Hamiltonians are time-independent. Several months ago I thought to myself, “What happens when the walls move out or in, or out *and* in, so they oscillate? Or, say it’s a finite-potential well. What happens when the strength of the potential increases or decreases?” I hadn’t encountered such questions before, and, as it turns out, I won’t be able to provide answers to all those questions, even for the pedantic case of the square well. At the same time, we here see that there are at least 70 pages of stuff to say—and a great deal more, in truth—so perhaps limiting ourselves to infinite square wells won’t be so limiting after all.

With that in mind, it is good to know what type of time dependence we are thinking about. Our present interest draws us to situations where the physical system is evolving in time: in a classical sense, the movement of particles in a balloon concerns us not at all, but rather expansion and contraction of the balloon itself. This is what I mean when I say “infinite square well with one moving wall”: one of the walls is moving, the other isn’t, so the system is either expanding or contracting. By “infinite square well” I mean, of course, that for a well of length  $\ell$ , the potential energy function is zero inside the well and infinite outside, so that a particle trapped in the well can never get out. This is all summed up in Figure 1.1.

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More specifically, the bulk of the following discussion pertains to an infinite square well with one linearly moving wall; that is, this square well may either expand or contract, and the well width linearly increases/decreases accordingly. We formulate our discussion from two different perspectives. The first proceeds from the Schrödinger equation, solving that differential equation to arrive at a set of eigenfunctions for the system. The second formulation begins on the classical side of the street, utilizing Feynman's "sum over all paths" to arrive at the same set of eigenfunctions. Once these eigenfunctions are known, we can go about the process of determining what they tell us about the system, the discussion of which fills out the second half of this paper. A few other tricks and surprises show up along the way, as well.



# 2

## The Schrödinger formulation

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Problems concerning quantum mechanical systems with moving boundaries have been studied several times in the past, using both approximate methods and exact solutions [4, 5, 6, 7, 8]. For exact solutions, the first system to have been solved was the one-dimensional infinite square well with one uniformly moving wall, as discussed by Doescher and Rice in 1969 [4]. Their paper served as the basis for much further work, both as a reference for approximate methods [7] and a comparative example for other exact studies [6, 8]. The following section introduces the system at hand from the perspective of the Schrödinger equation. Such a procedure starts with the basics and serves as a good mirror within which to view later, more advanced, arguments and commentary.

**2.1 Development of the Schrödinger Formulation** To begin, recall the stationary infinite square well. One starts with some wavefunction  $\Psi(x, t)$  and—when the Hamiltonian is independent of time—assumes a separable solution of  $\Psi(x, t) = \psi(x) f(t)$ . Through standard arguments found in the elementary quantum mechanics texts (see Griffiths [2]), this leads to a solution of

$$\psi(x, t) = \sum_n b_n u_n(x) \exp\left[-\frac{i}{\hbar} E_n t\right] \quad (2.1)$$

where

$$u_n = \sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\ell}\right] \quad \text{and} \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2m\ell^2}$$

Presently, we wish relax the constraint that the system be stationary by allowing  $\ell \rightarrow \ell(t)$ . In order to determine the time dependence of the system

we plug  $\Psi(x, t) = \psi(x) f(t)$  into the Schrödinger equation,  $\mathbf{H}\Psi = i\hbar \frac{\partial}{\partial t} \Psi$ , where the Hamiltonian  $\mathbf{H}$  is

$$\mathbf{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t)$$

$$\text{and the potential } V(x, t) = \begin{cases} 0 & \text{if } 0 \leq x \leq \ell(t) \\ \infty & \text{otherwise} \end{cases}$$

$\mathbf{H}$  would be constant in time if  $\ell(t) = \ell_0$ , a constant. In that case our separable solution assumption gives us

$$i\hbar \frac{1}{f} \frac{df}{dt} = E$$

where  $E$  is some constant. Integration with respect to time gives a solution of  $f(t) \exp[-iEt/\hbar]$ . From this point, putting the system into an infinite square well potential leads to discrete energy levels, stationary states, and all the rest. It would be nice if some form of those results carried over from the static to dynamic potential well. Note that, regardless of whether a wall is moving or not, at any instant in time the system can be written in terms of the eigenfunctions *at that instance*. Therefore we may as well start a discussion of the time dependent case by assuming an analogous set solutions, expanding the wavefunction as a sum of the instantaneous energy eigenfunctions<sup>1</sup>:

$$\psi(x, t) = \sum_n b_n(t) u_n(x, t) \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \quad (2.2.1)$$

$$u_n = \sqrt{\frac{2}{\ell(t)}} \sin\left[\frac{n\pi x}{\ell(t)}\right] \quad (2.2.2)$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m \ell(t)^2} \quad (2.2.3)$$

We need to figure out what the coefficients  $b_n(t)$  are. A natural step would be to plug equations (2.2) into the Schrödinger equation and see where that

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<sup>1</sup>The integral inside the exponential reflects the fact that the energy is not constant in time, but rather enters in/exits from the system as the wall moves in or out. These properties will be discussed in more depth throughout the text, but see especially §4.4 and §6.2.



leads us<sup>2</sup>. I here adopt the notation  $\frac{\partial}{\partial x} \equiv \partial_x$ . Looking at each side of the Schrödinger equation separately greatly reduces the amount of clutter in our argument.

I start with the left hand side (LHS):

$$\sum_n -\frac{\hbar^2}{2m} \partial_x^2 \psi_n = \sum_n -\frac{\hbar^2}{2m} \partial_x^2 \left\{ b_n \sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\ell}\right] \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \right\} \quad (2.3)$$

$$= \sum_n \frac{\hbar^2}{2m} b_n \sqrt{\frac{2}{\ell}} \frac{n^2 \pi^2}{\ell^2} \sin\left[\frac{n\pi x}{\ell}\right] \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \quad (2.4)$$

$$= \sum_n b_n E_n u_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \quad (2.5)$$

The RHS requires a little more work, given the time dependence of both the well-width  $\ell$  and the coefficients  $b_n$ :

$$\begin{aligned} \sum_n i\hbar \partial_t \psi_n &= i\hbar \sum_n \partial_t \left\{ b_n \sqrt{2} \ell^{-\frac{1}{2}} \sin\left[\frac{n\pi x}{\ell}\right] \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \right\} \\ &= -i\hbar b_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \left\{ -\sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\ell}\right] (\partial_t b_n) \right. \\ &\quad \left. + b_n \sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\ell}\right] \frac{1}{2\ell} \dot{\ell} \right. \\ &\quad \left. + b_n \sqrt{\frac{2}{\ell}} \cos\left[\frac{n\pi x}{\ell}\right] \frac{n\pi x}{\ell^2} \dot{\ell} \right. \\ &\quad \left. + b_n \sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\ell}\right] \frac{i n^2 \pi^2 \hbar^2}{\hbar 2m\ell^2} \right\} \end{aligned}$$

where dots denote differentiation with respect to time. Notice that we can write the cosine term as

$$\begin{aligned} b_n \sqrt{\frac{2}{\ell}} \cos\left[\frac{n\pi x}{\ell}\right] \frac{n\pi x}{\ell^2} \dot{\ell} &= -b_n \sqrt{\frac{2}{\ell}} \frac{\partial}{\partial t} \left( \sqrt{\frac{\ell}{2}} \sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\ell}\right] \right) \\ &= -b_n \sqrt{\frac{2}{\ell}} \frac{\partial}{\partial t} \left( \sqrt{\frac{\ell}{2}} u_n(x, t) \right) \end{aligned}$$

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<sup>2</sup>This argument follows how L.Schiff approaches time-dependent problems in his book [3]. See *Quantum Mechanics*, (1949), §31

Hence, the RHS of the Schrödinger equation is

$$\sum_n i\hbar \partial_t \psi_n = - \sum_n i\hbar \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \left\{ u_n \left[ \frac{b_n \dot{\ell}}{2\ell} + \frac{i}{\hbar} b_n E_n - \dot{b}_n \right] - b_n \sqrt{\frac{2}{\ell}} \partial_t \left( \sqrt{\frac{\ell}{2}} u_n \right) \right\} \quad (2.6)$$

Now we can set each side of the Schrödinger equation—equations (2.3) and (2.6)—equal to the other.

$$\begin{aligned} \sum_n b_n E_n u_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \\ = \sum_n \left\{ \dot{b}_n u_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \right. \\ \quad + b_n E_n u_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \\ \quad - i\hbar b_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] u_n \frac{\dot{\ell}}{2\ell} \\ \quad \left. + i\hbar b_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \left( \frac{\dot{\ell}}{2\ell} u_n + \dot{u}_n \right) \right\} \end{aligned}$$

where I have written  $\partial_t \left( \left( \frac{\ell}{2} \right)^{\frac{1}{2}} u_n \right)$  from (2.6) as  $\frac{\dot{\ell}}{2\ell} u_n + \dot{u}_n$ . Several terms in the above equation cancel. Specifically, the whole LHS cancels with the second term on the RHS, and the two terms on the RHS containing  $\dot{\ell}$  cancel. Two terms survive, and we move the one containing  $\dot{b}_n$  to the LHS, and write

$$\sum_n u_n \dot{b}_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] = \sum_n -b_n \dot{u}_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \quad (2.7)$$

Here we have an instance of Dirichlet's Theorem<sup>3</sup> where the function  $\dot{b}_n$  has been expanded in a series of sinusoids, namely, those contained in  $u_n$ . We can employ the standard Fourier's Trick and make use of the orthogonality of the wavefunctions  $u_n$ . Multiplying through on the left by  $u_k$  and integrating

<sup>3</sup>Basically, Dirichlet's says any (reasonably well-behaved) function  $f(x)$  can be ex-

from 0 to  $\ell$ , we have (let us omit the summations—we're looking at each term by itself)

$$\int_0^\ell u_k u_n \dot{b}_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] dx = -\int_0^\ell b_n u_k \dot{u}_n \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] dx$$

Looking at just the left hand side, we can expand out  $u_k$  and  $u_n$  and remove constants from the integral:

$$\dot{b}_n \frac{2}{\ell} \exp\left[-\frac{i}{\hbar} \int^t E_n(\tau) d\tau\right] \underbrace{\int_0^\ell \sin\left(\frac{k\pi x}{\ell}\right) \sin\left(\frac{n\pi x}{\ell}\right) dx}_{= \begin{cases} 0 & k \neq n \\ \frac{\ell}{2} & k = n \end{cases}}$$

The integral requires  $n \rightarrow k$ , and dividing by  $\exp\left[-\frac{i}{\hbar} \int^t E_k(\tau) d\tau\right]$  isolates  $\dot{b}_k$  to give us (now bringing the summation back)

$$\dot{b}_k = \sum_n \exp\left[\frac{i}{\hbar} \int^t (E_k - E_n) d\tau\right] \int_0^\ell -b_n u_k \dot{u}_n dx \quad (2.8)$$

We can, at this point, take the integral when  $\ell$  is a general function of time. With the help of *Mathematica*, we find that

$$\begin{aligned} \dot{b}_k &= \sum_n \int_0^\ell -b_n u_k \dot{u}_n dx \exp\left[\frac{i}{\hbar} \int^t (E_k - E_n) d\tau\right] \\ &= \sum_n \frac{2(-1)^{k+n} b_n k n \dot{\ell}}{(n^2 - k^2)\ell} \exp\left[-\frac{i}{\hbar} \int^t (E_n - E_k) d\tau\right] \end{aligned} \quad (2.9)$$

expanded in a Fourier series of sinusoids:

$$f(x) = \sqrt{\frac{2}{\ell}} \sum_n a_n \sin\left(\frac{n\pi x}{\ell}\right)$$

See M.Boas [9], chapter 7, for a good discussion Fourier series and conditions for expansion.

This blows up when  $n = k$ , but plugging that case into the integral yields zero, so we are simply left with

$$\dot{b}_k = \sum_{n \neq k} \frac{2(-1)^{k+n} b_n k n \dot{\ell}}{(n^2 - k^2)\ell} \exp \left[ -\frac{i\pi^2 \hbar}{2m} (n^2 - k^2) \int^t \frac{1}{\ell[\tau]^2} d\tau \right] \quad (2.10)$$

This is it: equation (2.10) is exact and equivalent to the Schrödinger equation for a particle in a box with time-dependent width. Once the function  $\ell(t)$  is specified, equation (2.10) can be simplified and solved. Let us now restrict the system to a uniformly moving wall,  $\ell(t) = \ell_0 + ut$ , and introduce the unitless variables

$$\xi = \frac{\ell(t)}{\ell_0} \quad \alpha = \frac{m\ell_0 v}{2\hbar} \quad (2.11)$$

in which case the coefficients are given by

$$\partial_\xi b_k = \sum_{n \neq k} b_n \frac{(-1)^{n+k}}{\xi} \frac{2nk}{(n^2 - k^2)} \exp \left[ -\frac{i\pi^2}{4\alpha} (n^2 - k^2) \left(1 - \frac{1}{\xi}\right) \right] \quad (2.12)$$

Unfortunately, there are many potential problems with these equations. Foremost, they constitute a set of coupled, first-order, nonlinear differential equations; it isn't clear how to go about solving exactly them at all. Second, the coefficients are time-dependent anyway, so it's a valid question to ask if we care about them to begin with. Still, as bad as these equations seem, they do reduce to the static case; setting  $\dot{\ell} = 0$  gives  $\dot{b}_k = 0$  for every  $k$ , which simply says that we have stationary states with energy probabilities determined by initial conditions. This reduction to the stationary case is good, but lends no real insight into the meaning of set of equations (2.12). It seems we must appeal to some other method to continue probing this system.

**2.2 Derivation of the eigenfunctions** In the last section we attempted to construct a wave function from a set of instantaneous eigenstates in a way analogous to that for the stationary system. We were in turn lead to a set of mathematically intractable equations<sup>4</sup> and at a loss for how to

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<sup>4</sup>Intractable for our case, in any event. I suppose there may be some system where (2.10) is solvable.

proceed with an exact treatment. We could have set out to solve (2.12) through perturbation methods provided by the standard quantum texts (eg. Schiff §31 [3], or Landau §40–45 [1]), as some have done in the past, but such is not our present interest. Doescher and Rice present an exact solution to this problem, so we should be able to derive. In the following I present my derivation of an exact wavefunction for a particle in an infinite square well with a single, uniformly moving wall.

I begin by rewriting the expansion of the wavefunction in the energy eigenstates, which I will call  $u_n(x, t)$ .

$$u_n(x, t) = \sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\ell}\right]$$

Later, I will need this in terms of  $\xi(t) = \frac{\ell(t)}{\ell_0} = 1 - \frac{u}{\ell_0}t$ , from which we have

$$u_n(x, \xi) = \sqrt{\frac{2}{\ell_0 \xi}} \sin\left[\frac{n\pi x}{\ell_0 \xi}\right] \quad \text{with energy} \quad E_n(t) = \frac{n^2 \pi^2 \hbar^2}{2m \ell(t)^2}$$

For an actual square well with a moving wall, we have a serious problem in that the system has no actual eigenfunctions to form a basis with—what is an eigenfunction at one instant is no longer an eigenfunction the next because the system has changed. But at each instant the system has eigenfunctions, so a useful thought is to, at any given instant in time, write the state of the system in terms of those instantaneous energy eigenfunctions.

$$\Psi(x, t) = \sum_n b_n(t) \psi_n(x, t) = \sum_n b_n(t) u_n(x, t) \exp\left[-\frac{i}{\hbar} \int_0^t E_n(\tau) d\tau\right] \quad (2.13)$$

The integral over energy in the exponential reflects both the fact that energy is time-dependent and that it is being drawn into/out of the system. Again, I refer the reader to §4.4 and §6.2 for more detail. Continuing, I rewrite the exponential, given that  $\ell(t) = \ell_0 + ut$

$$\begin{aligned} \exp\left[-\frac{i}{\hbar} \int_0^t E_n(\tau) d\tau\right] &\longrightarrow \exp\left[-\frac{i n^2 \pi^2 \hbar}{2m} \int_0^t \frac{1}{\ell_0 + u\tau} \tau\right] \\ &= \exp\left[-\frac{i n^2 \pi^2 \hbar}{2m} \left(\frac{t}{\ell_0(\ell_0 + ut)}\right)\right] \end{aligned} \quad (2.14)$$

Making use of the functional inversion  $\xi(t) = \frac{1}{\ell_0}(\ell_0 + ut) \rightarrow t(\xi) = \frac{\ell_0}{u}(\xi - 1)$ , I write

$$\begin{aligned} &= \exp \left[ -\frac{i n^2 \pi^2 \hbar}{2m} \left( \frac{\frac{\ell_0}{u}(\xi - 1)}{\ell_0(\ell_0 + u(\frac{\ell_0}{u}(\xi - 1)))} \right) \right] \\ &= \exp \left[ -\frac{i n^2 \pi^2 \hbar}{2mu} \frac{\xi - 1}{\ell_0 \xi} \right] \end{aligned}$$

Recalling that  $\alpha = \frac{m u \ell_0}{2\hbar}$ , the above becomes

$$\begin{aligned} &= \underbrace{\exp \left[ -\frac{i n^2 \pi^2}{4 \alpha} \left( 1 - \frac{1}{\xi} \right) \right]}_{\text{plug into (2.13):}} \\ \Psi(x, \xi) &= \sum_n b_n(\xi) \psi_n(x, \xi) \\ &= \sum_n b_n(\xi) u_n(x, \xi) \exp \left[ -\frac{i n^2 \pi^2}{4 \alpha} \left( 1 - \frac{1}{\xi} \right) \right] \quad (2.15) \end{aligned}$$

Our proposition is that from this set of eigenfunctions we can construct any wavefunction. Unfortunately, this is a particularly bad basis within which to do calculations because our coefficients  $b_n(\xi)$  are time dependent. Suppose instead that there exists some other way to write a wavefunction that doesn't have time dependent coefficients, but still is an expansion in energy eigenfunctions. We would then write

$$\Psi(x, \xi) = \sum_n a_n \phi_n(x, \xi) = \sum_n a_n u_n(x, \xi) \exp \left[ f(x, \xi) \right] \quad (2.16)$$

where the  $a_n$  are constant in time, the  $u_n$  are the instantaneous energy eigenfunctions, and the exponential term contains all other time and position dependence. We could think of this as placing all the time dependence from (2.15) into the exponential. Our goal is to determine what the function  $f(x, \xi)$  is, and then relate the coefficients  $a_n$  back to the true energy eigenfunction coefficients  $b_n$ . To that end, we rewrite the Schrödinger equation in terms of  $\xi$ , whereby  $\frac{\partial}{\partial t} f(t) = \frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial t} = \frac{u}{\ell_0} \frac{\partial f}{\partial \xi}$ :

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \phi(x, \xi) = \frac{i \hbar u}{\ell_0} \frac{\partial}{\partial \xi} \phi(x, \xi)$$

which is, substituting in for  $\alpha$ ,

$$\frac{i\ell_0^2}{4\alpha} \frac{\partial^2}{\partial x^2} \phi(x, \xi) = \frac{\partial}{\partial \xi} \phi(x, \xi) \quad (2.17)$$

We then plug  $\phi_n$  from (2.16) into (2.17) and are led to the following set of differential equations; all exponential terms, of course, canceled out:

$$\begin{aligned} \frac{1}{\sqrt{\ell_0 \xi}} \left\{ 4n\pi x \cos\left[\frac{n\pi x}{\xi \ell_0}\right] - \frac{1}{\alpha} i \ell_0 n^2 \pi^2 \sin\left[\frac{n\pi x}{\xi \ell_0}\right] + 2\ell_0 \xi \sin\left[\frac{n\pi x}{\xi \ell_0}\right] \right. \\ \left. - 4\ell_0 \xi^2 \sin\left[\frac{n\pi x}{\xi \ell_0}\right] \frac{\partial f}{\partial \xi} + \frac{1}{\alpha} 2i \ell_0^2 n\pi \xi \cos\left[\frac{n\pi x}{\xi \ell_0}\right] \frac{\partial f}{\partial x} \right. \\ \left. + \frac{1}{\alpha} i \ell_0^3 \xi^2 \sin\left[\frac{n\pi x}{\xi \ell_0}\right] \left(\frac{\partial f}{\partial x}\right)^2 + \frac{1}{\alpha} i \ell_0^3 \xi^2 \sin\left[\frac{n\pi x}{\xi \ell_0}\right] \frac{\partial^2 f}{\partial x^2} \right\} = 0 \end{aligned} \quad (2.18)$$

This looks a bit maladjusted for analytic purposes, but notice that there are two cosine terms and five sine terms. Let us assume that the cosine terms conspire to kill each other off and sine terms conspire to kill each other off independently. In that case we have two differential expressions, one containing only cosines, the other containing sines. These are added together to find the true solution. Looking at just the cosine terms, we have a differential equation in  $x$ :

$$\cos\left[\frac{n\pi x}{\xi \ell_0}\right] \left( 4n\pi x + i \frac{2}{\alpha} \ell_0^2 n\pi \xi \frac{\partial f}{\partial x} \right) = 0 \quad (2.19)$$

*Mathematica* quickly solves this:

$$f(x, \xi) \longrightarrow \frac{i \alpha x^2}{\ell_0^2 \xi} + A(\xi) \quad (2.20)$$

where  $A(\xi)$  is some function only of  $\xi$  yet to be determined. Unused at this point are the sine terms of (2.18), so we plug our partially determined function  $f(x, \xi)$  into the sine arguments, set the result equal to zero, and solve this new differential equation for  $A(\xi)$ . We find:

$$f(x, \xi) = \frac{i \alpha x^2}{\ell_0^2 \xi} + \frac{i n^2 \pi^2}{4 \alpha \xi} + B \quad (2.21)$$

where  $B$  is some constant. Because  $f$  is contained in a complex exponential, the constant  $B$  is some phase factor. We appeal to initial conditions to determine the factor:  $B$  must cancel every term when the wall is at its original length  $\ell_0$ , that is, when  $\xi = 1$ . Setting  $B = -\frac{in^2\pi^2}{4\alpha}$  accomplishes this. Therefore, we have discovered a basis within which to expand the wavefunction in terms of constant coefficients. This basis is

$$\begin{aligned}\phi_n(x, \xi) &= u_n(x, \xi) \exp\left[\frac{i\alpha x^2}{\ell_0^2 \xi} + \frac{in^2\pi^2}{4\alpha \xi} - \frac{in^2\pi^2}{4\alpha}\right] \\ &= \sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\xi \ell_0}\right] \exp\left[i\alpha \xi \frac{x^2}{\ell^2} - \frac{in^2\pi^2}{4\alpha} \left(1 - \frac{1}{\xi}\right)\right] \quad (2.22)\end{aligned}$$

$$= \sqrt{\frac{2}{\ell}} \sin\left[\frac{n\pi x}{\ell}\right] \exp\left[\frac{imu x^2}{2\hbar \ell} - \frac{in^2\pi^2\hbar}{2m\ell_0\ell} t\right] \quad (2.23)$$

Equation (2.22) agrees precisely with Doescher and Rice's stated solution. Equation (2.23) is equivalent Doescher and Rice's stated solution, but, as we shall see later, provides a more intuitive way to interpret the result.

Some aspects of the eigenfunctions and their derivation must be raised at this point. First, they are pointedly *not* stationary, but vary quite a bit with time. They don't shift around in any straightforward fashion, either. The time dependence shows up in no less than 5 different places: once in the normalizing coefficient, once in the sine function, twice in the first exponential term, and once in the last exponential term, when written as (2.22).

Second, one might wonder how easily this method of derivation could be applied to other types of wall movement. In answer, I would say not too well. First the time dependence must inverse-square integrable, as seen at (2.13). Right at that point we've discarded most every conceivable movement of the wall. Second, the calculation relies heavily on the functional inversion at (2.14). Usually that inversion doesn't exist. Finally, any remaining cases must then pass through the Schrödinger equation. End result: the odds are stacked against solving this problem almost always. What is amazing is that it can ever be solved at all, and furthermore, lead to the marvelously simple eigenfunctions written above.

**2.3 Properties of the eigenfunction** So far we have derived a solution to the Schrödinger equation for a square well with one moving wall—equation (2.22). It is my task in this section to evaluate this function and



see what we can learn from it. First note that setting the wall velocity  $u = 0$  entails  $\ell(t) \rightarrow \ell_0$  and  $\xi = 1$  for all time. This destroys the second exponential term. Further,  $\alpha \rightarrow 0$  kills the first exponential term, and we recover the stationary solution.

Equation (2.22) must also obey basic properties of wavefunctions. Plugging it into the Schrödinger equation does indeed show, with the quick help of *Mathematica*, that it is a solution. Taking the usual inner product of  $\phi_n^* \phi_k$ , we see

$$\int_0^\ell \phi_n^* \phi_k dx = \begin{cases} 0 & \text{for } n \neq k \\ 1 - \frac{\sin[2n\pi]}{2n\pi} = 1 & \text{for } n = k \end{cases}$$

The instantaneous eigenstates  $\phi_n$  remain normalized regardless of wall movement, and a particle in the  $n^{\text{th}}$  state at  $t = 0$  would remain in that state. Note, however, that the *state itself changes in time*:  $|n\rangle_0 \rightarrow |n\rangle_t$ , but  $|n\rangle_0 \neq |n\rangle_t$ <sup>5</sup>. As always, we can build any wavefunction out of linear combinations of the eigenfunctions with coefficients  $a_n$ :

$$\psi = \sum_n a_n \phi_n$$

Further study of the wavefunction becomes more transparent within a specific context. Therefore, consider a particle originally in the energy ground state. In that case we can find the coefficients  $a_n$  of the  $\phi_n$  representation of  $\psi(x, t)$ :

$$\begin{aligned} a_n &= \frac{2}{\ell_0} \int_0^{\ell_0} \phi_n^*(x, 0) \psi_1(x, 0) dx \\ &= \frac{2}{\ell_0} \int_0^{\ell_0} \exp\left[-i\alpha \left(\frac{x}{\ell_0}\right)^2\right] \sin\left[\frac{n\pi x}{\ell_0}\right] \sin\left[\frac{\pi x}{\ell_0}\right] dx \end{aligned} \quad (2.24)$$

If we expand the exponential term into its polar constituents

$$a_n = \frac{2}{\ell_0} \int_0^{\ell_0} \left( \cos\left[\frac{x^2\alpha}{\ell_0^2}\right] - i \sin\left[\frac{x^2\alpha}{\ell_0^2}\right] \right) \sin\left[\frac{\pi x}{\ell_0}\right] \sin\left[\frac{n\pi x}{\ell_0}\right] dx$$

---

<sup>5</sup>Here, I have used the Dirac notation to specify the state itself,  $|\phi\rangle$ , as opposed to the state in the position-representation,  $\phi_n$ .

we see that the coefficients are actually a combination of the Fresnel Integrals<sup>6</sup>

$$\mathcal{C}_1(x) = \sqrt{\frac{2}{\pi}} \int_0^x \cos(t^2) dt, \quad \text{and} \quad \mathcal{S}_1(x) = \sqrt{\frac{2}{\pi}} \int_0^x \sin(t^2) dt$$

The integral can be carried out and in general, each  $a_n$  has 16 terms, each written in terms a Fresnel integral. It isn't terribly illuminating to see them, so I suppress the list here; suffice it to say that we can numerically evaluate the  $a_n$ 's at any given point in time.

The next step is motivated by telling the story of our progress so far. We started with a wavefunction  $\psi(x, t)$  in an infinite square well. We then showed that we could write the wavefunction in terms of the instantaneous energy eigenfunctions  $u_n(x, t)$ . The problem with that coordinate system, however, is that it leads to the intractable coupled differential equations, so we switched to the basis  $\phi_n$  from (2.22), where the coefficients remain constant in time. From there we could find out how much of some wavefunction  $\psi$  is in each eigenstate  $\phi_n$  by the inner product:  $a_n = (\phi_n(x, 0) | \psi(x, 0))$ ; however, what we are really interested in is how much of the wavefunction is in each *energy* eigenstate,  $u_n(x, t)$ . That is, we want to know what the probabilities  $|b_n|^2$  are. We can accomplish this by setting our two methods of writing  $\psi(x, t)$  equal to each other:

$$\begin{aligned} \psi(x, t) &= \sum_n a_n \phi_n(x, t) = \sum_k b_k(t) u_k(x, t) \exp\left[-\frac{i}{\hbar} \int^t E_k(\tau) d\tau\right] \\ &= \sum_k C_k(t) u_k(x, t) \end{aligned} \quad (2.25)$$

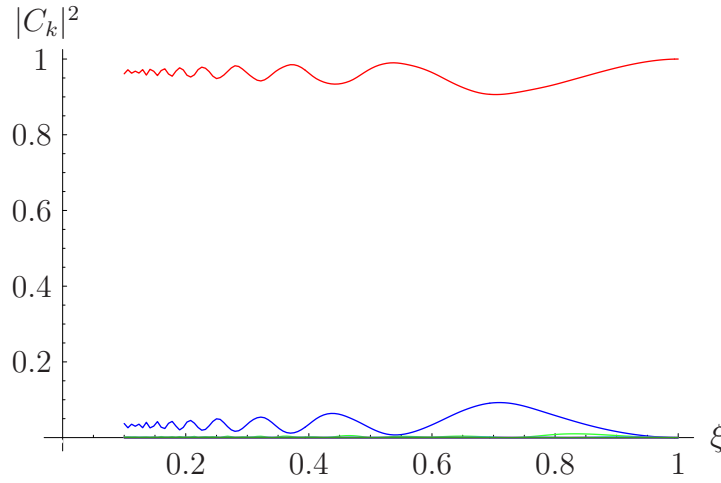
where  $C_k(t) = b_k \exp\left[-\frac{i}{\hbar} \int^t E_k(\tau) d\tau\right]$ . Note that  $|C_k|^2 = |b_k|^2$ . We can then

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<sup>6</sup>See the standard references for mathematical functions, such as Abramowitz&Stegun, §7.3, page 300 [10].

find the  $C_k$ 's:

$$\begin{aligned}
 C_k(t) &= (u_k|\psi) = (u_k|\sum_n a_n \phi_n) = \sum_n a_n \int_0^{\ell(t)} u_k(x,t) \phi_n(x,t) dx \\
 &= \sum_n \left\{ \left( \frac{2}{\ell_0} \int_0^{\ell_0} \exp[-i\alpha(\frac{x}{\ell_0})^2] \sin[\frac{\pi x}{\ell_0}] \sin[\frac{n\pi x}{\ell_0}] dx \right) \right. \\
 &\quad \left. \times \frac{2}{\ell_0} \int_0^{\ell(t)} \sin[\frac{k\pi x}{\ell}] \sin[\frac{n\pi x}{\ell}] \exp[i\alpha\xi(\frac{x}{\ell})^2 - i\frac{n^2\pi^2}{4\alpha}(1-\frac{1}{\xi})] dx \right\} \quad (2.26)
 \end{aligned}$$

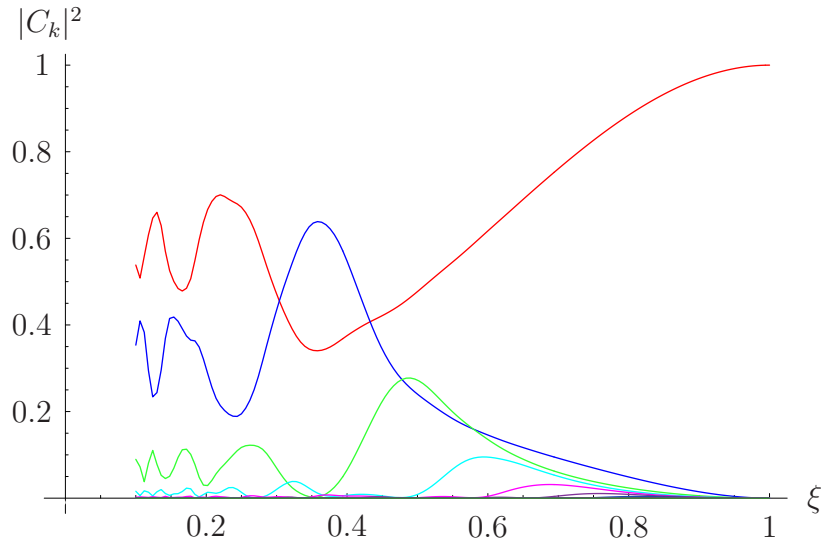


**Figure 2.1:** Energy probabilities  $|C_k|^2$  for  $k = 1-10$ , plotted versus  $\xi$  for  $\alpha = -1$ . This is a compression ( $\alpha$  is negative), so time flows right to left. The three visible probability lines are for  $k = 1$  (red),  $k = 2$  (blue), and  $k = 3$  (green).

Now, equations (2.26) require a grand amount of space to write down<sup>7</sup>, so we won't do that here. What we can do is check the validity of our expression using the relatively benign case where  $\xi = 1$ , i.e., at  $t = 0$ . This should simply give back  $C_k = \delta_{k,1}$ , meaning that the system is in the ground state. Plugging  $\xi = 1$  into (2.26) removes the second term from the second exponential and sets  $\ell(t) \rightarrow \ell(0) = \ell_0$ . Orthonormality of the sine functions under the integral forces  $k = 1$ . The second integral is now equivalent to the

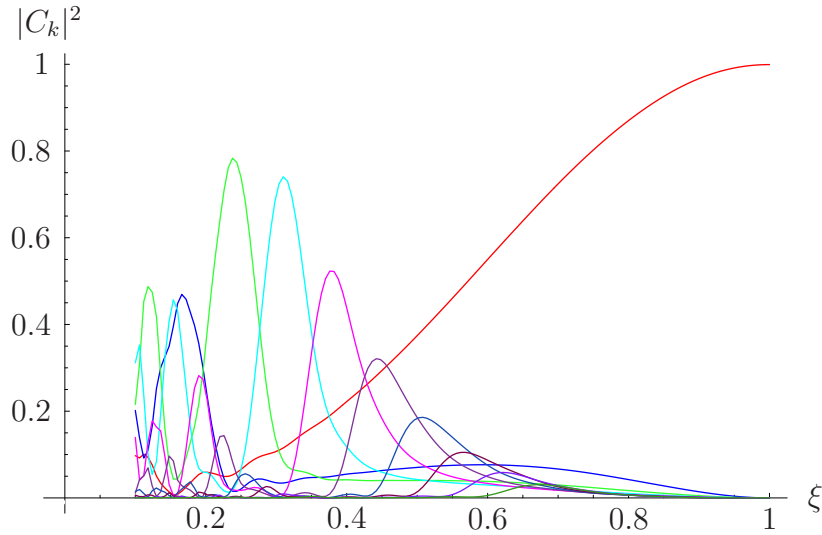
<sup>7</sup>In §5.1 the integral is carried out, in all the hirsute details, at (5.5); that is not for the ground state, however, but rather as a general case of (2.24).

first, with the exception of a minus sign in the exponential; that is, it is the complex conjugate of the first integral. The first integral is itself just  $a_n$ . We therefore have  $C_{k=1}(t=0) = \sum a_n a_n^* = \sum |a_n|^2 = 1$ . That's a nice result and indicates that we haven't misstepped in our inquiry thus far.



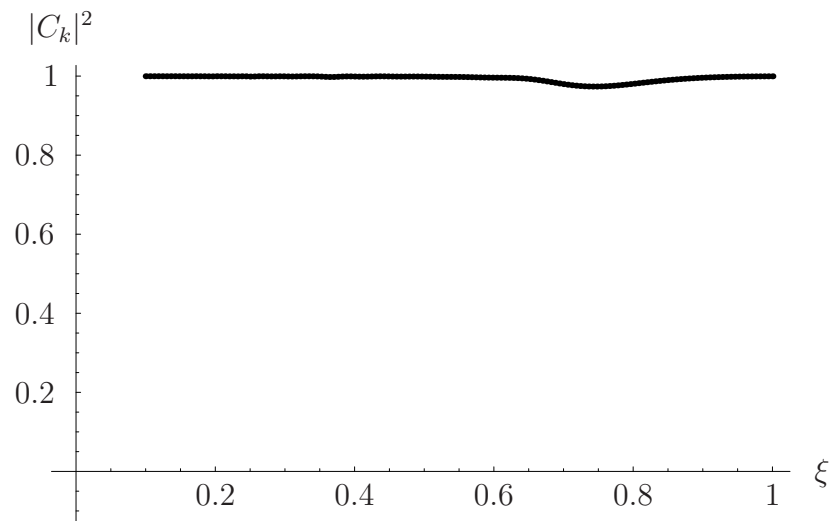
**Figure 2.2:** Energy probabilities  $|C_k|^2$  for  $k = 1-10$ , corresponding to colors red, blue, green, cyan, and purple, respectively; plotted versus  $\xi$  for  $\alpha = -4$ . This is a compression ( $\alpha$  is negative), so time flows right to left.

For other, less trivial, cases, one must proceed via numerical evaluation. Plotting the probabilities  $|C_k|^2$  for various eigenstates  $k$  and wall velocities  $\alpha$  clearly shows how the system evolves under compression and expansion. In particular, Figure 2.1 shows the probabilities for the first ten energy levels—only 3 are visible, the others having such small amplitudes—under a slowish compression,  $\alpha = -1$ . Figure 2.2 shows the probabilities for the first ten energy levels under a more rapid compression,  $\alpha = -4$ —again, after the 5<sup>th</sup> energy level the amplitudes are so small that the plots aren't visible. Finally, Figure 2.3 shows the probabilities for the first ten energy levels under a rapid compression,  $\alpha = -10$ . In that case all ten calculated coefficients contribute in an identifiable manner to the probabilities. Each plot is created from 151 points between  $\xi = .1$  and  $\xi = 1$  for each eigenstate; each point in each eigenstate was calculated to ten terms ( $n : 1 \rightarrow 10$  in equation (2.26)). These plots are in agreement with those produced by Doescher and Rice [4].



**Figure 2.3:** Energy probabilities  $|C_k|^2$  for  $k = 1-10$ , corresponding to colors red, blue, green, cyan, magenta, purple, dark blue, red-purple, purple-blue, and forest green, respectively; plotted versus  $\xi$  for  $\alpha = -10$ . Time flows right to left.

As this final, and rather boring, figure demonstrates, using 10 eigenstates calculated to 10 terms results in accurate data. Figure 2.4 shows the sum of all probabilities at each instant in time for a compression of  $\alpha = -10$ ; i.e., the sum of the plots in Figure 2.3. It is nearly a constant unity. The minimum is  $\sum |C_k|^2 = 0.974$  and occurs at  $\xi = 0.72$ . Note that this is the point of maximum contribution from the last calculated ( $k = 10$ ) eigenstate, as seen in Figure 2.3.



**Figure 2.4:** Summed energy probabilities  $|C_k|^2$  for  $k = 1-10$  at each point  $\xi$  for  $\alpha = -10$ . Time flows right to left. Minimum value of  $\sum |C_k|^2 = 0.974$  at  $\xi = 0.72$ .

# 3

## Classical Path Contributions: The Feynman Formulation

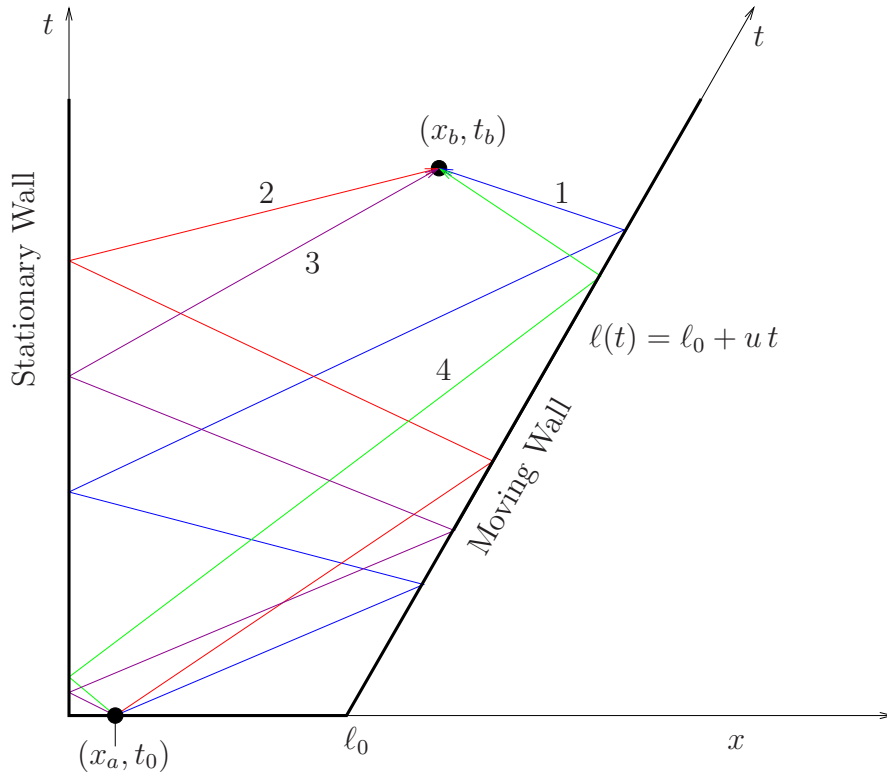
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**3.1 Introductory remarks** Much of quantum mechanics concerns itself with the construction of, and studies involving, the wavefunction. However, as is known to students of more advanced theories, there exists a deeper, and in some ways more powerful, entity lurking in the shadows of quantum theory: the propagator.

The propagator is, stripped to its bare essentials, a wavefunction that remembers its history. More to the point, it determines the evolution of a system that began at a specific point, which is to say it is a wavefunction that evolves from a delta function. By the end of our discussion, this should be clear in all the important ways: both mathematically and pictorially. The notion of a propagator was first proposed by Dirac (although he didn't use that term) whereby the wavefunction at one instant is related to the wavefunction a time interval  $\epsilon$  later via an exponential function of  $i\epsilon \times \mathcal{L}$ , where  $\mathcal{L}$  is the Lagrangian [11]. From its roots, then, the propagator describes how the wavefunction evolves in state-space. Knowing the propagator provides easy access to wavefunctions in any representation for a quantum state, a feature we will exploit in section §4.2.

Now, in the last chapter we derived and explored a basis of wavefunctions for the uniformly expanding/contracting infinite square well. This was a purely quantum mechanical discussion. This chapter, on the other hand, develops the propagator through a “sum over paths” as prescribed by the Feynman formulation of quantum mechanics. At its foundations, Feynman's sum utilizes only classical aspects of a particle in an infinite square well.

That is, as N. Wheeler writes in *Feynman Quantization in a box* where he studies the analogous stationary system [12], “the quantum properties of the system are entirely implicit in its classical properties.” This is quite a departure from our previous probing of the system, and one we will ruminate on farther down the road. The following argument follows a paper written by M. da Luz and B. Cheng [6], though with a number of changes to create a clearer presentation.



**Figure 3.1:** Example subset of all classical paths  $(x_b, t_b) \leftarrow (x_a, t_a)$ . Labeled are each class of path  $x(t) : (x_b, t_b) \leftarrow (x_a, t_0)$ . 1 hits the moving wall first and last; 2 hits the moving wall first and stationary wall last; 3 hits the stationary wall first and last; 4 hits the stationary wall first and moving wall last.

Consider a particle moving in a square well with one wall moving at velocity  $u$ . This is depicted in Figure 3.1, where wall velocity is positive and hence the system expands; note that the following argument works just as well when the wall velocity is negative. Here we see that four possible classes



of paths carry a free particle along  $x(t) : (x_a, t_0) \rightarrow (x_b, t_b)$ . In particular, a particle can (Figure 3.1):

1. First bounce off the moving wall, last bounce off the stationary wall
2. First bounce off the moving wall, bounce off the moving wall
3. First bounce off the stationary wall, bounce off the moving wall
4. First bounce off the stationary wall, bounce off the stationary wall

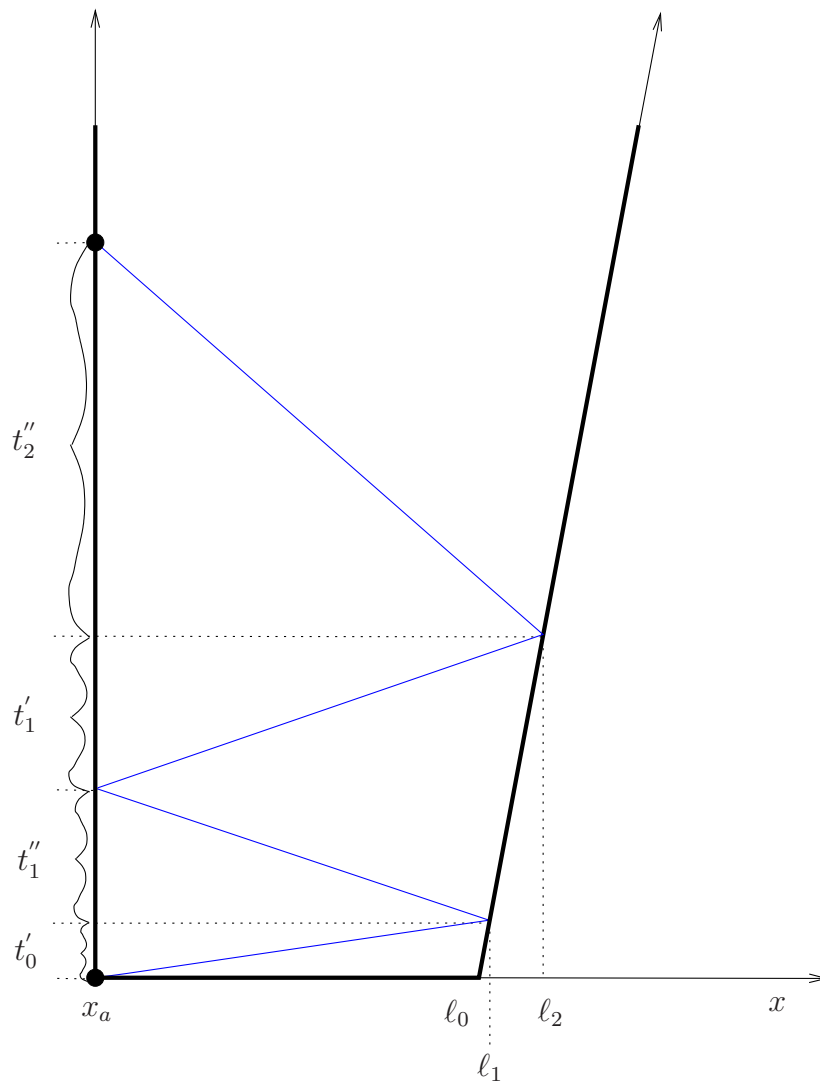
with any number of bounces between the first and last collisions. The total number of bounces is, in each case, 1) even; 2) odd; 3) even; and 4) odd. This will be important later.

The classical action for a free particle is given by  $S_{cl} = \frac{m}{2} \frac{(\Delta x)^2}{\Delta t}$ , which utilizes the fact that the velocity for a free particle traveling from  $(x_a, t_a)$  to  $(x_b, t_b)$  is simply  $v = \frac{x_b - x_a}{t_b - t_a}$ . In our case, however, when the particle bounces off the moving wall it rebounds with a new velocity given by  $v_{\text{after}} = v_{\text{before}} - 2u$ , where  $u$  is the velocity of the wall. We must therefore consider how many total bounces a particle has undergone and break up our evaluation of the action into time intervals between one bounce off the moving wall and the next, during which time the particle's velocity is constant.

In order to find a good way to index time, we presently restrict ourselves to a simple case of Path 2, where both the initial and final particle positions are at the origin  $x = 0$ , as in Figure 3.2. Accordingly, time is indexed:

- $l_j$ : position of the moving wall at the  $j^{\text{th}}$  bounce;
- $t_j''$ : time *after* the  $j^{\text{th}}$  bounce the for particle to travel from  $x = l_j$  to  $x = 0$
- $t_j'$ : time *after* the  $j^{\text{th}}$  bounce when the particle travels from  $x = 0$  to the next moving wall bounce at  $x = l_{j+1}$ ;

Note that some time  $t_j'$  refers not the temporal distance from  $t = 0$ , but instead to the time between the  $j^{\text{th}}$  and  $(j + 1)^{\text{th}}$  wall collisions. The actual time for any given path can be found by adding to and subtracting from this initial set of time intervals. We can now quantitatively analyze this (*still classical!*) system.



**Figure 3.2:** An example of path class 1. The length of the well for the  $j^{\text{th}}$  bounce off the moving wall is called  $l_j$ .

**3.2 Foundational case:**  $x_a = x_b = 0$  To see how the sum over paths works, we begin with the special case of path 2 shown in Figure 3.2, where a particle starts at  $(x_a, t_a)$  and travels via some path—that is, via some number of wall-collisions  $n$ —to  $(x_b, t_b)$ . Using Figure 3.2 as a guide, we can write down the following relations between the position of the moving wall the time-intervals between collisions with either wall:

$$(v - u)t'_0 = \ell_1 \quad (3.1.1)$$

$$(v - 2u)t''_1 = \ell_1 \quad (3.1.2)$$

$$(v - 2u)t'_1 = \ell_2 \quad (3.1.3)$$

$$(v - 4u)t''_2 = \ell_2 \quad (3.1.4)$$

$$(v - 4u)t'_2 = \ell_3 \quad (3.1.5)$$

$$\vdots$$

$$(v - 2ku)t''_k = \ell_k \quad (3.1.6)$$

$$(v - 2ku)t'_k = \ell_{k+1} \quad (3.1.7)$$

Eventually, the particle loses enough velocity and  $(v - 2ku) \leq u$ , after which the particle cannot catch up to the wall. We'll assume that doesn't happen; in fact, we will eventually calculate the what the initial velocity must be in order to arrive at  $(x_b, t_b)$  after  $n$  encounters with the moving wall. Between collisions, the wall itself moves distances

$$u(t''_1 + t'_1) = \ell_2 - \ell_1 \quad (3.2.1)$$

$$u(t''_2 + t'_2) = \ell_3 - \ell_2 \quad (3.2.2)$$

$$u(t''_3 + t'_3) = \ell_4 - \ell_3 \quad (3.2.3)$$

$$\vdots$$

$$u(t''_k + t'_k) = \ell_{k+1} - \ell_k \quad (3.2.4)$$

Additionally, we have an initial condition that defines  $t'_0$  and the initial

well size  $\ell_a$ :

$$\begin{aligned} ut'_0 &= \ell_1 - \ell_a & (3.3) \\ \ell_a &= \ell_1 - ut'_0 \\ t'_0 &= \frac{\ell_1 - \ell_a}{u} \end{aligned}$$

Between the set of equations (3.1), (3.2), and (3.3) we have written down all the information we need. The following two pages simply rearrange that information into a format conducive to analysis via the Feynman formalism. We first look at the length of the well at each successive collision. For  $\ell_1$  we have

$$\ell_1 = vt'_0$$

Plugging in for  $t'_0$  from equation (3.3)

$$\ell_1 = \frac{v\ell_a}{v-u} \tag{3.4.1}$$

For  $\ell_2$ , (3.2.1) says

$$\begin{aligned} \ell_2 &= \ell_1 + u(t''_1 + t'_1) \\ \text{and} \quad (t''_1 + t'_1) &= \frac{\ell_1 + \ell_2}{v-2u} \quad \text{from (3.1.2) and (3.1.3)} \end{aligned}$$

Employing (3.4.1), we solve for  $\ell_2$

$$\ell_2 = \frac{v\ell_a}{v-3u} \tag{3.4.2}$$

Repeating this argument for one more level, we have from (3.2.2)

$$\begin{aligned} \ell_3 &= \ell_2 + u(t''_2 + t'_2) \\ (t''_2 + t'_2) &= \frac{\ell_2 + \ell_3}{v-4u} \quad \text{from (3.1.4) and (3.1.5)} \end{aligned}$$

so that application of (3.4.2) gives us

$$\ell_3 = \frac{v\ell_a}{v-5u} \tag{3.4.3}$$

We see this pattern continues, so that the  $j^{\text{th}}$  wall collision is given by

$$\ell_j = \frac{v\ell_a}{v - (2j - 1)u} \quad (3.4.4)$$

Relations for the time intervals are derived in a similar vein. Equations (3.1.3) and (3.1.2) give

$$t'_1 = \frac{\ell_2}{v - 2u} \quad t''_1 = \frac{\ell_1}{v - 2u}$$

and from our just discovered expressions (3.4.1) and (3.4.2), we have

$$t'_1 = \frac{v\ell_a}{(v - 3u)(v - 2u)} \quad t''_1 = \frac{v\ell_a}{(v - u)(v - 2u)} \quad (3.5.1)$$

Again, from the appropriate equations (3.1)

$$t'_2 = \frac{\ell_3}{v - 4u} \quad t''_2 = \frac{\ell_2}{v - 4u}$$

together with lengths  $\ell_2$  and  $\ell_3$  provided by (3.4.2) and (3.4.3), we see

$$t'_2 = \frac{v\ell_a}{(v - 5u)(v - 4u)} \quad t''_2 = \frac{v\ell_a}{(v - 3u)(v - 4u)} \quad (3.5.2)$$

After this clear iteration we have the two equations

$$t'_j = \frac{v\ell_a}{[v - (2j + 1)u][v - 2ju]} \quad (3.5.3)$$

$$t''_j = \frac{v\ell_a}{[v - (2j - 1)u][v - 2ju]} \quad (3.5.4)$$

To sum up, by iteration we have found the following equations

$$\ell_j = \frac{v\ell_a}{v - (2j - 1)u} \quad (3.6.1)$$

$$t'_j = \frac{v\ell_a}{[v - (2j + 1)u][v - 2ju]} \quad (3.6.2)$$

$$t''_j = \frac{v\ell_a}{[v - (2j - 1)u][v - 2ju]} \quad (3.6.3)$$

We can now continue on with our analysis. Remembering that so far we are dealing with a particle that begins/ends at the stationary wall and makes contact with the moving wall  $n$  times ( $n$  an even number in this case), we can write down the total elapsed time for the motion  $(x_a, t_a) \rightarrow (x_b, t_b)$ :

$$T = t_b - t_a = \sum_{j=1}^n (t'_{j-1} + t''_j)$$

Using *Mathematica*, the above summation collapses to a surprisingly simple, elegant result:

$$T = \frac{2n\ell_a}{v - 2nu}$$

This tells us that, in order to hit the moving wall  $n$  times and arrive at  $(x_b, t_b)$ , the particle needs an original velocity

$$v_n \equiv 2nu + \frac{2n\ell_a}{T}$$

Noting that the moving wall itself traverses a distance  $uT = \ell_b - \ell_a$ , we arrive at the expression for what the original velocity needs to be for the particular path with  $n$  collisions:

$$v_n = \frac{2n\ell_b}{T}$$

We are now in a position to write down the classical action for a particle that encounters the moving wall  $n$  times. The action is

$$S_n = \frac{m}{2} \left\{ \int_0^{t'_0} v_n^2 dt + \sum_{j=1}^{n-1} \int_0^{t_j} (v_n - 2ju)^2 dt + \int_0^{t''_n} (v_n - 2nu)^2 dt \right\} \quad (3.7)$$

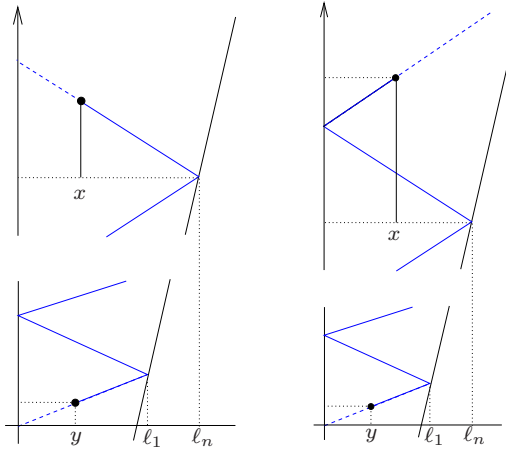
for  $t_j = t''_j + t'_j$ . Plugging the above expression into *Mathematica*, we quickly recover the answer presented by da Luz and Cheng:

$$S_n[0, t_b; 0, t_a] = 2mn^2 \frac{\ell_b \ell_a}{T} \quad (3.8)$$

When the wall is stationary,  $\ell_b = \ell_a \equiv \ell_0$ ,  $T = \frac{2n\ell_0}{v}$ , and the total distance traveled is  $2n\ell_0$ . The action is then

$$S_{u=0} = 2mn^2 \frac{\ell_0^2 v}{2n\ell_0} = \frac{m(2n\ell_0)^2}{2(t_b - t_a)}$$

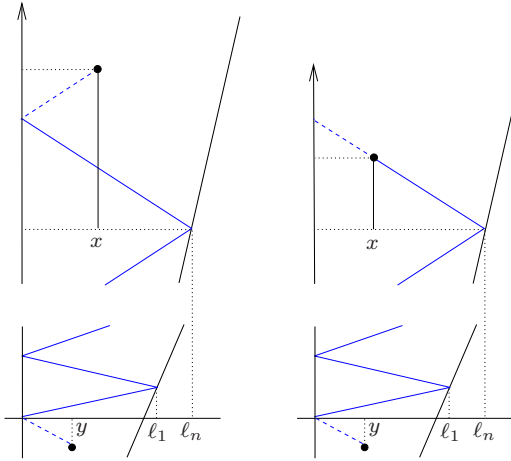
which is the regular classical action for a particle bouncing in a box with stationary walls.



**Figure 3.3:** Path Class 1[right] and 2[left]. Compared to the  $x_a = x_b = 0$  case, the particle travels added/subtracted distances  $-y + x$  for Path 1 and  $-y - x$  for Path 2, making for corresponding changes the time interval  $T_0$ .

**3.3 Arbitrary linear paths** At this point we need to expand our discussion to include all types of paths  $(x_a, t_a) \rightarrow (x_b, t_b)$ . Recall that these are (see Figure 3.3 and Figure 3.4)

1. First bounce off the moving wall, last bounce off the stationary wall
2. First bounce off the moving wall, last bounce off the moving wall
3. First bounce off the stationary wall, last bounce off the moving wall
4. First bounce off the stationary wall, last bounce off the stationary wall



**Figure 3.4:** Path Class 3[right] and 4[left]. Compared to the  $x_a = x_b = 0$  case, the particle travels distances  $+y - x$  for Path 3 and  $y + x$  for Path 4, making for corresponding changes to the time interval  $T_0$ .

Above, we worked out a special case of Path 2 (Figure 3.3), with both the first and last bounces off the moving wall and the particle starting and ending at the stationary wall. All other paths can be created by adding-on/subtracting-off additional lengths from our special case, as indicated in Figures 3.3 and 3.4. It is under that guiding thought that we now enumerate all paths

$$(x_a, t_a) \xrightarrow[n \text{ bounces}]{} (x_b, t_b)$$

To begin, we note that equation (3.1.1) has changed, and now reads

$$vt'_0 + x_a = \ell_1$$

This changes (3.4.1) to read

$$\ell_1 = \frac{v\ell_a - x_a u}{v - u} \tag{3.9}$$

Subsequently, all iterated wall positions shift by the same amount. However, this equation only holds for paths 1 and 2. If we let  $x$  and  $y$  be defined, for each path, to be



1.  $y = -x_a; x = x_b$
2.  $y = -x_a; x = -x_b$
3.  $y = x_a; x = -x_b$
4.  $y = x_a; x = x_b$

We can then write the  $j^{\text{th}}$  well length, along with the  $j^{\text{th}}$  time intervals, as

$$\ell_j = \frac{v\ell_a + yu}{v - (2j - 1)u} \quad (3.10)$$

$$t'_j = \frac{v\ell_a + yu}{[v - 2(j + 1)u][v - 2ju]} \quad (3.11)$$

$$t''_j = \frac{v\ell_a + yu}{[v - 2(j - 1)u][v - 2ju]} \quad (3.12)$$

where we plug in the appropriate  $x$  and  $y$  for the path at hand. The travel times can easily be determined by adding and subtracting from the simple case considered in the previous section. That time was

$$T_0 \equiv T[(0, t_a; 0, t_b)] = \frac{2n\ell_0}{v - 2nu} \quad (3.13)$$

Note that for that case we set  $t_a = 0$ , so that  $\ell_a = \ell_0$ . Now we have  $\ell_a = \ell_0 + u\frac{y}{v}$ . Using equation (3.13) and looking at Figure 3.3, we see that for Path 1 the travel time is

$$T_1 \equiv T_0 - \frac{y}{v} + \frac{x}{v - 2nu}$$

Substituting in  $\ell_0 = \ell_a - \frac{uy}{v}$  into  $T_0$  gives us

$$T_1 = \frac{2n\ell_a - y + x}{v - 2nu} \quad (3.14)$$

For Path 2, the particle meets the moving wall on the first and last collisions, and travels a distance  $y + x$  less than the path for  $T_0$ . Therefore, the total time of flight is

$$T_2 \equiv T_0 - \frac{y}{v} - \frac{x}{v - 2nu} = \frac{2n\ell_a - y - x}{v - 2nu} \quad (3.15)$$

In the same manner we find the time-of-flight for Paths 3 and 4

$$T_3 = \frac{2n\ell_a + y - x}{v - 2nu} \quad (3.16)$$

$$T_4 = \frac{2n\ell_a + y + x}{v - 2nu} \quad (3.17)$$

Or, in a simpler fashion

$$T = \frac{2n\ell_a + y + x}{v_j - 2nu} \quad (3.18)$$

where we have used the  $x, y$  conventions defined above. We now know that for a particle to take some path  $(x_a, t_a) \xrightarrow[n \text{ collisions}]{\hspace{1.5cm}} (x_b, t_b)$  it must have initial velocity

$$v_{n,j} = \frac{2nuT}{T} + \frac{2n\ell_a + y + x}{T}$$

But  $uT = \ell_b - \ell_a$ , so

$$v_{n,j} = \frac{2n\ell_b + y + x}{T} \quad (3.19)$$

The corresponding actions will then be (using  $k$  to designate path-class)

$$S_n^{(k)} = \frac{m}{2} \left\{ \sum_{j=1}^n \left( \frac{\ell_j^2}{t'_{j-1}} + \frac{\ell_j^2}{t'_j} \right) + \frac{x^2}{x/(v - 2nu)} + \frac{y^2}{y/v} \right\}$$

Upon entry into *Mathematica*, this reduces (again!) to the marvelously simple result

$$S_n^k = \frac{m}{2T} \left[ 4\ell_a\ell_b n^2 + 4(\ell_b y + \ell_a x)n + (y + x)^2 \right] \quad (3.20)$$

where we must make sure  $x$  and  $y$  have the appropriate signs for each path class. Note that (3.20) reduces to (3.8) (page 28) in the case  $x_a = x_b = 0$ .

Make a note at this point. We are now carrying the argument from its classical beginnings towards its quantum destination. The leap from classical action to the propagator was explained by Feynman, and entails for a free particle [11] (which is what we have in our box)

$$K = \sqrt{\frac{m}{2i\pi\hbar T}} e^{\frac{i}{\hbar} S_{cl}[x(t)]}$$

In our case, we have a sum over all such paths  $(x_a, t_a) \rightarrow (x_b, t_b)$ , and must include a phase factor of  $\pi$  due to paths with odd numbers of reflections; those are paths 2 and 4. Taking that into account, the semi-classical propagator is then given by

$$K[x_b, t_b; x_a, t_a] = \sqrt{\frac{m}{2\pi i \hbar T}} \sum_{j=1, n=0}^{4, \infty} \left\{ (-1)^{j+1} e^{\frac{i}{\hbar} S_n^{(j)}} \right\}$$

Now notice that when  $n \rightarrow -n$ ,  $S^{(1)} = S^{(3)} \equiv S^{\text{even}}$ , and  $S^{(2)} = S^{(4)} \equiv S^{\text{odd}}$ . We can therefore write the propagator as

$$= \sqrt{\frac{m}{2\pi i \hbar T}} \sum_{n=-\infty}^{\infty} e^{\frac{i}{\hbar} S_n^{\text{even}}} - e^{\frac{i}{\hbar} S_n^{\text{odd}}} \quad (3.21)$$

Working now explicitly for a single action term, without inserting  $x, y$  for any specific case, we have

$$K' = \left( \frac{m}{2\pi i \hbar T} \right)^{\frac{1}{2}} \sum_{n=-\infty}^{\infty} \exp \left\{ \frac{im}{2\hbar T} \left[ 4\ell_a \ell_b n^2 + 4(\ell_b y + \ell_a x)n + (y+x)^2 \right] \right\}$$

where the prime on  $K$  is to remind us that *we are presently only considering one action term, of which there are two*. Rewriting, we have

$$K' = \left( \frac{m}{i\hbar T} \right)^{\frac{1}{2}} \sum_{n=-\infty}^{\infty} e^{\frac{im}{2\hbar T} (y+x)^2} e^{\frac{i}{\hbar} \frac{m}{T} (2\ell_a \ell_b n^2 - 2(-\ell_b y - \ell_a x)n)}$$

It turns out that our analysis would benefit from the introduction of Jacobi's theta function. In order to do that, we introduce the dimensionless variables

$$\beta = \frac{2m\ell_a \ell_b}{\hbar T} \quad \xi = -\frac{\ell_b y m}{\hbar T} \quad \zeta = -\frac{\ell_a x m}{\hbar T}$$

We then have, in general,

$$K' = \left( \frac{m}{i\hbar T} \right)^{\frac{1}{2}} \sum_{n=-\infty}^{\infty} e^{\frac{im}{2\hbar T} (x+y)^2} e^{i \left( \frac{\beta}{\pi} n^2 - 2(\xi + \zeta)n \right)} \quad (3.22)$$

The theta function itself is defined as

$$\Theta_3(z, \tau) = \sum_{n=-\infty}^{\infty} e^{i[\pi\tau n^2 - 2zn]}$$

The propagator, now named  $K_{B,A}$  and *including all terms*, is

$$K_{B,A} = \left(\frac{m}{i\hbar T}\right)^{\frac{1}{2}} \left[ e^{\frac{im}{2\hbar T}(x_b-x_a)^2} \Theta_3\left(\zeta - \xi, \frac{\beta}{\pi}\right) - e^{\frac{im}{2\hbar T}(x_a+x_b)^2} \Theta_3\left(\zeta + \xi, \frac{\beta}{\pi}\right) \right] \quad (3.23)$$

As introduced to me by N. Wheeler<sup>1</sup>, the theta function has this useful property:

$$\Theta_3(z, \tau) = \sqrt{i/\tau} e^{\frac{z^2}{i\pi\tau}} \Theta_3\left(\frac{z}{\tau}, -\frac{1}{\tau}\right) \quad (3.24)$$

Application of the identity results in

$$K_{B,A} = \left(\frac{m}{i\hbar T}\right)^{\frac{1}{2}} \left[ e^{\frac{im}{2\hbar T}(x_b-x_a)^2} \sqrt{\frac{i\pi}{\beta}} e^{\frac{(\zeta-\xi)^2}{i\beta}} \Theta_3\left(\frac{\pi(\zeta-\xi)}{\beta}, -\frac{\pi}{\beta}\right) - e^{\frac{im}{2\hbar T}(x_b+x_a)^2} \sqrt{\frac{i\pi}{\beta}} e^{\frac{(\zeta+\xi)^2}{i\beta}} \Theta_3\left(\frac{\pi(\zeta+\xi)}{\beta}, -\frac{\pi}{\beta}\right) \right] \quad (3.25)$$

At this point we can use the (other) definition of the theta function

$$\Theta_3(z, \tau) = 1 + 2 \sum_{n=1}^{\infty} e^{n^2 i\pi\tau} \cos 2nz \quad (3.26)$$

to carry this argument to its completion. Doing so, and plugging in for  $\xi$ ,  $\zeta$ , and  $\beta$ , we find ourselves face to face with this complicated looking beast

$$K_{B,A} = \sqrt{\frac{m}{i2\pi\hbar T}} \sqrt{\frac{i\pi\hbar T}{2m\ell_a\ell_b}} \left\{ \exp \left[ \frac{im}{2\hbar T}(x_b - x_a)^2 - \frac{i\hbar T \left(\frac{m}{\hbar T}(x_a\ell_b - x_b\ell_a)\right)^2}{2\ell_a\ell_b m} \right] \right. \\ \times \left( 1 + 2 \sum_{n=1}^{\infty} e^{-\frac{i\hbar n^2 \pi^2 T}{2m\ell_a\ell_b}} \cos \left[ \frac{\hbar n \pi T}{m\ell_a\ell_b} \left( \frac{m\ell_b x_a - m\ell_a x_b}{\hbar T} \right) \right] \right) \\ - \exp \left[ \frac{im}{2\hbar T}(x_b + x_a)^2 - \frac{i\hbar T \left(\frac{m}{\hbar T}(x_a\ell_b + x_b\ell_a)\right)^2}{2\ell_a\ell_b m} \right] \\ \left. \times \left( 1 + 2 \sum_{n=1}^{\infty} e^{-\frac{i\hbar n^2 \pi^2 T}{2m\ell_a\ell_b}} \cos \left[ \frac{\hbar n \pi T}{m\ell_a\ell_b} \left( \frac{m\ell_b x_a + m\ell_a x_b}{\hbar T} \right) \right] \right) \right\}$$

<sup>1</sup>*Applied Theta Functions*, Wheeler (1997), page 7. A clear and encompassing exposition on theta functions is contained in *A Brief Introduction to Theta Functions*, Bellman (1961) [13].

Now, this looks terrible, but *blue* is actually equal to *red*. Let us call these terms *exp#1*. Inside the braces, we are left with

$$\left\{ \left( 1 + 2 \sum \text{exp} \cdot \cos \right) - \left( 1 + 2 \sum \text{exp} \cdot \cos \right) \right\}$$

The 1's cancel, and both the purple exponential terms are the same, call them *exp#2*. The two cosine terms differ only by a minus sign; that is, they are of the form  $\cos(A - B) - \cos(A + B) = 2 \sin(A) \sin(B)$ . Also, within  $A$  and  $B$ , the  $\hbar$ ,  $m$  and  $T$  cancel, resulting in  $A = \frac{n\pi x_a}{\ell_a}$  and  $B = \frac{n\pi x_b}{\ell_b}$ . Finally, writing the time as  $T = \frac{\ell_b - \ell_a}{u}$  greatly reduces *exp#1*, which then becomes  $\exp\left[\frac{imu}{2\hbar}\left(\frac{x_b^2}{\ell_b} - \frac{x_a^2}{\ell_a}\right)\right]$ . We then have

$$\sqrt{\text{constants}} \cdot \text{exp\#1} \left( \sum \text{exp \#2} [\sin \#1 \cdot \sin \#2] \right)$$

Writing everything out explicitly, this is the propagator in its final form:

$$\begin{aligned} K[x_b, t_b; x_a, t_a] &= \frac{2}{\sqrt{\ell_a \ell_b}} \exp\left[\frac{imu}{2\hbar}\left(\frac{x_b^2}{\ell_b} - \frac{x_a^2}{\ell_a}\right)\right] \\ &\times \sum_{n=1}^{\infty} \exp\left[\frac{i\hbar n^2 \pi^2}{2mu}\left(\frac{1}{\ell_b} - \frac{1}{\ell_a}\right)\right] \sin\left(\frac{n\pi x_a}{\ell_a}\right) \sin\left(\frac{n\pi x_b}{\ell_b}\right) \quad (3.27) \end{aligned}$$

Take note of two things: first, this result is in agreement with the literature, specifically with da Luz and Cheng [6] and, presumably, all their references. Second, this result is exact, describing the evolution of any wavefunction in linearly expanding or contracting infinite-potential square wells.



# 4

## Analysis of the Derived Propagator

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**4.1 A short pause** I feel that a short rest is in order at this point. In the previous chapter I went through quite the non-trivial calculation culminating in, I would say, the unexpected result of an exact propagator. Of course, Chapter 2 includes a derivation of exact eigenfunctions for this system, so naturally an exact propagator must exist. At the same time, without having *previously* discovered those eigenstates it is not obvious that an exact propagator exists for a system with a time-dependent potential. Furthermore, the propagator was derived utilizing *only classical information*; we considered a particle in a box, worked out how it traveled classically through the box, and from that, with the help of the Jacobi's theta function, came to our answer. Introduction of the theta function essentially spurred a shift from a particle-like, classical discussion to a wave-like, quantum mechanical discussion. With that in mind, we can begin to probe this propagator, and see what it tells us about the system at hand.

**4.2 Analysis of the propagator** Now that we have the propagator for particle motion in an expanding box we should check it against what is already known to see if it makes sense. Before we do that, though, I'd like to rewrite the propagator. Generally, we are interested in how systems evolve with time, but, as equation (3.27) displays it, time is buried within the wall speed,  $u$ , and the final well length  $\ell_b$ . Now, the origin of time is a free parameter, so let us designate  $t_a = 0$  and call  $t_b = t$ ; this means  $\ell_a$  is the original length of the wall, so we call it  $\ell_0$ , and let  $\ell_b = \ell(t)$ . Renaming the variables in that way makes the velocity of the wall  $u = (\ell(t) - \ell_0)/t$ . Finally,

in keeping with convention, let us call the initial particle position  $x_a = y$  and final particle position  $x_b = x$ . Then the propagator is (I can think of two ways to write the summation)

$$K[x, t; y, 0] = \frac{2}{\sqrt{\ell_0 \ell(t)}} \exp\left[\frac{imu}{2\hbar}\left(\frac{x^2}{\ell(t)} - \frac{y^2}{\ell_0}\right)\right] \\ \times \sum_{n=1}^{\infty} \exp\left[\frac{in^2\pi^2\hbar}{2mu}\left(\frac{1}{\ell(t)} - \frac{1}{\ell_0}\right)\right] \sin\left(\frac{n\pi y}{\ell_0}\right) \sin\left(\frac{n\pi x}{\ell(t)}\right) \quad (4.1.1)$$

---


$$\text{OR} \quad \times \sum_{n=1}^{\infty} \exp\left[-\frac{in^2\pi^2\hbar}{2m\ell_0\ell(t)} t\right] \sin\left(\frac{n\pi y}{\ell_0}\right) \sin\left(\frac{n\pi x}{\ell(t)}\right) \quad (4.1.2)$$

These two expressions are exactly the same. Getting to the second from the first simply requires that  $u$  be written  $(\ell(t) - \ell_0)/t$  and straightforward algebra provides the rest. So, the only difference between the two equations is how the second exponential term is written. Because the energy of the system lives within the exponential term, this difference can lead to some confusion<sup>1</sup> on how to *define* the energy of the system. Doing so is not, on the surface, a transparent endeavor, but requires a bit of argument. Interestingly, (4.1.2) agrees in form with the eigenfunctions provided by Doescher and Rice (see (2.23), page 14), whereas (4.1.1) agrees with da Luz and Cheng, as well as Berry and Klein [5]. Again, both ways of writing the propagator are equivalent, but I believe my way (4.1.2) avoids confusion when finding the spectral resolution of the propagator. Section 4.4 clarifies the distinction between the two.

Continuing, recall the development of propagators for time independent Hamiltonians. Generally, the Schrödinger equation tells us

$$\mathbf{H}\psi(x, t) = i\hbar\frac{\partial}{\partial t}\psi(x, t) \quad (4.2.1)$$

When  $\mathbf{H}$  is independent of time, separation of variables allows us to write

$$\mathbf{H}\psi(x) = E\psi(x) \quad (4.2.2)$$

---

<sup>1</sup>da Luz and Cheng mention in their article ([6], *J.Phys.A: Math. Gen.*, **25**, 1992, page L1047) that Doescher and Rice include an extra term in their wavefunction, stating that the term does not appear in the propagator. In fact, it appears explicitly in the propagator written as (4.1.2).



Such a system has a set of orthonormal, complete eigenstates  $|\psi_n\rangle$ , in the sense that

$$\sum_n |\psi_n\rangle\langle\psi_n| = \mathbf{1} \quad \text{and} \quad \langle\psi_n|\psi_m\rangle = \delta_{mn} \quad (4.2.3)$$

where we are now using the Dirac notation, as described in [14]. The  $n^{\text{th}}$  eigenstate  $|\psi_n\rangle$  has energy  $E_n$ . The set of  $|\psi_n\rangle$  is a basis, so we can write anything in the space in terms of them. In particular, we can write

$$\mathbf{H} = \sum_n |\psi_n\rangle E_n \langle\psi_n| \quad (4.2.4)$$

and, because of orthonormality,

$$\mathbf{H}^k = \sum_n |\psi_n\rangle E_n^k \langle\psi_n| \quad (4.2.5)$$

Now, the propagator for a system with a time-independent Hamiltonian is  $K = \exp(-i/\hbar \mathbf{H}t)$ . By expansion in a formal series, and use of (4.2.5), we can write the propagator as a weighted sum of the associated eigenstates

$$K(x, t; y, 0) = \sum_n |\psi_n\rangle e^{-i/\hbar E_n t} \langle\psi_n| \quad (4.2.6)$$

which is, stepping now out of the Dirac notation and into that of wavefunctions,

$$= \sum_n e^{-i/\hbar E_n t} \psi_n(x) \psi_n^*(y) \quad (4.2.7)$$

Our propagator, in either flavor found at (4.1), looks strikingly similar to this. If we decide to directly compare our derived propagator with (4.2.7), we would write, in the SECOND (4.1.2) case

$$\psi_n(x) = \sqrt{\frac{2}{\ell_b}} \exp\left[\frac{imux^2}{2\hbar\ell_b}\right] \sin\left(\frac{n\pi x}{\ell_b}\right) \quad (4.3)$$

$$\psi_n^*(y) = \sqrt{\frac{2}{\ell_0}} \exp\left[-\frac{imuy^2}{2\hbar\ell_0}\right] \sin\left(\frac{n\pi y}{\ell_0}\right) \quad (4.4)$$

$$\text{with energy} \quad E_n(t) = \frac{\hbar^2 n^2 \pi^2}{2m\ell_0\ell_b} \quad (4.5)$$

where I have distributed the coefficient  $\frac{2}{\sqrt{\ell_0 \ell_b}}$  between  $\psi(x)$  and  $\psi(y)$  in the seemingly appropriate fashion.

Now think about the propagator as suggested by (4.1.1). The exponential term in this case doesn't adhere closely to the form  $\exp(-i/\hbar E_n t)$ , but if we just separate out the initial and final wavefunctions like so

$$\psi_n(x) = \sqrt{\frac{2}{\ell_b}} \exp\left[\frac{imux^2}{2\hbar\ell_b} + \frac{in^2\pi^2\hbar}{2mul_b}\right] \sin\left(\frac{n\pi x}{\ell_b}\right) \quad (4.6)$$

$$\psi_n^*(y) = \sqrt{\frac{2}{\ell_0}} \exp\left[-\frac{imuy^2}{2\hbar\ell_0} - \frac{in^2\pi^2\hbar}{2mul_0}\right] \sin\left(\frac{n\pi y}{\ell_0}\right) \quad (4.7)$$

then the energy is buried in each:

$$E_n(t; \psi_n(x)) = -\frac{n^2\pi^2\hbar^2}{2mul_b} \quad \text{or} \quad E_n(t; \psi_n(y)) = -\frac{n^2\pi^2\hbar^2}{2mul_0}$$

$$\text{and in general we write} \quad E_n(t) = -\frac{n^2\pi^2\hbar^2}{2ul(t)} \quad (4.8)$$

First off, there's a problem with the sign of the energy; it seems to come in negative, the opposite of what we would expect. Second, it is unclear if the full exponential in (4.6) and (4.7) needs to be included in the energy, or just one of the terms. Either way these wavefunctions don't agree with the wavefunction at (4.3). Conflict arises between the two conceptions because they each have different purported energies. In former case the denominator of the energy goes as

$$\ell_0\ell_b = \ell_0(\ell_0 + ut) = \ell_0^2 + \ell_0 ut$$

whereas in the latter case the denominator is

$$ul(t) = \frac{\ell_b - \ell_0}{t} \ell_b = \ell_b^2/t - \ell_0\ell_b/t$$

For now, note that there is a conflict in energy. See §4.4 for a proper discussion and proposed resolution of this problem, but in the meantime accept that the wavefunctions as written at (4.3) are correct, whereas the wavefunctions written as (4.6) are not.

Moving forward, recall that  $\ell_b$  evolves in the straightforward fashion  $\ell_b(t) = \ell_0 + ut$  which we designate  $\ell \equiv \ell(t)$ , the time dependent length

of the well. Working from (4.1.2), we are now in position to write down  $\psi_n(x)$ , the “stationary-state”-esque wavefunction at any time  $t > 0$ :

$$\psi_n(x) = \sqrt{\frac{2}{\ell}} \exp\left[\frac{imux^2}{2\hbar\ell}\right] \sin\left(\frac{n\pi x}{\ell}\right) \quad (4.9)$$

with “eigenvalue”-esque energy

$$E_n(t) = \frac{\hbar^2 n^2 \pi^2}{2m\ell_0\ell} \quad (4.10)$$

But look at this! When the wall doesn’t move,  $u = 0$ ,  $\ell(t) = \ell_0$ , and we have exactly the energy eigenstates and eigenvalues for a particle in an infinite square well. Apparently, we have crept up to the classic example from behind, and lent some credence to the notion<sup>2</sup> of letting the wave function in a time-dependent Hamiltonian acquire its time dependence by taking normally stationary items—energy, wall length, ...—and writing them in time parametrized form.

There is, however, one extra bit. In addition to the straightforward insertion of time into a formerly static problem, the eigenfunctions pick up the exponential factor  $\exp\left(\frac{imux^2}{2\hbar\ell}\right)$ . It is unclear, as yet, where that comes from *physically*, what its significance may be, or how to interpret its inclusion in the wavefunction. Its existence raises several questions. I find particular interest in whether similar factors arise in other time dependent systems, and, if they do, how those factors relate for various types of systems. Based on the present discussion, I would expect something analogous to appear in the wavefunctions and propagators for an expanding spherical shell, or a well with an oscillating wall, or any number of other circumstances<sup>3</sup>.

Regardless, we have at (4.1) the propagator written in its spectral representation, based on the associated Hamiltonian, from which we have pulled out a set of eigenfunctions. It is interesting to note that, as promised, nowhere in our argument was the wall velocity  $u$  assumed to be positive. It follows that, as long as the final position of the particle is inside the final well width ( $0 \leq x_b \leq \ell_b$ ) this derivation works equally well for compressions as for expansions. Furthermore, if the well is expanding a particle inside of it loses

<sup>2</sup>See Doescher and Rice’s brief paper [4] and §2.2 of the present work.

<sup>3</sup>A paper by Berry and Klein [5] seems to address this issue, among others. Section §6.2 in the current work briefly dances with the idea, but a full and detailed discussion proved to be outside the scope of this paper.

velocity with each interaction with the wall. This is another way of saying that the system is *losing energy to, or doing work on*, its surroundings; in the same way, when the well is compressed a particle gains velocity with each interaction and thus the system gains energy. In this way, our derivation supports our intuition about what should happen within the system when we vary the size of the well.

There is still more we can discover by analyzing our results. Note that we actually have two, *mathematically disparate*, forms of the propagator, one from before application of the theta function, and one after. As N. Wheeler points out<sup>4</sup> the former description applies to a particle representation and the latter to a wave representation. The theta function, in effect, brought us from statements about particle trajectories and classical actions to Fourier sine series and wave mechanics.

Above we interpreted our results for the wave representation, so now recall the particle description (3.21). After following our renaming scheme as above ( $x_a \rightarrow y$ ,  $x_b \rightarrow x$ ,  $\ell_a \rightarrow \ell_0$ ,  $t_a \rightarrow 0$ ,  $t_b \rightarrow t$ ), we write the propagator in the particle representation as

$$K[x, t; y, 0] = \sqrt{\frac{m}{iht}} \sum_{n=-\infty}^{\infty} \left( \exp \left[ \frac{im}{2\hbar t} (x - y)^2 \right] \exp \left[ \frac{im}{\hbar t} (2\ell_0 \ell_b n^2 - 2(\ell_b y - \ell_a x)n) \right] \right. \\ \left. - \exp \left[ \frac{im}{2\hbar t} (y + x)^2 \right] \exp \left[ \frac{im}{\hbar t} (2\ell_0 \ell_b n^2 + 2(\ell_b y + \ell_a x)n) \right] \right) \quad (4.11)$$

Removing the presently excessive details, this is

$$K = \sqrt{\frac{1}{t}} \sum_{n=-\infty}^{\infty} e^{(\text{imaginary})\frac{n^2}{t}} \left( e^{(\text{real})n} e^{(\text{imaginary})\frac{1}{t}} - e^{(\text{real})n} e^{(\text{imaginary})\frac{1}{t}} \right) \quad (4.12)$$

Every time it appears, time  $t$  is *downstairs*, in the denominator, whereas in the wave representation found at (4.1) time is always up top. This is, apparently, a general feature of all systems suitably described in terms of theta functions. Compare this to the cases of a particle confined to a one dimensional ring or stationary box as discussed in *Applied Theta Functions* by Wheeler [15], where in the short-time limit ( $t \downarrow 0$ ) quantum mechanics

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<sup>4</sup>See *Applied Theta Functions* (1992) as well as *Feynman Quantization in a Box* from *Feynman Formalism for Polygonal Domains: Research 1971-76*, N. Wheeler.

becomes, in a sense, classical; the same is usually said when  $\hbar \downarrow 0$ . Both the particle and wave representations should exhibit this characteristic, though it is more easily seen in the particle representation, to which we now divert our attention.

**4.3 Short-time limit and the delta function** A propagator essentially tells a system how to evolve in time. Therefore, a general feature of a propagator  $K[x_b, t_b; x_a, t_a]$  is that for short time intervals  $(t_b - t_a) \downarrow 0$ , it should become a delta function<sup>5</sup>. That is, the propagator is a wavefunction, specifically the wavefunction that evolves from a delta function. A delta function, of course, is a function Dirac invented while working out his version of quantum mechanics. Briefly, Dirac needed

$$\psi_q = \int a(p - q)\psi_p dp$$

so he wrote

$$\int_{-\infty}^{\infty} \delta(x) dx = 1$$

resulting in, after some formal setup work,

$$\int_{-\infty}^{\infty} f(x)\delta(x - a) dx = f(a)$$

At this point, Wheeler steps in with the Gaussian, a function applicable to a great variety of subjects but especially relevant for probabilistic discussions, to write

$$k(x - a; \epsilon) \equiv \frac{1}{\epsilon\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x - a}{\epsilon}\right)^2\right) \quad (4.13)$$

Again familiar in the context of probability theory,  $\epsilon$  describes the width of the Gaussian, and, when  $\epsilon \downarrow 0$  the function increasingly becomes a spike of area 1; that is, a delta function. Bringing this knowledge to bear on the

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<sup>5</sup>I here follow Wheeler Ch. 0 pp. 43–44[14], who in turn follows Dirac §22 [16]. Dirac writes of the constraints on the  $\delta$  function from its inception and, if one knows the answer in advance, it is clear that a Gaussian can fit the bill nicely.

present topic, we can say that any kernel described as a Gaussian should, in some limit, become a delta function. Looking back to the propagator for an expanding/contracting square well found at (4.11), we identify these important elements:

- $x \rightarrow x$
- $a \rightarrow y$
- $\epsilon \rightarrow \sqrt{\frac{i\hbar t}{m}}$

“Wait!” one might exclaim, “we don’t have a Gaussian at (4.11), but rather a sum and product of Gaussians!” True as that may be, it doesn’t affect our argument, as sums and products of Gaussians are still Gaussians, and when the time interval becomes small, our propagator, evidently, becomes sharply peaked, and in the limit turns into a delta function. Thus, if  $t_a = 0$  and  $t_b = t$ , we have

$$\psi(x) = \int K[x, t; y, 0]\psi(y)dx \quad (4.14)$$

Borrowing the notation at (4.13), this is

$$= \int K[x - y; t]\psi(y)dx \quad (4.15)$$

which becomes, for  $t \downarrow 0$

$$\lim_{t \downarrow 0} \psi(x) = \lim_{t \downarrow 0} \int K[x - y; t]\psi(y)dx = \psi(y) \quad (4.16)$$

In section §5.2 we calculate this numerically and display it graphically as well.

**4.4 Energy defined** In the previous section I began an (unresolved) discussion of the energy of the system. The inherent problem facing us there was that, as yet, the energy was not a well defined concept, but rather one

that needs some meaning given to it. This section attempts to do so by appealing to the work-energy principle, whereby

$$\nabla E = -\mathbf{F}$$

By way of setup, consider the case of a stationary square well. The energy is

$$E_n = \frac{n^2\pi^2\hbar^2}{2m\ell^2}$$

We can think of the work energy principle as telling us that, in order for the wall *not* to move it must exert a force on the system of

$$F = -\frac{dE_n}{d\ell} = \frac{n^2\pi^2\hbar^2}{m\ell^3}$$

This implies the existence of some sort of “quantum pressure,” which I presume relates to the mass, volume, energy, and other properties of a system in an analogous fashion to thermodynamics<sup>6</sup>. If we were to integrate this from  $\ell_0$  to  $\infty$  we would find the total work the system can do on its surrounding to be  $\frac{n^2\pi^2\hbar^2}{2m\ell_0^2}$ . As expected, the system cannot do more work than the energy it started with.

With general concept of this argument now spelled out, we can turn attention to the current speculation. Specifically, we have at §4.2 placed on the table several ways to conceptualize energy. Which way(s) make sense, given the work energy principle? Let us start with the energy supplied through the Schrödinger formulation of §2.2.3:

$$E_n = \frac{n^2\pi^2\hbar^2}{2m\ell_0\ell} \tag{4.17}$$

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<sup>6</sup>As an example, the now standard magneto-optical trap (MOT), used to trap/cool atoms via interaction with and between laser beams, essentially exhibits this feature. In that case the size of the magnetic bowl is constant, so we would expect more atoms, that is, more mass, in the same size bowl to require more “force,” supplied by the intensity of the laser, to keep the system stable. In the same way, more powerful lasers should enable the experimenter to trap more atoms. Such seems to be the case, although a colleague—N.Tompkins—who works with MOT’s knows of no published document exploring the relation between laser intensity and number of trapped atoms.

The wall moves like  $\ell = \ell_0 + ut$ . This expansion<sup>7</sup> defines a change in energy recognized as work done by the system on its surroundings. That is, the system exerts a force on the wall of

$$F = \frac{dE_n}{d\ell} = -\frac{n^2\pi^2\hbar^2}{2m} \frac{1}{\ell_0\ell^2} \quad (4.18)$$

We then ask the question, “What is the total work the system can do?” We find this by integrating the force from  $\ell_0$  to  $\infty$

$$\int_x F \cdot dx = \int_{\ell_0}^{\infty} \frac{dE_n}{d\ell} d\ell = E_n \Big|_{\ell_0}^{\infty} = -\frac{n^2\pi^2\hbar^2}{2m\ell_0^2} \quad (4.19)$$

This is precisely what we expect: the system can “give back” the initial energy, but no more.

Now we look to the other possible energies defined by the propagator. da Luz and Cheng<sup>8</sup> seem to identify only part of the exponential term with energy. We know energy in a square well comes in the form  $\exp(-i/\hbar E_n t)$ , so we identify:

$$E_n = \frac{in^2\pi^2\hbar^2}{2m\ell t} \quad (4.20)$$

but  $u = \frac{1}{t}(\ell - \ell_0)$ , so we write the above as

$$E_n = \frac{in^2\pi^2\hbar^2}{2m(\ell^2 - \ell\ell_0)} \quad (4.21)$$

For expansion, the system exerts a force on the wall of

$$F = \frac{dE_n}{d\ell} = -\frac{in^2\pi^2\hbar^2}{2m} \frac{2\ell - \ell_0}{\ell^2(\ell - \ell_0)^2} \quad (4.22)$$

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<sup>8</sup>*J. Phys. A: Math. Gen.***25**(1992). See page L1047, equation (33):

$$\psi_n(x, t) \sqrt{\frac{2}{\ell}} \exp\left(\frac{imux^2}{2\hbar\ell}\right) \sin\left(\frac{n\pi x}{\ell}\right) \exp\left(\frac{in^2\pi^2\hbar}{2m\ell t}\right)$$

Their dissection of the exponential term seems to associate the second exponential term with energy and the first with... something else.



Integrated from  $\ell_0$  to  $\infty$  gives

$$-\frac{in^2\pi^2\hbar^2}{2m} \frac{1}{\ell_0^2 - \ell_0^2} \quad (4.23)$$

and we have a problem. Apparently, this gives back infinite energy. But perhaps we must include the entire exponential term from (4.1.1). This is:

$$\frac{imu x^2}{2\hbar\ell} + \frac{in^2\pi^2\hbar^2}{2mul} = \frac{i}{\hbar} \left( \frac{m^2 u^2 x^2 + n^2 \pi^2 \hbar^2}{2mul} \right) \quad (4.24)$$

Again, using  $u = (\ell - \ell_0)\frac{1}{t}$ , this is

$$\frac{i}{\hbar} \left( \frac{m^2 \left( (\ell - \ell_0)\frac{1}{t} \right)^2 x^2 + n^2 \pi^2 \hbar^2}{2m(\ell^2 - \ell\ell_0)} \right) t$$

Therefore, we identify the energy to be

$$\frac{m^2 \left( (\ell - \ell_0)\frac{1}{t} \right)^2 x^2 + n^2 \pi^2 \hbar^2}{2m(\ell^2 - \ell\ell_0)} \quad (4.25)$$

At this point we evaluate the energy at  $\infty$  and  $\ell_0$  and see that both limits contribute an infinite amount of energy. That's not physically admissible, so we conclude that this is not a valid energy, but the proposed energy at (4.17) is valid. This is in agreement with Doescher and Rice [4], and follows naturally from the propagator as written at (4.1.2). Additionally, while the propagator written as (4.1.1) is correct and exactly equivalent to (4.1.2), it is somewhat misleading. Rather than explicitly containing the time information, that kernel buries it in two places: first in the wall velocity  $u$ , then again in the wall length  $1/\ell_b$ . Because of this, da Luz and Cheng determined that Doescher and Rice had an extra term, where in fact there was none. da Luz and Cheng simply seem to have misinterpreted their result.

I would like to briefly entertain a discussion of this “quantum pressure” idea. Above we studied the energy of our system by taking derivatives of the energy  $E$  with respect to the volume, in this case the well width  $\ell$ :  $\frac{\partial E}{\partial \ell} \equiv -p$ . In general this is what we mean by pressure. Say we have some amount of gas, for instance, surrounded by a balloon; the gas expands to form a sphere, the shape which minimizes its energy, until the pressure outside the balloon

is the same as that within. A change in the volume of the balloon corresponds to a change in energy, and thus determines the pressure of the system.

In our case we find the pressure from the energy of the system (4.17):

$$\frac{\partial}{\partial \ell} E_n = \frac{\partial}{\partial \ell} \left( \frac{n^2 \pi^2 \hbar^2}{2m \ell_0 \ell} \right) = \frac{dE_n}{d\ell} = -\frac{n^2 \pi^2 \hbar^2}{2m} \frac{1}{\ell_0 \ell^2}$$

so that our pressure is

$$p \equiv -\partial_\ell E_n = \frac{n^2 \pi^2 \hbar^2}{2m \ell_0 \ell} \frac{1}{\ell} = \frac{E_n}{\ell}$$

Note that this has units of force. It seems that a one dimensional pressure is a force. I suppose there is no mystery in the origin of this pressure, but rather it is analogous to thermodynamic pressure. Thermodynamically, pressure arises from statistical interactions of large numbers of particles with an enclosing container. The smaller the space in which these particles are confined, the more they collide with their boundaries, and hence the more pressure they exert. Either way, we have a system where it is energetically favorable to fill all of space. Restricting it from doing so necessarily increases its energy.

# 5

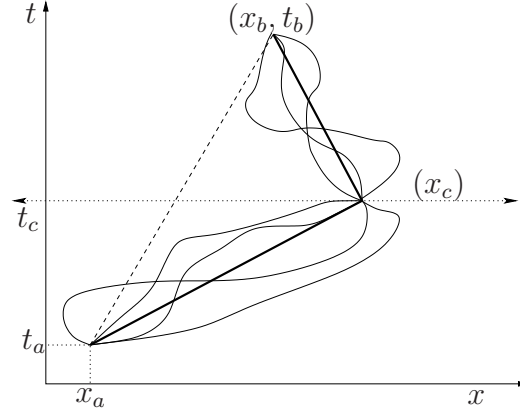
## Convolved Kernels and Arbitrary Wall Movement

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The discussions of the previous three chapters have found at their end all the equations governing one dimensional square wells with one wall uniformly evolving in time. From these, all properties of the system one normally calculates—probability densities, movement expectation values, etc.—are computationally approachable. In the grand scheme of things, however, it would be nice to know about other, less admittedly pedantic, systems. The question then arises, *can we apply what we have learned so far to more complex systems?* We may wish, for instance, to study expanding/contracting shells, higher-dimensional boxes, boxes with odd shapes, wells accelerating walls, or any number of related systems. Many of those systems, while physically related to the present one, may be mathematically or computationally far removed, in which case the answers to questions about them may require more information than we now possess. At the moment, though, we are in a wonderful position to probe some formal aspects of closely related scenarios.

**5.1 Convolution** Our goal in this section is to describe systems with arbitrary wall movement. To do so we need to know how propagators interact with one another, the reasons for which will become clear momentarily. To that end, recall how we first introduced the kernel on page 32 at (3.3):

$$K = a \int_{\text{all paths}} e^{\frac{i}{\hbar} S_{cl}[x(t)]}$$



**Figure 5.1:** Path of a free particle traveling  $A \rightarrow C \rightarrow B$ . The corresponding kernel results from the convolution of the kernels  $K[C, B]$  and  $K[A, C]$ , integrated over all possible values of  $x_c$  at  $C$ . Thick lines are the dynamical path for each stage, thin lines represent all possible paths, the dotted line represents integration over  $x_c$ , and the dashed is the dynamical path  $A \rightarrow B$  for a free particle.

where  $a$  is just some constant. Say the particle under study traveled from  $x_a$  to  $x_c$  and then from  $x_c$  to  $x_b$ . The action for the total movement  $x_a \rightarrow x_b$  is simply the action of the first leg added to the second:

$$S[B, A] = S[B, C] + S[C, A]$$

in which case the propagator is

$$\begin{aligned} K[B, A] &= \int e^{\frac{i}{\hbar} S_{cl}[x(t)]} = \int e^{\frac{i}{\hbar} (S[B, C] + S[C, A])} \\ &= \int e^{\frac{i}{\hbar} S[B, C]} e^{\frac{i}{\hbar} S[C, A]} \end{aligned}$$

Summing over paths entails, as suggested in Figure 5.1, integrating over the point  $x_c$  at time  $t_c$ . Thus the total propagator is the convolution of two sub-propagators

$$K[B, A] = \int K[B, C] K[C, A] dx_c$$

Any path can be dissected in this manner, whether or not any physical event or change occurs at the intervening time. The notation implies reading  $K[B, A]$  as “the propagator for  $A \rightarrow B$ , passing through  $C$ .”

**Example: Free Particle**

Consider the case of a free particle where the kernel is

$$K[B, A] = \sqrt{\frac{m}{i\hbar(t_b - t_a)}} e^{\frac{i}{\hbar} \frac{m}{2} \frac{(x_b - x_a)^2}{t_b - t_a}} \quad (\text{Ex.1})$$

For the situation shown in Figure 5.1, we would write the convolution as

$$K[B, A] = \int \sqrt{\frac{m}{i\hbar(t_b - t_c)}} e^{\frac{i}{\hbar} \frac{m}{2} \frac{(x_c - x_b)^2}{t_c - t_b}} \sqrt{\frac{m}{i\hbar(t_c - t_a)}} e^{\frac{i}{\hbar} \frac{m}{2} \frac{(x_c - x_a)^2}{t_c - t_a}} dx_c$$

Collecting and removing from the integral everything that doesn't depend on  $x_c$ , this is

$$= \sqrt{\alpha} \sqrt{\beta} e^{-\left(\frac{\alpha}{2} x_a^2 + \frac{\beta}{2} x_b^2\right)} \int_{-\infty}^{\infty} e^{-\frac{\alpha + \beta}{2} x_c^2 - (\alpha x_a + \beta x_b) x_c} dx_c$$

where  $\alpha = \frac{m}{i\hbar(t_b - t_c)}$  and  $\beta = \frac{m}{i\hbar(t_c - t_a)}$

This integral has solution

$$= \sqrt{\alpha\beta} \sqrt{\frac{2\pi}{\alpha + \beta}} e^{-\frac{\alpha\beta(x_a - x_b)^2}{2(\alpha + \beta)}}$$

Plugging  $\alpha$  and  $\beta$  back into the above reproduces precisely the free particle propagator (Ex.1) for  $A \rightarrow B$ , as it should.

Note that writing (5.1) doesn't rely on the particle itself doing anything. Rather, any time any aspect of the system changes that results in a change in the propagator, we can write down a total propagator as the convolution of one before and one after the event. Returning to the specific case of a particle in a box, we can perform the analogous computation of  $K[B, A]$  to find the propagator for the path  $(x_a, t_a) \rightarrow (x_c, t_c) \rightarrow (x_b, t_b)$  in the case where the wall changes velocity from  $u$  to  $v$ .  $v$ , of course, can assume any (real) value.

Pay close attention because this calculation is a bit of a beast. First recall that the propagator of a particle in an expanding/contracting square well is, from (4.1.2),

$$K[x_b, t; x_a, 0] = \frac{2}{\sqrt{\ell_a \ell_b}} \exp\left[\frac{imu}{2\hbar}\left(\frac{x_b^2}{\ell_b} - \frac{x_a^2}{\ell_a}\right)\right] \times \sum_{n=1}^{\infty} \exp\left[-\frac{in^2\pi^2\hbar}{2m\ell_a\ell_b}t\right] \sin\left(\frac{n\pi x_a}{\ell_a}\right) \sin\left(\frac{n\pi x_b}{\ell_b}\right) \quad (5.2)$$

Using the propagator clothed as such, the convolved propagator is

$$K[B, A] = \int K[B, C]K[C, A]dx_c = \int \frac{2}{\sqrt{\ell_a \ell_c}} \exp\left[\frac{imu}{2\hbar}\left(\frac{x_c^2}{\ell_c} - \frac{x_a^2}{\ell_a}\right)\right] \frac{2}{\sqrt{\ell_c \ell_b}} \exp\left[\frac{imv}{2\hbar}\left(\frac{x_b^2}{\ell_b} - \frac{x_c^2}{\ell_c}\right)\right] \times \sum_{n=1}^{\infty} \exp\left[-\frac{in^2\pi^2\hbar}{2m\ell_a\ell_c}(t_c - t_a)\right] \sin\left(\frac{n\pi x_a}{\ell_a}\right) \sin\left(\frac{n\pi x_c}{\ell_c}\right) \times \sum_{\nu=1}^{\infty} \exp\left[-\frac{i\nu^2\pi^2\hbar}{2m\ell_c\ell_b}(t_b - t_c)\right] \sin\left(\frac{\nu\pi x_c}{\ell_c}\right) \sin\left(\frac{\nu\pi x_b}{\ell_b}\right) dx_c \quad (5.3)$$

Some of this can be extracted from the integral

$$\frac{4}{\ell_c \sqrt{\ell_a \ell_b}} e^{\frac{im}{2\hbar}(v\frac{x_b^2}{\ell_b} - u\frac{x_a^2}{\ell_a})} \sum_{n,\nu} \exp\left[-\frac{i\pi^2\hbar}{2m\ell_c}\left(\frac{1}{\ell_a}(t_c - t_a)n^2 + \frac{1}{\ell_b}(t_b - t_c)\nu^2\right)\right] \times \sin\left(\frac{n\pi x_a}{\ell_a}\right) \sin\left(\frac{\nu\pi x_b}{\ell_b}\right) \int_0^{\ell_c} e^{\frac{im}{2\hbar}\frac{(u-\nu)}{\ell_c}x_c^2} \sin\left(\frac{n\pi x_c}{\ell_c}\right) \sin\left(\frac{\nu\pi x_c}{\ell_c}\right) dx_c \quad (5.4)$$

This is a series of integrals of the form

$$\int e^{ax^2} \sin\left(\frac{n\pi}{\ell_c}x\right) \sin\left(\frac{\nu\pi}{\ell_c}x\right) dx$$

which we previously encountered at (2.24) in section 2.3. This isn't surprising at all, as we arrived at that integral while determining the coefficients  $a_n$  of the eigenfunctions  $\phi_n$ ; the propagator is a superposition of these eigenfunctions to begin with. Unfortunately, as we found when studying the  $\phi_n$ 's as well, this integral cannot be solved analytically, but only numerically. Furthermore, whereas the previous case involved a single sum from 0 to  $\infty$ , now we have two such summations—one over  $n$  and one over  $\nu$ .

Briefly, the integral is

$$\begin{aligned} \sqrt{\frac{\pi}{32a}} e^{-\frac{i\pi^2}{4al_c^2}(n+\nu)^2} & \left\{ e^{\frac{i\pi^2 n\nu}{al_c^2}} \left( \mathcal{C} \left[ \frac{2al_c^2 + \pi(n-\nu)}{\sqrt{2\pi a} l_c} \right] + i\mathcal{S} \left[ \frac{2al_c^2 + \pi(n-\nu)}{\sqrt{2\pi a} l_c} \right] \right) \right. \\ & - e^{\frac{i\pi^2 n\nu}{al_c^2}} \left( \mathcal{C} \left[ \frac{-2al_c^2 + \pi(n-\nu)}{\sqrt{2\pi a} l_c} \right] + i\mathcal{S} \left[ \frac{-2al_c^2 + \pi(n-\nu)}{\sqrt{2\pi a} l_c} \right] \right) \\ & + \left( \mathcal{C} \left[ \frac{-2al_c^2 + \pi(n+\nu)}{\sqrt{2\pi a} l_c} \right] + i\mathcal{S} \left[ \frac{-2al_c^2 + \pi(n+\nu)}{\sqrt{2\pi a} l_c} \right] \right) \\ & \left. - \left( \mathcal{C} \left[ \frac{2al_c^2 + \pi(n+\nu)}{\sqrt{2\pi a} l_c} \right] + i\mathcal{S} \left[ \frac{2al_c^2 + \pi(n+\nu)}{\sqrt{2\pi a} l_c} \right] \right) \right\} \end{aligned} \quad (5.5)$$

where the constant  $a$  is

$$\frac{m(u-v)}{2\hbar l_c}$$

and the Fresnel integrals are defined [10]

$$\mathcal{C}(z) \equiv \int_0^z \cos(\pi/2 t^2) dt \quad \mathcal{S}(z) \equiv \int_0^z \sin(\pi/2 t^2) dt \quad (5.6)$$

Let us name the expression (5.5)  $\mathcal{F}(t_c; n, \nu)$  because the time  $t_c$  completely determines every term and  $n$  and  $\nu$  make quick reference to the appropriate summations.

Feigning nonchalance in the face of this tangled mess of equations, let us consider the propagator of two such changes in wall velocities. Say the particle moves along the path  $A \rightarrow C \rightarrow D \rightarrow B$ . Then the propagator is given by

$$\begin{aligned} K[D, A] &= \int K[D, C]K[C, A]dx_c \\ &\downarrow \\ &= \text{bad, as above. And then the second convolution is} \\ K[B, A] &= \int K[B, D]K[D, A]dx_d \\ &= \int K[B, D] \left( \int K[D, C]K[C, A]dx_c \right) dx_d \end{aligned}$$

Now look back at  $\mathcal{F}$  and note that it *does not depend on any  $x$* , and hence can be pulled through any integral. Additionally, call the different wall velocities  $u_1, u_2, u_3, \dots$ , and the summation indices  $n_1, n_2, n_3, \dots$ . Then we can write the above as

$$\begin{aligned}
 K[B, A] &= \int_0^{\ell_d} \frac{2}{\sqrt{\ell_d \ell_b}} \exp\left[\frac{im u_3}{2\hbar} \left(\frac{x_b^2}{\ell_b} - \frac{x_d^2}{\ell_d}\right)\right] \sum_{n_3=1}^{\infty} \exp\left[-\frac{in_3^2 \pi^2 \hbar}{2m \ell_d \ell_b} (t_b - t_d)\right] \\
 &\quad \times \sin\left(\frac{n_3 \pi x_d}{\ell_d}\right) \sin\left(\frac{n_3 \pi x_b}{\ell_b}\right) \left\{ \frac{4}{\ell_c \sqrt{\ell_a \ell_d}} e^{\frac{im}{2\hbar} \left(u_2 \frac{x_d^2}{\ell_d} - u_1 \frac{x_a^2}{\ell_a}\right)} \right. \\
 &\quad \times \sum_{n_1, n_2} \exp\left[-\frac{i\pi^2 \hbar}{2m \ell_c} \left(\frac{1}{\ell_a} (t_c - t_a) n_1^2 + \frac{1}{\ell_d} (t_d - t_c) n_2^2\right)\right] \\
 &\quad \left. \times \sin\left(\frac{n_1 \pi x_a}{\ell_a}\right) \sin\left(\frac{n_2 \pi x_d}{\ell_d}\right) \mathcal{F}(t_c; n_1, n_2) \right\} dx_d \quad (5.7)
 \end{aligned}$$

Once again, several terms can be pulled out front and combined, and the propagator can be written

$$\begin{aligned}
 &= \frac{8}{\ell_c \ell_d \sqrt{\ell_a \ell_b}} e^{\frac{im}{2\hbar} \left(u_3 \frac{x_b^2}{\ell_b} - u_1 \frac{x_a^2}{\ell_a}\right)} \sum_{n_1, n_2, n_3} \left\{ \right. \\
 &\quad \times \exp\left[-\frac{i\pi^2 \hbar}{2m} \left(\frac{1}{\ell_a \ell_c} (t_c - t_a) n_1^2 + \frac{1}{\ell_d \ell_c} (t_d - t_c) n_2^2 + \frac{1}{\ell_d \ell_b} (t_b - t_d) n_3^2\right)\right] \\
 &\quad \times \sin\left(\frac{n_1 \pi x_a}{\ell_a}\right) \sin\left(\frac{n_3 \pi x_b}{\ell_b}\right) \mathcal{F}(t_c; n_1, n_2) \\
 &\quad \left. \times \int e^{\frac{im}{2\hbar} \frac{u_2 - u_3}{\ell_d} x_d^2} \sin\left(\frac{n_3 \pi x_d}{\ell_d}\right) \sin\left(\frac{n_2 \pi x_d}{\ell_d}\right) dx_d \right\}
 \end{aligned}$$

This last integral we have a name for— $\mathcal{F}(t_d; n_2, n_3)$ —so we write the propagator as

$$\begin{aligned}
 K[B, A] &= \frac{8}{\ell_c \ell_d \sqrt{\ell_a \ell_b}} e^{\frac{im}{2\hbar} \left(u_3 \frac{x_b^2}{\ell_b} - u_1 \frac{x_a^2}{\ell_a}\right)} \sum_{n_1, n_2, n_3} \left\{ \right. \\
 &\quad \times \exp\left[-\frac{i\pi^2 \hbar}{2m} \left(\frac{1}{\ell_a \ell_c} (t_c - t_a) n_1^2 + \frac{1}{\ell_d \ell_c} (t_d - t_c) n_2^2 + \frac{1}{\ell_d \ell_b} (t_b - t_d) n_3^2\right)\right] \\
 &\quad \left. \times \sin\left(\frac{n_1 \pi x_a}{\ell_a}\right) \sin\left(\frac{n_3 \pi x_b}{\ell_b}\right) \mathcal{F}(t_c; n_1, n_2) \mathcal{F}(t_d; n_2, n_3) \right\} \quad (5.8)
 \end{aligned}$$



A pattern is starting to develop. Continually inserting successive divisions of time and wall velocity movements adds factors of  $\frac{2}{\ell_i}$  out front, and factors

$$\exp\left[-\frac{i\pi^2\hbar}{2m}\frac{(t_j-t_i)}{\ell_j\ell_i}n_i^2\right] \quad \text{and} \quad \mathcal{F}(t_i; n_{i-1}, n_i)$$

inside the summation. Therefore, in general, the propagator for  $x(t) : A \rightarrow B$ , for (presumably) any wall motion approximated by  $f$  time-divisions is

$$\begin{aligned} K[B, A] &= \prod_{i=1}^f \left(\frac{2}{\ell_i}\right) \frac{2}{\sqrt{\ell_a\ell_b}} e^{\frac{im}{2\hbar}\left(u_f\frac{x_b^2}{\ell_b}-u_1\frac{x_a^2}{\ell_a}\right)} \sum_{n_1, \dots, n_f} \left\{ \right. \\ &\quad \times \exp\left[-\frac{i\pi^2\hbar}{2m} \sum_i \frac{1}{\ell_{i-1}\ell_i} (t_i - t_{i-1}) n_i^2\right] \\ &\quad \left. \times \sin\left(\frac{n_1\pi x_a}{\ell_a}\right) \sin\left(\frac{n_f\pi x_b}{\ell_b}\right) \prod_i \mathcal{F}(t_i; n_{i-1}, n_i) \right\} \quad (5.9) \end{aligned}$$

Taking the limit as  $f \rightarrow \infty$  makes this exact.

We can, at this point, pause and check if the current result makes sense. In particular, we should ask if it reduces to the case of constant wall movement when  $u = v$ . For that purpose it is sufficient to check this collapse for a single kink in the wall's velocity, say at time  $t_c$  and wall position  $\ell_c$ . To that end, review the integral in (5.4) that leads to  $\mathcal{F}$ ; when  $u = v$  the exponential term goes to 1. The integral is then simply

$$\int_0^{\ell_c} \sin\left(\frac{n\pi x}{\ell_c}\right) \sin\left(\frac{\nu\pi x}{\ell_c}\right) dx = \begin{cases} \frac{\ell_c}{2} & \text{for } n = \nu \\ 0 & \text{for } n \neq \nu \end{cases}$$

The integral forces  $\nu = n$  and brings out the constant  $\frac{\ell_c}{2}$ , which cancels with the factor of  $\frac{2}{\ell_c}$  at the front of the propagator<sup>1</sup>. With the removal of all off diagonal elements in the summation, the normalizing factor of  $2/\sqrt{\ell_a\ell_b}$  out front is correct, the exponential term out front is correct, and the two sine

---

<sup>1</sup>When we consider the case of many time divisions, as in (5.9), the collapse of each  $\mathcal{F}_i$  into  $\frac{\ell_i}{2}$  cancels with its corresponding  $\frac{2}{\ell_i}$  out front. In this way the entire first product in (5.9) cancels with the last product.

terms within the summation are correct. What is left is the exponential term inside the summation, to which we now turn our attention. It is

$$\exp\left[-\frac{i\pi^2\hbar}{2m}\left(\frac{1}{\ell_a\ell_c}(t_c-t_a)n^2+\frac{1}{\ell_b\ell_c}(t_b-t_c)n^2\right)\right]$$

which is

$$= \exp\left[-\frac{i\pi^2\hbar n^2}{2m}\left(\frac{(\ell_c-\ell_a)(t_c-t_a)}{(\ell_c-\ell_a)\ell_a\ell_c}+\frac{(\ell_b-\ell_c)(t_b-t_c)}{(\ell_b-\ell_c)\ell_b\ell_c}\right)\right]$$

But  $\frac{t_i-t_j}{\ell_i-\ell_j} = u$  the wall velocity, so

$$= \exp\left[-\frac{i\pi^2\hbar}{2mu}\left(\frac{1}{\ell_a}-\frac{1}{\ell_c}+\frac{1}{\ell_c}-\frac{1}{\ell_b}\right)\right]$$

The two  $1/\ell_c$ 's cancel, and, all told, we are left with

$$\frac{2}{\sqrt{\ell_a\ell_b}} e^{\frac{imu}{2\hbar}\left(\frac{x_b^2}{t_b}-\frac{x_a^2}{t_a}\right)} \sum_n \exp\left[-\frac{i\pi^2\hbar}{2mu}\left(\frac{1}{\ell_a}-\frac{1}{\ell_b}\right)\right] \sin\left(\frac{n\pi x_a}{\ell_a}\right) \sin\left(\frac{n\pi x_b}{\ell_b}\right)$$

which is precisely the derived propagator  $K[x_b, t_b; x_a, t_a]$  at (4.1).

**5.2 Approximations** The argument concluded by equation (5.9) presents a formal method for writing down the propagator for arbitrarily moving boundaries. Unfortunately, the simple elegance of the result is marred by its basic worthless functionality; that is to say, (5.9) is really long and complicated, thus preventing one from actually using it. We can, in this situation, ask what assumptions can be made to better illuminate the transpiring physics. In particular, what happens when the wall velocity changes at only one instant in time, and, further, that the unique “kink” is small? To answer that let us first explicitly write out the propagator in that case. Let the change occur at time  $t_c$ , wall length  $\ell_c$ , with the former velocity being  $u$  and the latter  $v$ . Then, working from (5.4) the propagator is

$$\begin{aligned} K[B, A] &= \frac{2}{\ell_c} \frac{2}{\sqrt{\ell_a\ell_b}} e^{\frac{im}{2\hbar}\left(v\frac{x_b^2}{t_b}-u\frac{x_a^2}{t_a}\right)} \sum_{n, \nu=1}^{\infty} \left\{ \right. \\ &\quad \times \exp\left[-\frac{i\pi^2\hbar}{2m\ell_c}\left(\frac{1}{\ell_a}(t_c-t_a)n^2+\frac{1}{\ell_b}(t_b-t_c)\nu^2\right)\right] \\ &\quad \left. \times \sin\left(\frac{n\pi x_a}{\ell_a}\right) \sin\left(\frac{\nu\pi x_b}{\ell_b}\right) \int_0^{\ell_c} e^{\frac{imx_c^2}{2\hbar}(u-v)} \sin\left(\frac{n\pi x}{\ell_c}\right) \sin\left(\frac{\nu\pi x}{\ell_c}\right) dx \right\} \quad (5.10) \end{aligned}$$

We can expand the exponential inside the integral in terms of  $r \equiv u - v$ . In that case the integral is, to first order in  $r$ ,

$$\begin{aligned} & \int_0^{\ell_c} \left(1 + \frac{imrx^2}{2\hbar} - \dots\right) \sin\left(\frac{n\pi x}{\ell_c}\right) \sin\left(\frac{\nu\pi x}{\ell_c}\right) dx \\ &= \begin{cases} \frac{2i(-1)^{n+\nu}\ell_c^3 m\nu r}{\hbar\pi^2(n^2-\nu^2)^2} & \text{for } n \neq \nu \\ \frac{\ell_c}{2} + \frac{im\ell_c^3 r}{12\hbar} - \frac{im\ell_c^3 r}{8\hbar\pi^2 n^2} & \text{for } n = \nu \end{cases} \end{aligned} \quad (5.11)$$

A note of caution at this point: in throwing out higher order terms, we have removed ourselves from a true propagator, and the object now under discussion may have lost some of the necessary properties, such as being normalized and turning into the delta function on small timescales. At the end of the present argument, we must carefully consider the meaning of our result and determine just how far we have traveled from a real propagator.

That caution aside, let us strip the propagator to its bare essentials and look at only first-order perturbations. Splitting the propagator into two summations helps clarify the proceeding steps. The first summation is over  $n = \nu$ , and contains (from the  $\ell_c/2$  term in (5.11)) the unperturbed propagator, along with on-diagonal corrections. The second summation is over both  $n$  and  $\nu$ , with  $n \neq \nu$ . Sans constants, the propagator is

$$\begin{aligned} K[B, A] &\sim \sum_{\nu=n} e^{-i(n^2+n^2)} \sin(n\pi x) \sin(n\pi y) \left(1 + ir - \frac{ir}{n^2}\right) \\ &\quad + \sum_{\substack{n,\nu \\ n \neq \nu}} e^{-i(n^2+\nu^2)} \sin(n\pi x) \sin(\nu\pi y) \frac{i(-1)^{n+\nu} n\nu r}{(n^2 - \nu^2)^2} \end{aligned}$$

This is interesting. Call the  $n^{\text{th}}$  term of the unperturbed propagator  $k_n$ ; that is,  $k_n = \exp(-2i(n^2)) \sin(n\pi x) \sin(n\pi y)$ . Then the first summation is the unperturbed kernel added to a scaled, imaginary version of itself:

$$\begin{aligned} K' &= \sum_n k_n + ir \sum_n \left(k_n - \frac{k_n}{n^2}\right) \\ &= K_{\text{no kink}} + ir K_{\text{no kink}} - ir \sum_n \frac{k_n}{n^2} \end{aligned}$$

where the prime on  $K'$  indicates that we are looking only at the diagonal ( $n = \nu$ ) terms. Now call the  $(n, \nu)^{\text{th}}$  trigonometric part of the *off diagonal*

terms  $k'_{n,\nu}$ ; that is,  $k'_{n,\nu} = \exp(-i(n^2 + \nu^2)) \sin(n\pi x) \sin(\nu\pi y)$ . Then the off diagonal summation is

$$K'' = ir \sum_{n,\nu} k'_{n,\nu} \frac{(-1)^{n+\nu} n\nu}{(n^2 - \nu^2)^2}$$

This falls off rapidly for terms where the difference  $n - \nu$  is large, and all the more so when either  $n$  or  $\nu$  is large by itself. If we write the fraction in terms of the difference  $a$  so that  $\nu \equiv n + a$ , we see:

$$\begin{aligned} \frac{n\nu}{(n^2 - \nu^2)^2} &= \frac{n(n+a)}{(n^2 - (n+a)^2)^2} = \frac{n^2 + na}{(n + (n+a))^2 (n - (n+a))^2} \\ &= \frac{1 + a/n}{(1 + (1 + a/n))^2 (n - (n+a))^2} \end{aligned}$$

which, when  $n \rightarrow \text{big}$ , is

$$\frac{1}{2^2 a^2} = \frac{1}{4(n - \nu)^2}$$

In which case

$$K'' = ir \sum_{n,\nu} k'_{n,\nu} \frac{(-1)^{n-\nu}}{2^2 (n - \nu)^2}$$

Our summation over two indices defines a matrix  $\mathbb{K}$ , where the  $(n, \nu)^{th}$  element of our summation is  $K_{n\nu}$ . The summation itself amounts to adding all the elements of the matrix together. Now,  $K''$  quickly approaches zero as the difference  $n - \nu$  becomes greater. This means only the diagonal and close to diagonal elements of  $K_{n\nu}$  matter; everything else adds an increasingly insignificant amount to the summation. Therefore, we essentially never need to keep more terms than  $\sim 3N$  terms ( $N$  diagonal terms, and about  $N$  terms on either side of the diagonal). To first order, then, the basic form of the total propagator is

$$\begin{aligned} K &= \sum_n e^{-2in^2} \sin(n\pi x) \sin(n\pi y) \left(1 + ir - \frac{ir}{n^2}\right) \\ &+ ir \sum_{\substack{n,\nu \\ |n-\nu| < 1}} \frac{(-1)^{n-\nu}}{2^2 (n - \nu)^2} e^{-i(n^2 + \nu^2)} \sin(n\pi x) \sin(\nu\pi y) \end{aligned}$$

I include the above simply for ease of reading. Below is the actual total propagator, with all terms and constants included.

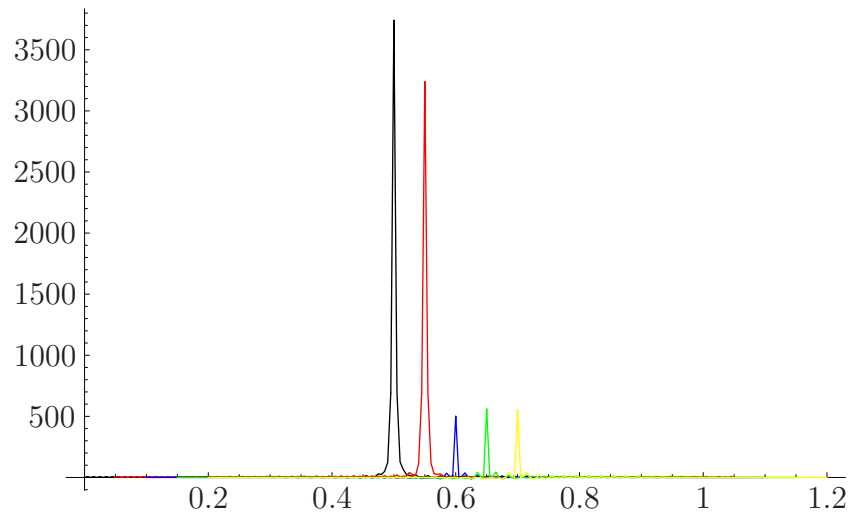
$$\begin{aligned}
K = \frac{2}{\sqrt{\ell_a \ell_b}} e^{\frac{im}{2\hbar}(v \frac{x_b^2}{\ell_b} - u \frac{x_a^2}{\ell_a})} \left\{ \right. \\
\sum_{n=1}^{\infty} \exp \left[ -\frac{i\pi^2 \hbar}{2m\ell_c} \left( \frac{1}{\ell_a} (t_c - t_a) n^2 + \frac{1}{\ell_b} (t_b - t_c) n^2 \right) \right] \\
\times \sin \left( \frac{n\pi x_a}{\ell_a} \right) \sin \left( \frac{n\pi x_b}{\ell_b} \right) \left( 1 + \frac{im\ell_c^2 r}{6\hbar} - \frac{im\ell_c^2 r}{4\hbar\pi^2 n^2} \right) \\
+ \sum_{\substack{n,\nu \\ |n-\nu| < 1}} \exp \left[ -\frac{i\pi^2 \hbar}{2m\ell_c} \left( \frac{1}{\ell_a} (t_c - t_a) \nu^2 + \frac{1}{\ell_b} (t_b - t_c) n^2 \right) \right] \\
\times \sin \left( \frac{n\pi x_a}{\ell_a} \right) \sin \left( \frac{\nu\pi x_b}{\ell_b} \right) \frac{im\ell_c^2 r (-1)^{n-\nu}}{2\hbar\pi^2 (n-\nu)^2} \left. \right\} \quad (5.12)
\end{aligned}$$

Numerical calculations have shown that discarding terms  $|n - \nu| > 1$  only changes the value of  $K$  at any given point by  $< 1\%$  when  $n \sim 2000$ . More to the point, the percent difference between keeping all terms and throwing away terms  $|n - \nu| < 1$  for  $n \sim 20$  is still *less than 5%*. We conclude that our approximation is valid.

Despite its apparent complexity, equation (5.12) is a wonderful expression for numerical analysis, allowing one to generate plots of the probability density  $KK^*$ . Plotted as a function of position within the well, this tells you the probability of a particle, initially at some point  $x_a$  to be at any given spot in the well after some time  $t_b$ .

**5.3 Plots** Recall that the kernel is a wavefunction that evolves from a delta function. We can check both the validity of our numerical calculations and that general property of the kernel calculating and plotting  $|K|^2$  across the breadth of the well. I find the best way to do so is to parametrize time according to well length and wall velocity, then plot  $|K|^2$  as a function of  $\ell(t)$ ; that is, write the propagator as a function  $K[x_a, x_b, \ell_b, \ell_c, \ell_a, u, r]$ , where the final point  $x_b$  is varied in order to produce a graph. Setting  $\ell_b$  very close to  $\ell_a$  corresponds to a short time limit. The resulting plot over all values of  $x_b$  will then be a delta function. This is demonstrated in Figure 5.2, where the kernel

has been calculated for a short time interval to various precision in the off-diagonal elements. The lowest order precision is the black line (call it  $K_{\text{black}}$ ), with  $n = 1000$  and  $|n - \nu| = 1$ . Red corresponds to  $|n - \nu| \leq 5$ , and blue is the difference between black and red.  $|K|^2$  is not actually shown for green and yellow, but rather just the differences  $K_{\text{black}} - K_{\text{green}}$  and  $K_{\text{black}} - K_{\text{yellow}}$ . Green corresponds to  $|N - \nu| \leq 10$ , and yellow  $|n - \nu| \leq 15$ . I'd like to emphasize that *Each successive plot is shifted to the right by  $0.05\ell$  to facilitate visibility.* The actual delta functions all stack up over  $x_b = 0.5\ell$ . This explains why the well width apparently ranges  $\ell : 0 \rightarrow 1.2$  instead of  $\ell : 0 \rightarrow 1$ .

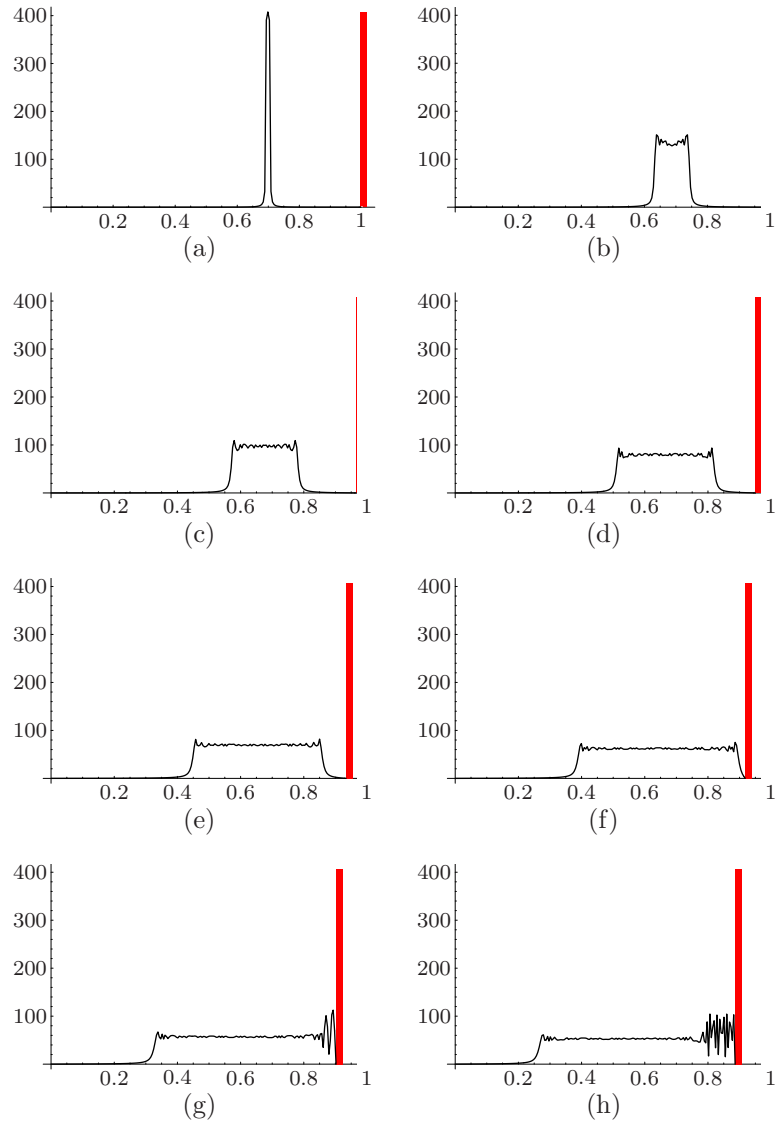


**Figure 5.2:** Plot of  $|K|^2$ , summed to 1000 terms ( $n = \nu = 1000$ ), for a very short amount of time for a particle initially sitting in the middle of the square well. The black line contains terms out to 1 off the diagonal, the red line contains terms out to 5 off the diagonal. The blue line shows the difference between the black and red lines. The green and yellow lines are the differences between the black line and kernels (not displayed) for 10 and 15 off diagonal terms, respectively. Each successive plot was shifted to the right by  $0.05 \ell$  for better visibility. Maximum variance of  $\sim 13\%$  between the lower order approximation (black line) and the better approximations (red, blue, green, and yellow lines) occurs at the peak of the delta function.

There are several things to note in Figure 5.2. First, based on the displayed differences, the maximum variance between the worst approximation (black line) and the approximations where more off diagonal terms are re-

tained is about 13%. This is in marked contrast to the value of  $< 1\%$  difference claimed above. However, this difference is, in fact, circumstantial. The delta function is an object one must expect to run into trouble with during a numeric calculation. So, although our value is off by roughly 13% percent at the peak of the delta function, I claim that, overall, it's just fine. In support of that, look carefully at the width of the difference profiles (blue, green, yellow). In each case the difference rapidly drops to zero on either side of the delta function, so that the approximation is valid up  $\pm 0.003 \ell_c$  from the peak of the delta function. That's pretty damn good, any way you package it.

Figures 5.3, 5.4, and 5.4 show the evolution of the kernel in an expanding square well. In this case the change in wall velocity has been set to zero. As shown, the kernel starts as a delta function, initial peaked about  $0.7\ell$ , and begins collapsing. Because it is off-centered, one side of the collapsing delta function hits a wall before the other. Those right-going-waves reflect off the moving wall (Figure 5.3(g)) and travel back towards the stationary wall. Meanwhile, the left-going-waves eventually bounce off the stationary wall (Figure 5.4(e)) and begin travelling back towards the moving wall. The two wave packets, now quite spread out, begin to interfere with each other at Figure 5.4(h), after which point there seem to be a degree of states it can be in, ranging from mostly disordered, as at Figure 5.5(d), to mostly ordered. And then there are the multiply-ordered states, as seen in Figure 5.4(i) or Figure 5.5(c). As recently pointed out to me by N. Wheeler, similar figures can probably be generated by looking at the moments of launched classical particles; for details concerning that situation, see



**Figure 5.3:** *Evolution of the propagator in a contracting well, frames 1–8.*



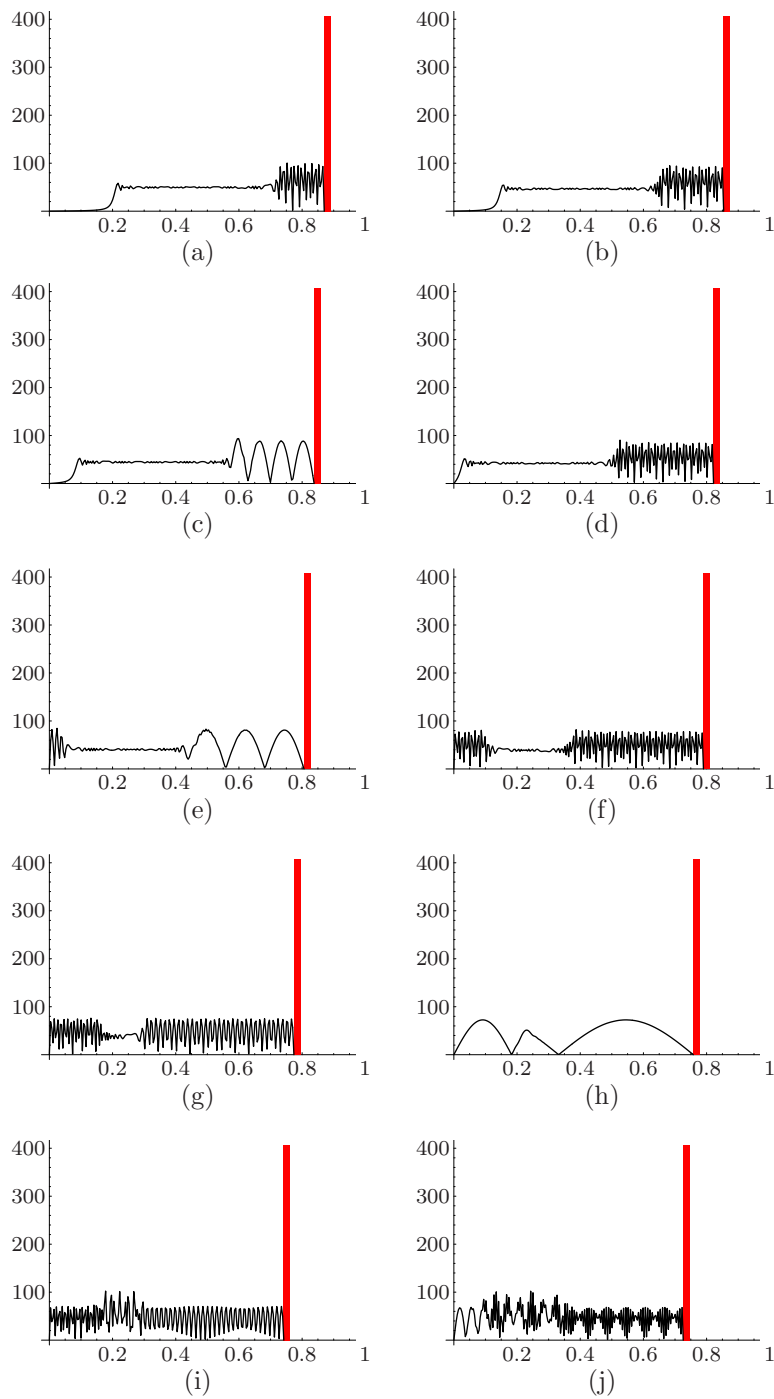
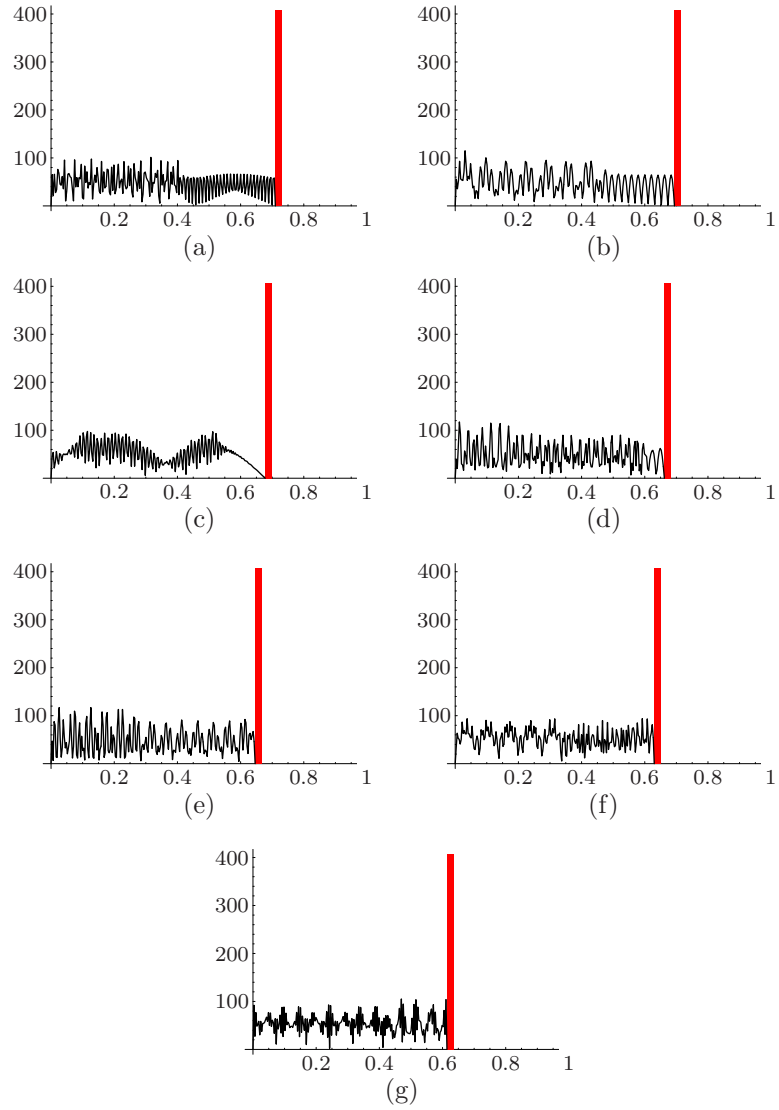


Figure 5.4: Evolution of the propagator in a contracting well, frames 9–18.



**Figure 5.5:** *Evolution of the propagator in a contracting well, frames 19–25.*

# 6

## Related Systems

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**6.1 Another brief pause** Before I delve into the proceeding discussion, I'd like to raise a quick flag. This chapter is, in some respects, disjoint in form and content from the preceding chapters. Previously we concerned ourselves with the discovery and development of properties of the linearly expanding/contracting infinite square well. We found eigenfunctions, energy eigenvalues, wrote down an exact propagator, formally extended that argument to write down other propagators, made charts and graphs of probability densities, and performed other similar tasks. Now we are briefly changing gears before the end of the road to address a question must have been—and indeed, *should* have been—on your mind through the entire trip. The question is, “How often can we actually do this?” That is, under what conditions does an analytic solution to the moving boundary problem exist. For this chapter I simply present an argument for when we can find exact solutions to the wave equation. *How* one might arrive at those solutions is another matter entirely, and one that simply begs for exploration, but for the moment must wait for another day.

**6.2 Derivation of related systems** To begin, consider a system with an isotropic, time dependent potential  $V(x, t)$ , parametrized via some moving boundary  $\ell(t)$ . Say, also, that as the system evolves in time the strength of the potential can fluctuate, and call that allowed fluctuation  $\alpha(\ell(t))$ . Given a Hamiltonian with those dials to twist it turns out we can answer our question. To do so we follow an argument provided by Berry and Klein [5]. Our Hamiltonian is

$$H(\mathbf{r}, \mathbf{p}, \ell(t)) = \frac{p^2}{2m} + \alpha(\ell(t))V\left(\frac{\mathbf{r}}{\ell(t)}\right) \quad (6.1)$$

The basic idea is that, when  $\alpha(\ell)$  and  $\ell(t)$  are suitably chosen, a particle under the influence of this Hamiltonian can be considered to move in a conservative field. Conservative fields are of special interest to us because the forces can be expressed as spatial derivatives of potentials:  $F = -\nabla \cdot V(\mathbf{r})$ . In all such cases a set of eigenfunctions exists that any wavefunction can be expanded in. It follows, then, that when we are able to switch to a coordinate system where the fields are conservative then there must exist eigenstates for wavefunctions satisfying the Schrödinger equation. This is a powerful statement, for it entails time-independent treatment of time-dependent systems through some transformations of the Hamiltonian.

Using (6.1), we can write down Newton's equations of motions:

$$m \frac{\partial^2 \mathbf{r}}{\partial t^2} = -\alpha \frac{\partial}{\partial \mathbf{r}} V\left(\frac{\mathbf{r}}{\ell}\right) \quad (6.2)$$

Changing variables to  $\boldsymbol{\rho} = \frac{\mathbf{r}}{\ell}$  and some scaled time  $\tau = \tau(t)$ , we have

$$\frac{m\ell^2\dot{\tau}^2}{\alpha} \frac{\partial^2 \boldsymbol{\rho}}{\partial \tau^2} + \frac{2m\ell\dot{\tau}}{\alpha} \frac{\partial \boldsymbol{\rho}}{\partial \tau} + \frac{m\ell\ddot{\tau}}{\alpha} \boldsymbol{\rho} = -\frac{\partial}{\partial \boldsymbol{\rho}} V \quad (6.3)$$

which is

$$\frac{m\ell^2\dot{\tau}}{\alpha} \frac{\partial^2 \boldsymbol{\rho}}{\partial \tau^2} + \frac{m}{\alpha} \frac{d}{dt}(\ell^2\dot{\tau}) \frac{\partial \boldsymbol{\rho}}{\partial \tau} + \frac{m\ell\ddot{\tau}}{\alpha} \boldsymbol{\rho} = -\frac{\partial}{\partial \boldsymbol{\rho}} V \quad (6.4)$$

where dots denote derivatives with respect to  $t$ . We want this to look like only conservative forces are at work, so we go about twisting the dial  $\alpha(t)$ ,  $\tau(t)$ , and  $\ell(t)$  to make it so. First, we must get rid of the dissipative (second) term. This forces

$$\frac{d}{dt}(\ell^2\dot{\tau})$$

so that

$$\ell^2\dot{\tau} = \text{constant} \quad (6.5)$$

Without loss of generality, we can set that constant to 1, and let  $\tau(0) = 0$ . This is to say,

$$\dot{\tau} = \frac{1}{\ell^2} \quad \text{or} \quad \tau(t) = \int_0^t \frac{1}{\ell(t)^2} dt \quad (6.6)$$

Given the value of  $\dot{\tau}$ , and in keeping with the form of (6.2), the first term of (6.4) requires

$$\alpha = \frac{1}{\ell^2} \quad (6.7)$$

Finally, the last term on the LHS of (6.4) can continue to exist provided it doesn't depend on time. In that case we can nail down  $\ell(t)$ . Noting that the mass  $m$  is already constant, we have

$$\ell^3 \ddot{\ell} = \text{constant} \equiv \frac{k}{m} \quad (6.8)$$

We can easily solve this differential equation to find

$$\ell(t) = \sqrt{at^2 + 2bt + c} \quad (6.9)$$

and equation (6.8) then requires that our constants relate as

$$ac - b^2 = \frac{k}{m} \quad (6.10)$$

Noting all these requirements, equation (6.4) becomes

$$m \frac{\partial \boldsymbol{\rho}}{\partial \tau} + k \boldsymbol{\rho} = - \frac{\partial V}{\partial \boldsymbol{\rho}}$$

which we write as

$$m \frac{\partial \boldsymbol{\rho}}{\partial \tau} = - \frac{\partial}{\partial \boldsymbol{\rho}} (V + \frac{1}{2} k \rho^2) \quad (6.11)$$

We have now switched to an accelerating reference frame where clocks measure  $\tau$  and meter sticks measure  $\boldsymbol{\rho}$ . This result is contingent on the existence of time  $\tau$ , which means the integral at (6.6) must converge. Additionally, equation (6.9) tells us exactly which time-dependent systems have sets of eigenfunctions.

Note that the rescaling of time  $\tau = \int \frac{1}{\ell^2}$  resolves my earlier confusion on the nature of the integral at (2.13). The integral at that point enters because of the rescaling of time; although this may relate to the inclusion/extrusion of energy from the system, mathematically the integral derives from time re-parametrization.



# 7

## Concluding Remarks

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Throughout the last 69 pages, I believe that most properties of this infinite potential well with one linearly moving wall have been discussed in a respectable amount of depth. At the same time, while being far from trivial in execution, the present endeavor has served primarily as an illustrative example of how to begin to approach a problem where the physical parameters of the system fluctuate temporally. Bringing the methodologies encountered here to bear on other, similar systems may lead to new discoveries to be discussed and pondered over. So, while there is much left to say about these systems, time constraints being what they are, it is now time to end our journey and take stock of what we have come to find out.

We began by considering the innocent-looking case of the quantum mechanics arising from an infinite potential well with a time dependent potential function. Our general idea was to impose time dependent boundary conditions and proceed as one normally would when solving for the static case. As it turned out, even this conceptually basic case was no trivial problem, but through a wonderful—and in some ways unexpected—turn of affairs the argument settled into an exactly solved, analytic solution. Again amazingly, these exact solutions stemmed from two mathematically and conceptually removed methods of analysis: on the one hand solving a differential equation provided by Schrödinger, on the other hand performing the “sum over all [classical] paths” of an imaginary classical particle as directed by Feynman. Somehow these two disjoint paths managed to meet and kiss in the middle for our entertainment.

Discovering the propagator and eigenfunctions supplied several tools to continue probing the system with. First, it allowed us to define and contemplate the energy of the system, leading to an interesting connection between

quantum systems with moving boundaries and analogous thermodynamical systems. Understanding the energy allowed us, briefly, to discuss the pressure of the system, what is meant by that, and how it relates to other pressures we see.

As a final task, we took the exact propagator and tried to stretch it away from its roots to shed light on other, related situations. The procedure provided a wonderful formal result which was, unfortunately, a bit too analytically inflexible to extract more information from. At the same time, application of the computational “brute-force” method provided some good numerical results and pretty pictures for simple cases of wall movement. Adding numerous changes in the wall velocity generates, of course, more computational hardships, and I am under the impression that systems with arbitrary wall movements are both analytically and computationally intractable unless one has the time and resources to throw many CPU’s at the problem. This shouldn’t come as a surprise, though; most systems one can imagine aren’t particularly well behaved anyway.

That sums up the present results, but several unresolved issues now adorn the workbench. I would like to end by simply posing a few questions. When we make the transition from a stationary wall moving wall, the eigenfunctions of the system pick up an extra exponential factor (see §4.4, starting page 44). Does a similar factor arise in other systems such as ones of higher dimensions or non-linearly moving walls? If so, how does it relate to/vary between one system and the next? Can we find a way to predict what it will be for a given system? Is there a better numerical process for studying these time dependent systems? What happens when we vary the strength of a finite potential well?



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