Adiabatic changes of the wave function in the quantum box with moving wall

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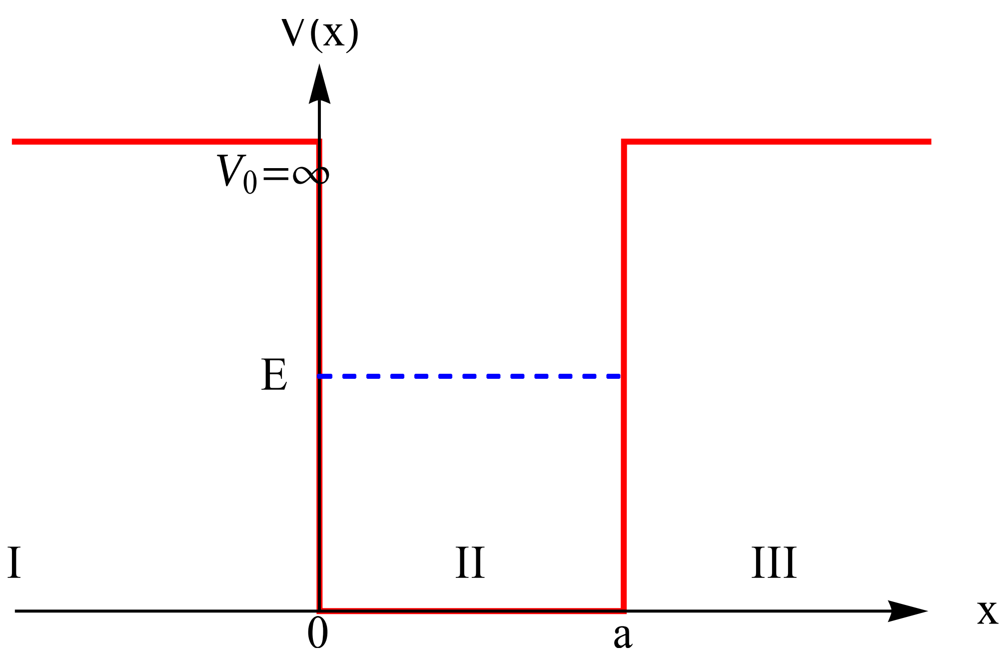
The problem of a quantum box (a particle in a one-dimensional infinite square-well potential with stationary wall) is one of the examples in elementary quantum mechanics. Here we consider a slightly more complicated situation where one of the walls is allowed to move slowly with a constant velocity provides an instructive example for the adiabatic change in the perturbation. Doescher and Rice found an exact solution for the time dependent Schrödinger equation for the infinite square-well potential with a moving wall. I found this problem in a book of Griffiths (Introduction to quantum mechanics). I solve this problem using the Mathematica.

1. Review of one-dimensional quantum box.



$$\hat{H} = \frac{\hat{p}^2}{2m}$$

$$H\varphi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) = E\varphi(x) = \frac{\hbar^2 k^2}{2m}\varphi(x)$$

The solution of this equation is

$$\varphi(x) = A\sin(kx) + B\cos(kx)$$

where

$$E = \frac{\hbar^2 k^2}{2m}$$

Using the boundary condition:

$$\varphi(x=0) = \varphi(x=a) = 0$$

we have

$B = 0$ and $A \neq 0$.

$$\sin(ka) = 0$$

$$ka = n\pi \quad (n = 1, 2, \ldots)$$

Note that $n = 0$ is not included in our solution because the corresponding wave function becomes zero. The wave function is given by

$$\varphi_n(x) = \langle x|\varphi_n\rangle = A_n \sin(\frac{n\pi x}{a}) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$$

with

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

((**Normalization**))

$$1 = \int_0^a A_n^{\ 2}\sin^2(\frac{n\pi x}{a})dx = \frac{a}{2}A_n^{\ 2}$$

Griffiths Problem 10-1

2. Adiabatic change (prediction)

We suppose that we prepare a particle in the ground state of the infinite square well:

$$\varphi_{n=1}^{\ (i)}(x) = \sqrt{\frac{2}{a}}\sin(\frac{\pi x}{a})$$

Suppose that the right wall of the infinite square moves at the constant velocity. The width of the wall is

$$w(t) = a + vt\,.$$

If the wall moves slowly, it is expected that the system remains in the ground state as

$$\varphi_{n=1}^{\ (f)}(x) = \sqrt{\frac{2}{w(t)}}\sin(\frac{\pi x}{w(t)})\,.$$

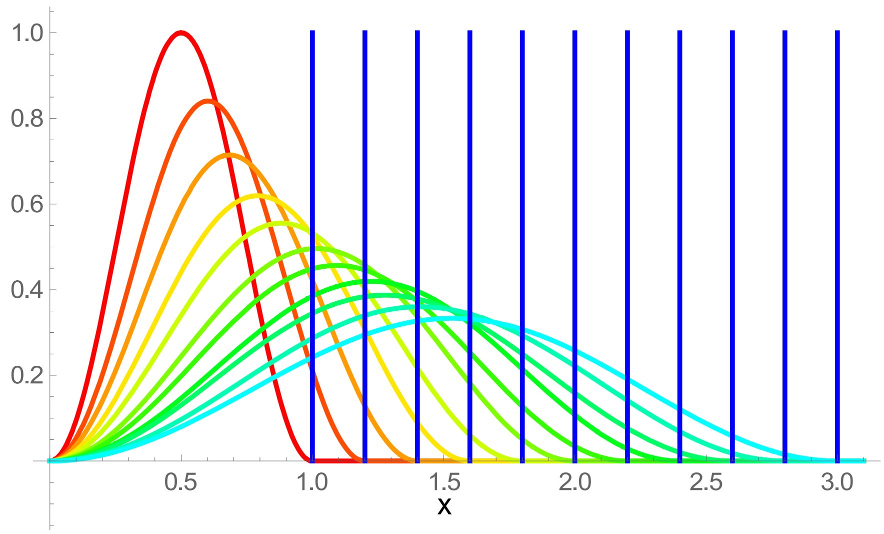


Fig. The initial state: the ground state. The right wall of the infinite square potential moves adiabatically at the constant velocity. The probability as a function of x is plotted where the time is changed constantly.

3. Adiabatic perturbation: Griffiths Problem 10-1

D.J. Griffiths, Introduction to Quantum Mechanics, second edition (Cambridge, 2017).
S.W. Doescher and M.H. Rice, "Infinite Square-Well Potential with a Moving Wall," Am. J. Phys. 37, 1246 (1969).

$***$**Problem 10.1** The case of an infinite square well whose right wall expands at a *constant* velocity (v) can be solved *exactly*.[2] A complete set of solutions is

$$\Phi_n(x,t) \equiv \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w}x\right) e^{i(mvx^2 - 2E_n^i at)/2\hbar w}, \qquad [10.3]$$

where $w(t) \equiv a + vt$ is the (instantaneous) width of the well and $E_n^i \equiv n^2\pi^2\hbar^2/2ma^2$ is the nth allowed energy of the *original* well (width a). The *general* solution is a linear combination of the Φ's:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Phi_n(x,t); \qquad [10.4]$$

the coefficients c_n are *independent of* t.

(a) Check that Equation 10.3 satisfies the time-dependent Schrödinger equation, with the appropriate boundary conditions.

(b) Suppose a particle starts out ($t = 0$) in the ground state of the initial well:

$$\Psi(x, 0) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right).$$

Show that the expansion coefficients can be written in the form

$$c_n = \frac{2}{\pi}\int_0^{\pi} e^{-i\alpha z^2} \sin(nz)\sin(z)\, dz, \qquad [10.5]$$

where $\alpha \equiv mva/2\pi^2\hbar$ is a dimensionless measure of the speed with which the well expands. (Unfortunately, this integral cannot be evaluated in terms of elementary functions.)

(c) Suppose we allow the well to expand to twice its original width, so the "external" time is given by $w(T_e) = 2a$. The "internal" time is the *period* of the time-dependent exponential factor in the (initial) ground state. Determine T_e and T_i, and show that the adiabatic regime corresponds to $\alpha \ll 1$, so that $\exp(-i\alpha z^2) \cong 1$ over the domain of integration. Use this to determine the expansion coefficients, c_n. Construct $\Psi(x, t)$, and confirm that it is consistent with the adiabatic theorem.

(d) Show that the phase factor in $\Psi(x, t)$ can be written in the form

$$\theta(t) = -\frac{1}{\hbar}\int_0^{t} E_1(t')\, dt', \qquad [10.6]$$

where $E_n(t) \equiv n^2\pi^2\hbar^2/2mw^2$ is the *instantaneous* eigenvalue, at time t. Comment on this result.

((**Solution**))

$w(t) = a + vt$

$$\psi_n(x,t) = \sqrt{\frac{2}{w(t)}}\sin[\frac{n\pi}{w(t)}x]\exp[i\frac{(mvx^2 - 2E_n^i at)}{2\hbar w(t)}],$$

where

$$E_n^i = \frac{n^2\pi^2\hbar^2}{2ma^2}.$$

((**Mathematica**)) This equation satisfies the Schrődinger equation.
((**Proof**))

```
Clear["Global`"];
w[t1_] := a + v t1;
E1[n1_] := (n1^2 π^2 ℏ^2)/(2 m a^2);
ψ[x_, t_, n_] :=
  Sqrt[2/w[t]] Sin[(n π)/w[t] x] Exp[ⅈ ((m v x^2 - 2 E1[n] a t))/(2 ℏ w[t])];


s1 = ⅈ ℏ D[ψ[x, t, n], t] // Simplify;

s2 = (-ℏ^2)/(2 m) D[ψ[x, t, n], {x, 2}] // Simplify;

s1 - s2 // Simplify

0
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At $t = 0$,

$$\psi(x,t=0) = \sum_{n=1}^{\infty} C_n \psi_n(x,t=0)$$
$$= \sum_{n=1}^{\infty} C_n \sqrt{\frac{2}{a}} \sin[\frac{n\pi}{a}x] \exp(i\frac{mvx^2}{2\hbar a})$$

where C_n is independent of *t*,

$$\psi_n(x,t=0)=\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})\exp(i\frac{mvx^2}{2\hbar a})$$

Then we get the expression of C_n as

$$C_n=\sqrt{\frac{2}{a}}\int_0^a dx\,\psi(x,t=0)\sin(\frac{n\pi x}{a})\exp(-i\frac{mvx^2}{2\hbar a})$$

where

$$\int_0^a dx\sin(\frac{k\pi x}{a})\sin(\frac{n\pi x}{a})=\frac{a}{2}\delta_{n.k}$$

When

$$\psi(x,t=0)=\sqrt{\frac{2}{a}}\sin(\frac{\pi x}{a})$$

C_n can be evaluated as

$$C_n=\frac{2}{a}\int_0^a dx\sin(\frac{\pi x}{a})\sin(\frac{n\pi x}{a})\exp(-i\frac{mvx^2}{2\hbar a})$$

For simplicity we use $z=\frac{\pi x}{a}$. C_n can be rewritten as

$$C_n=\frac{2}{\pi}\int_0^\pi dz\sin(z)\sin(nz)\exp(-i\alpha z^2)$$

where

$$\alpha=\frac{mva}{2\pi^2\hbar}.$$

The value of C_n can be evaluated using Mathematica numerically. The solution of the Schrődinger equation (in general case) is

$$\psi(x,t) = \sum_{n=1}^{\infty} C_n \sqrt{\frac{2}{w(t)}} \sin[\frac{n\pi}{w(t)} x] \exp[i \frac{(mvx^2 - 2E_n^i at)}{2\hbar w(t)}$$

3. Condition for the adiabatic change

We define the two characteristic times T_e and T_i. The time T_e is defined as

$$T_e = \frac{a}{v}$$

at which $w(T_e) = 2a$.

The phase factor of the wave function in the ground state is

$$\exp(-i \frac{E_1^i t}{\hbar})$$

The time T_i is defined as

$$\frac{E_1^i T_i}{\hbar} = 2\pi$$

at the phase is on the order of 2π. Then we have

$$T_i = \frac{2\pi\hbar}{E_1^i} = \frac{4ma^2}{\pi\hbar}$$

The adiabatic perturbation is valid when

$$T_i << T_e$$

leading to

$$\frac{4ma^2}{\pi\hbar} << \frac{a}{v}, \qquad \text{or} \qquad \frac{4mva}{\pi\hbar} << 1.$$

This condition implies that

$$\alpha = \frac{mva}{2\pi^2\hbar} << 1$$

Suppose that $\alpha = 0$, then we have

$$C_n = \frac{2}{\pi}\int_0^{\pi} dz \sin(z)\sin(nz) = \delta_{n,1}$$

So the wave function is approximated as

$$\psi(x,t) = \sqrt{\frac{2}{w(t)}}\sin(\frac{\pi x}{w(t)})\exp[i\frac{mvx^2 - 2E_1^i at}{2\hbar w(t)}]$$

which is the ground state of the instantaneous well, of width $w(t)$. Note that

$$\frac{mvx^2}{2\hbar w(t)} \approx \frac{mva^2}{2\hbar a} = \frac{mva}{2\hbar} << 1$$

So $\psi(x,t)$ can be rewritten as

$$\psi(x,t) \approx \sqrt{\frac{2}{w(t)}}\sin(\frac{\pi x}{w(t)})\exp[-i\frac{E_1^i at}{\hbar w(t)}]$$

where

$$\frac{E_1^i at}{\hbar w(t)} = \frac{at}{\hbar w(t)}\frac{\pi^2\hbar^2}{2ma^2} = \frac{\pi^2\hbar t}{2maw(t)}$$

Note that

$$E_n^i = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

4. Phase factor

$$\begin{aligned}
\theta(t) &= -\frac{1}{\hbar}\int_0^t E_1(t')dt' \\
&= -\frac{1}{\hbar}\int_0^t \frac{\pi^2\hbar^2}{2m[w(t')]^2}dt' \\
&= -\frac{\pi^2\hbar}{2m}\int_0^t \frac{1}{(a+vt')^2}dt' \\
&= \frac{\pi^2\hbar}{2mv}\left(\frac{1}{a+vt}-\frac{1}{a}\right) \\
&= -\frac{\pi^2\hbar}{2m}\left(\frac{t}{a(a+vt)}\right) \\
&= -\frac{\pi^2\hbar t}{2maw(t)}
\end{aligned}$$

where

$$E_n(t) = \frac{n^2\pi^2\hbar^2}{2m[w(t)]^2}.$$

Using this phase factor, we have

$$\psi(x,t) \approx \sqrt{\frac{2}{w(t)}}\sin\left(\frac{\pi x}{w(t)}\right)\exp[i\theta(t)].$$

It adiabatically expands well with the width $w(t)$ replaced by a. We note that $\theta(t) = -\frac{\pi^2\hbar t}{2maw(t)}$ is equal to

$$\frac{E_1(t)}{\hbar} = \frac{\pi^2\hbar}{2m[w(t)]^2} \approx \frac{\pi^2\hbar}{2maw(t)},$$

where

$$E_1(t) = \frac{\pi^2\hbar^2}{2m[w(t)]^2}.$$

5. Probability

$$\psi(x,t) = \sum_{n=1}^{\infty} C_n \sqrt{\frac{2}{w(t)}} \sin[\frac{n\pi}{w(t)} x] \exp[i \frac{(mvx^2 - 2E_n^i at)}{2\hbar w(t)}],$$

with

$$C_n = \frac{2}{\pi} \int_0^{\pi} dz \sin(z) \sin(nz) \exp(-i\alpha z^2).$$

We use new variables and parameters to simplify the form of wave function.

$$t_0 = \frac{vt}{a}, \qquad x_0 = \frac{x}{a}, \qquad p = \frac{mva}{\hbar}$$

and

$$\frac{\psi(x,t)}{\sqrt{2/a}} = \sum_{n=1}^{\infty} C_n \sqrt{\frac{1}{1+t_0}} \sin(\frac{n\pi x_0}{1+t_0}) \exp[i(\frac{p}{2} \frac{x_0^2}{1+t_0} - \frac{n^2\pi^2}{2p} \frac{t_0}{1+t_0})]$$

Note that the parameter p is related to the ratio T_i / T_e

$$p = \frac{\pi}{4} \frac{T_i}{T_e} \approx \frac{T_i}{T_e}.$$

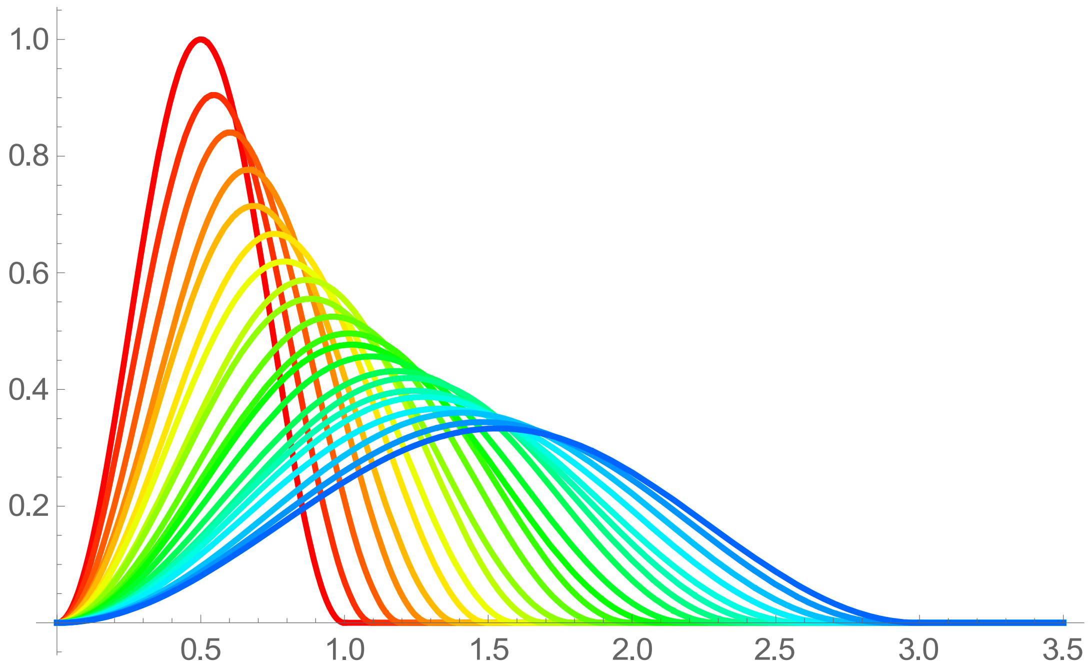

Fig. $p = 0.2$. Plot of $\left|\dfrac{\psi(x,t)}{\sqrt{2/a}}\right|^2$ as a function of x. $t = 0, 0.1, 0.2, 0.3, \ldots, 1.9$, and 2.0.

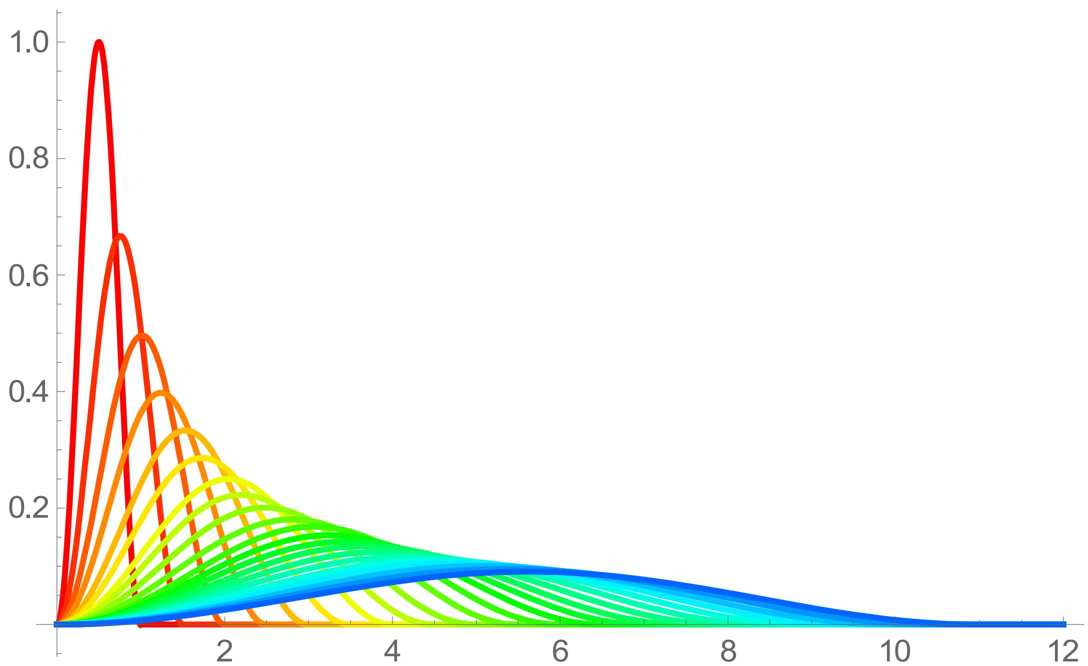

Fig. $p = 0.2$. Plot of $\left|\dfrac{\psi(x,t)}{\sqrt{2/a}}\right|^2$ as a function of x. $t = 0, 0.5, 1, 1.5, \ldots, 9.5, 10$.

REFERENCES

D.J. Griffiths, Introduction to Quantum Mechanics, second edition (Cambridge, 2017).

S.W. Doescher and M.H. Rice, "Infinite Square-Well Potential with a Moving Wall," Am. J. Phys. 37, 1246 (1969).