

PATH INTEGRALS IN QUANTUM MECHANICS

BENJAMIN MCKAY

ABSTRACT. These notes are intended to introduce the mathematically inclined reader to the formulation of quantum mechanics via path integrals.

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“ I’m not making this up, you know.”

Anna Russell, The Ring of the Nibelung

1. INTRODUCTION

This material is drawn largely from Feynman & Hibbs [2]. It is also helpful to take a look the list of errata given by Styer [4]. I would like to thank the mathematicians who sat through these lectures, and particularly Aaron Bertram, Jim Carlson, Javier Fernandez and Steve Gersten for helpful comments.

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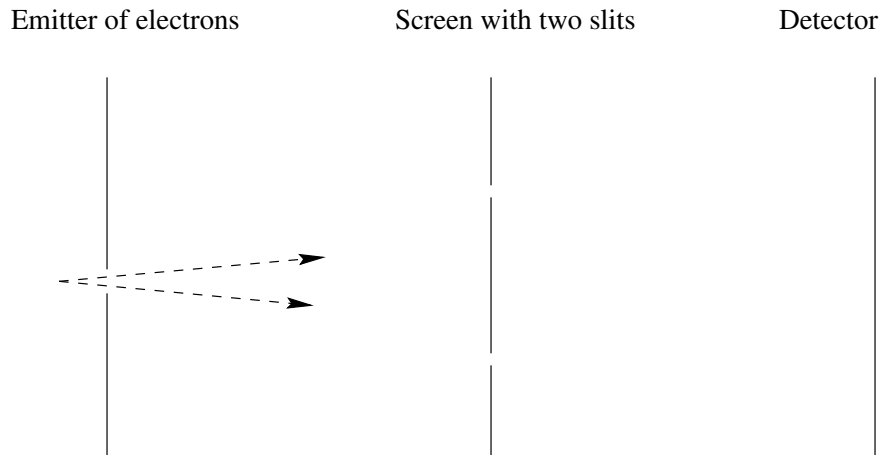


FIGURE 1. The two slit experiment

2. THE TWO SLIT EXPERIMENT

In the experiment shown in figure 2 we watch electrons strike a detector; each one arrives like a drop of rain. Each electron is counted with a “click” and its approximate location recorded. The electrons coming in are counted up, and we find the numbers of them (actually, the density) graphed in figure 2 on the next page. What is it?

Guesses

- (1) Each electron passes through either hole 1 or hole 2.
- (2) The number of electrons per second striking a spot on the detector is the sum of the number/second coming through hole 1 with the number/second coming through hole 2.

Lets check. Close hole 2, as in figure 2 on the facing page. The distribution of electrons is drawn in figure 2 on page 4. Now close hole 1. This is not working. Guess 2 is wrong! It would give us Imagine a breakwater in a harbour with two gaps for ships to pass through. What do the waves look like? Suppose we have two breakwaters: Ships go up and down like oscillating. The magnitude squared of this wave form looks a lot like the counting of electrons in the two slit experiment. Guess:

Guesses

- (3) For each point of the screen, there are complex numbers ϕ_1 and ϕ_2 (representing contributions from each of the two holes) called *amplitudes* so that the probability of seeing an electron at that point of the screen is $|\phi_1 + \phi_2|^2$ with both holes open.
- (4) If we close a hole, say hole 2, then ϕ_2 is replaced by 0.

This works. The humps in figures 2 on page 4 and 2 on page 5 show $|\phi_1|^2$ and $|\phi_2|^2$ but adding $\phi_1 + \phi_2$ gives interference from phases.

Now lets try lots of holes as in figure 2 on page 7: Then we have to add up complex amplitudes for each hole at each point of the detector screen. Suppose we have lots of screens too, as in figure 2 on page 8. Then we have to add up not just

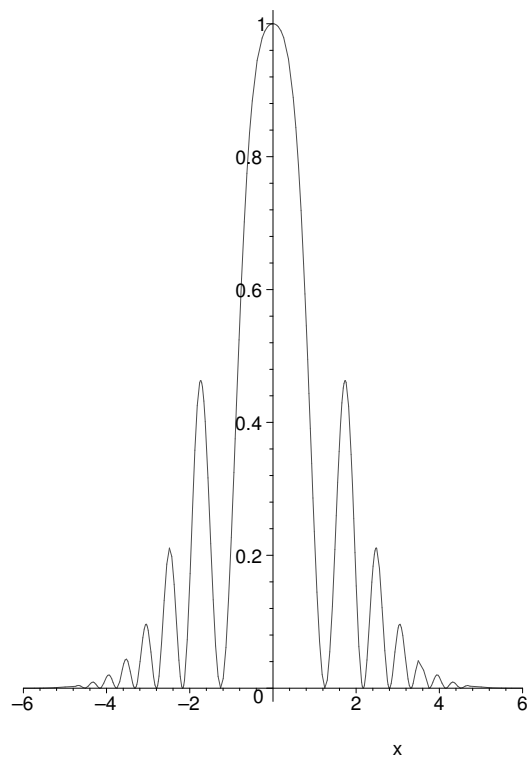


FIGURE 2. The density of electrons coming in at the detector

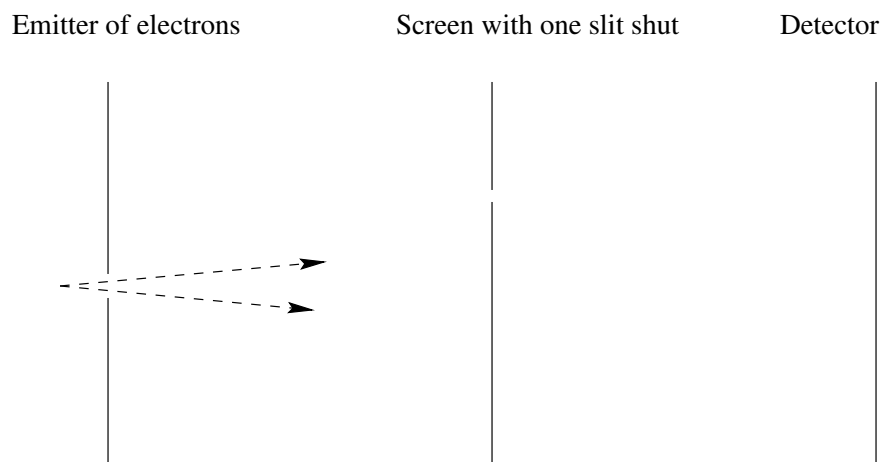


FIGURE 3. Closing one hole

a contribution from each hole, but from a choice of which hole to pass through in each screen: a choice of route that the electron could pick in travelling from emitter to screen.

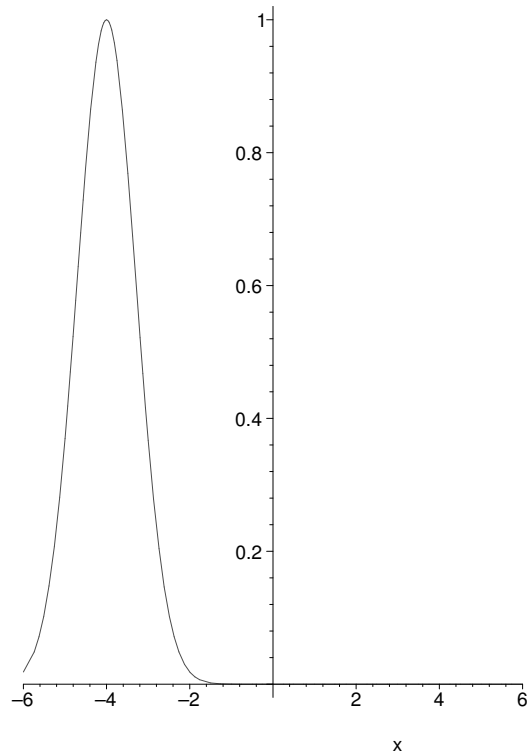


FIGURE 4. The density of electrons after we close the right hole

In the limit, we have a continuum of screens, but each of them is *all holes*. (So there aren't actually any screens at all.) We find the sum over possible routes becomes a *path integral*. So the probability of finding an electron at a point x_1 of the screen is

$$\text{Prob}(x_1) = \left| \int [dx] \phi[x(t)] \right|^2$$

where the integral sums over all paths $x(t)$ from the emitter to the point x_1 , and $\phi[x(t)]$ means the amplitude for this path.

3. HOW TO FIND THE AMPLITUDE OF A PATH

A plane wave in empty space has linearly evolving phase. By analogy, in order to get wave-like behaviour of amplitudes, we expect to have evolution of phase along a product of paths to be the sum of the phases for each. This suggests:

Guesses

(5)

$$\phi\left(\cdot \xrightarrow{A} \cdot \xrightarrow{B} \cdot\right) = \phi\left(\cdot \xrightarrow{A} \cdot\right) \phi\left(\cdot \xrightarrow{B} \cdot\right)$$

in other words: amplitudes for events in succession multiply.

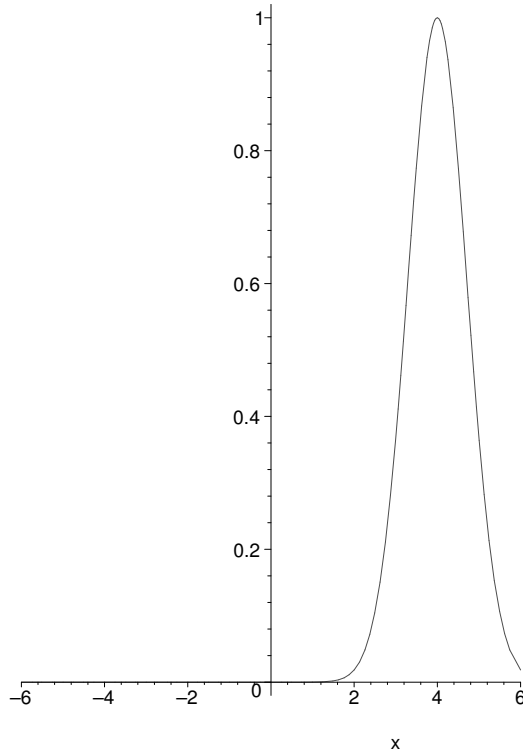


FIGURE 5. The density of electrons after we close the left hole

With this given, finding amplitudes is a local problem. In particular, for a path which is just a single point

$$\phi(\cdot) = 1$$

by the multiplication of amplitudes. Let us find the amplitude of a little piece of path, say infinitesimally large. This is just a tangent vector to the path. So

$$\phi(\longrightarrow) = 1 + \text{correction}.$$

To have pure linear evolution of phase in empty space, we want the correction to just push the phase around, (i.e. to be tangent to the unit circle in the complex numbers) so to be imaginary:

$$\phi(\longrightarrow) = 1 + iL$$

for some quantity L which depends only on the tangent vector to our curve (so L is a real valued function on the tangent bundle). Multiplying together the contributions along a whole curve:

$$\phi[x(t)] = e^{i \int L(x(t), \dot{x}(t)) dt}.$$

To make rescaling easier, we will include a rescaling constant \hbar . This \hbar must have the same units as L . Why? Because to take an exponential

$$e^z = 1 + z + \frac{z^2}{2} + \dots$$

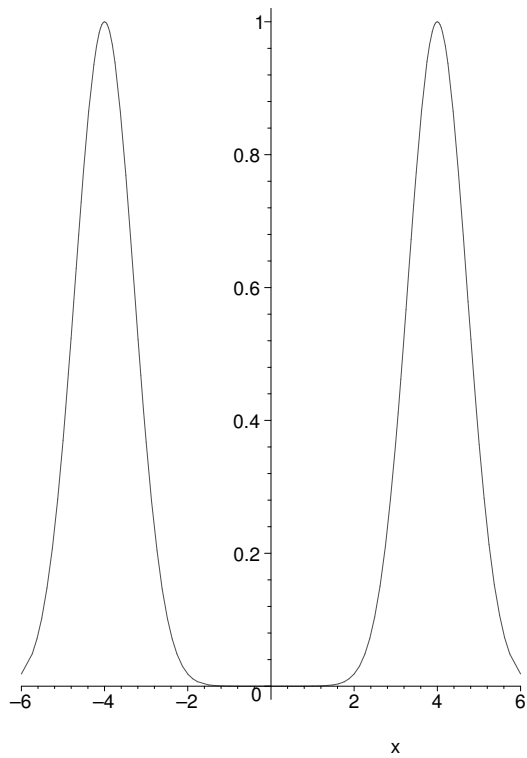


FIGURE 6. The density of electrons expected to come in at the detector
 First breakwall: one hole Second breakwall: two holes Ships tie up here

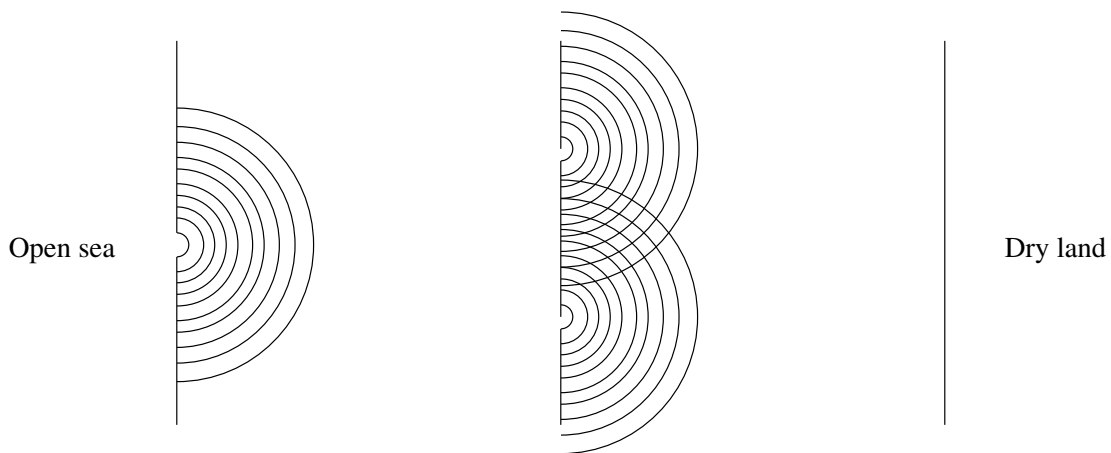


FIGURE 7. A harbour

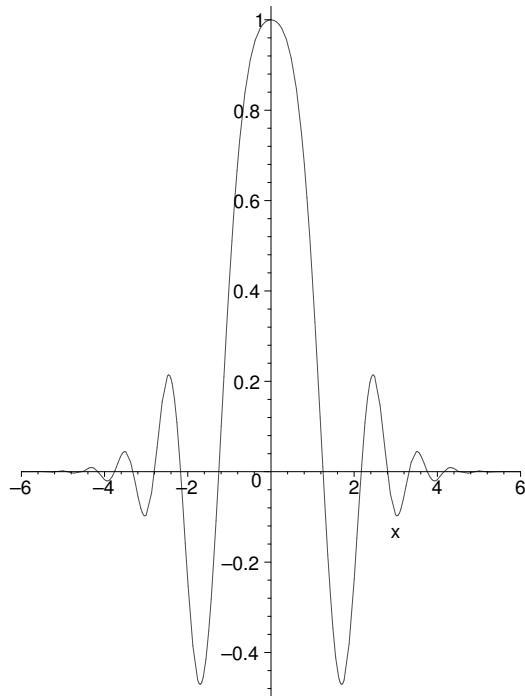


FIGURE 8. Waves lifting ships in a harbour

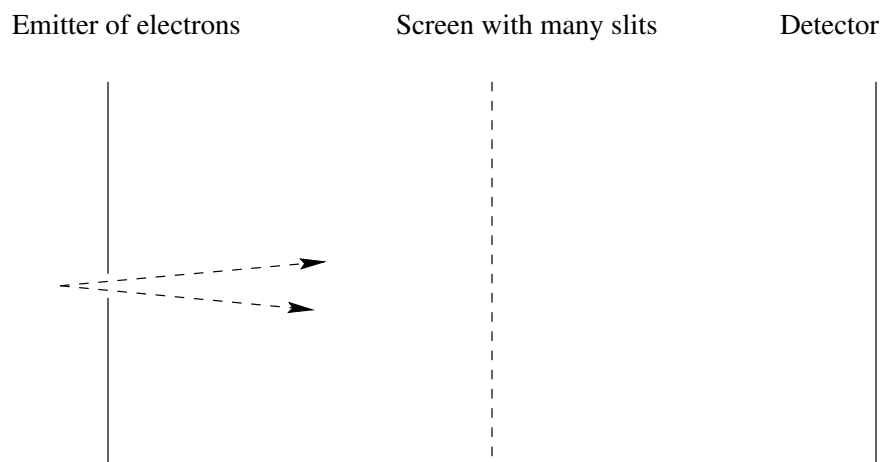


FIGURE 9. Lots of holes

we have to be able to add together all powers of z . But the units of z^2 will only equal those of z if z is unitless. Therefore we put in an \hbar just to balance off the units.

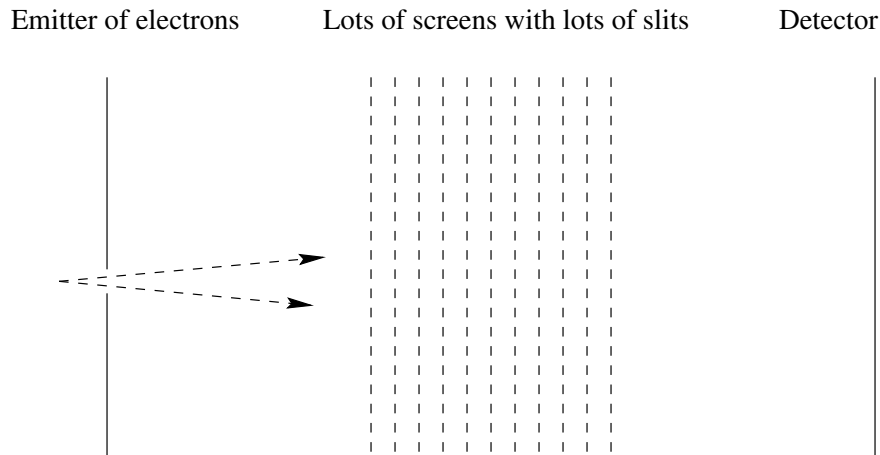


FIGURE 10. Lots of screens with lots of holes

Summing up (both literally and figuratively), the probability of seeing an electron at x_1 is

$$\text{Prob}(x_0) = \left| [dx] e^{\frac{i}{\hbar} \int dt L(x(t), \dot{x}(t))} \right|^2$$

where the integral is over all paths from emitter to x_1 . What is L ?

Guesses

- (6) L is the Lagrangian of the classical theory.

Justifications

- It works!
- The Lagrangian is the only function we know on the tangent bundle which can determine the entire classical theory, i.e. the classical paths.

Remark 1 The paths we sum over include those going back and forth many times, as in figure 3 on the facing page.

Remark 2 Aaron’s lectures only allowed Lagrangians to depend on position and velocity. Sometimes it is convenient to allow them to depend on time as well—but not for studying fundamental physics where we want to assume that the laws of physics are independent of time. However, in a lab, the potential energy function (which is part of the Lagrangian) may change with time because objects in the lab equipment might move over time. We keep track of this in the potential energy, in lieu of trying to keep track of all particles in the universe directly in our mathematical model. How we go about “averaging” all of the ambient universe into a potential function is a serious question which we probably won’t return to. But these issues are already present in classical physics.

4. THE CLASSICAL LIMIT

If L is a typical Lagrangian like

$$L = \frac{m}{2} \left| \frac{dx}{dt} \right|^2 - V(x)$$

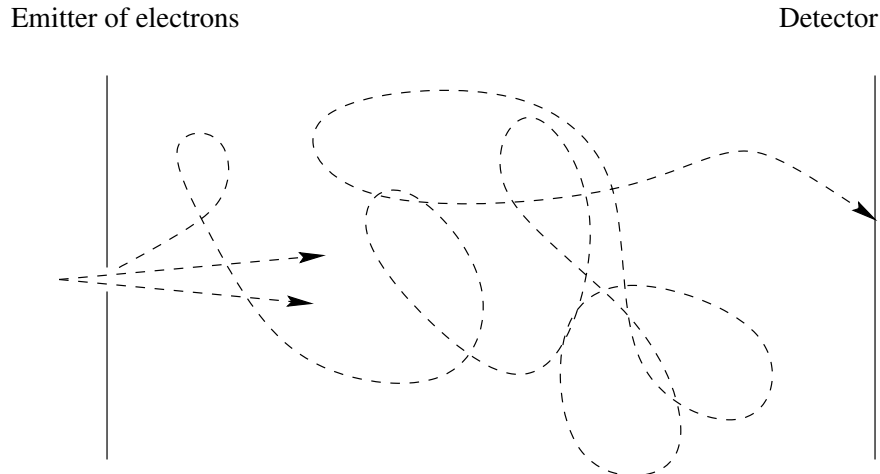


FIGURE 11. A path which doubles back several times before hitting the detector

then the action $S = \int L dt$ has units of mass length²/time, and therefore to obtain unitless quantities S/\hbar in our exponential, \hbar has the same units. If we fix a length scale to measure in based on the size of physical phenomena we want to study, then having \hbar small is the same as studying large objects (or very massive ones).

The numbers

$$S = \int dt L$$

will become huge, and vary enormously with slight changes in path, and the complex numbers $e^{\frac{i}{\hbar}S}$ will oscillate wildly in phase (i.e. direction in the complex plane). But near a classical path, the integral of the Lagrangian does not vary as much as it does at other places, so that these numbers $e^{\frac{i}{\hbar}S}$ all point in nearly the same direction for paths close to a classical path. These add up to a large contribution, compared to the wildly varying phases away from a classical path, which (we imagine) cancel each other out.

In the $\hbar \rightarrow 0$ (semiclassical) limit, only classical paths contribute, explaining their significance in large scale physics.

5. CUTTING AND PASTING

The rule

$$\phi \left(\cdot \xrightarrow{A} \cdot \xrightarrow{B} \cdot \right) = \phi \left(\cdot \xrightarrow{A} \cdot \right) \phi \left(\cdot \xrightarrow{B} \cdot \right)$$

which obviously holds for

$$\phi = e^{\frac{i}{\hbar}S}$$

allows us to cut the path integral in two. First, let's write

$$\langle x_1, t_1 | x_0, t_0 \rangle = \int [dx]_{x_0, t_0}^{x_1, t_1} e^{\frac{i}{\hbar}S}$$

where the integral is carried out over paths which leave the point x_0 at time t_0 and arrive at x_1 at time t_1 . Then splitting paths in two at an intermediate time t_m

Emitter of electrons

Detector

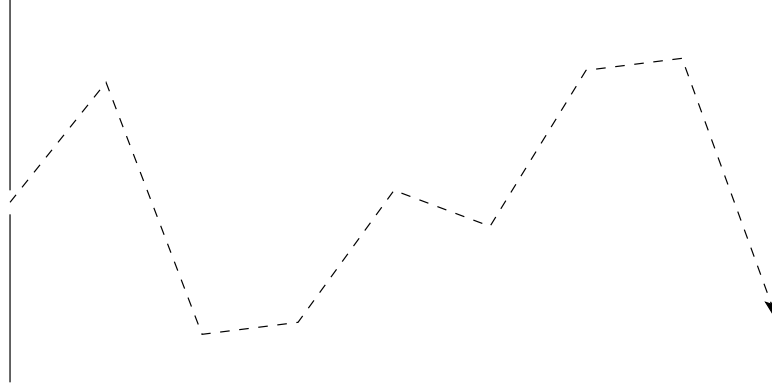


FIGURE 12. Path made of linear pieces

(m =middle) between t_0 and t_1 gives

$$\langle x_1, t_1 | x_0, t_0 \rangle = \int dx_m \langle x_1, t_1 | x_m, t_m \rangle \langle x_m, t_m | x_0, t_0 \rangle$$

where the integral is over the choice of which point x_m the path will get to at time t_m .

6. EXAMPLE: THE FREE PARTICLE

Our Lagrangian is

$$L = \frac{m}{2} \left(\frac{dx}{dt} \right)^2$$

in one dimension $x \in \mathbb{R}$. First lets calculate $\int dt L$ over a lot of paths. Approximate any path by little linear pieces as in figure 6. Looking at a single piece, a linear path

$$x(t) = x_0 + \frac{t - t_0}{t_1 - t_0} (x_1 - x_0)$$

we see that L is constant:

$$L = \frac{m}{2} \left(\frac{x_1 - x_0}{t_1 - t_0} \right)^2$$

and we calculate that the action $S = \int dt L$ is

$$S = \frac{m}{2(t_1 - t_0)} (x_1 - x_0)^2.$$

Now if we put two pieces together, one from x_0 to y and one from y to x_1 , each taking time $\Delta t = (t_1 - t_0)/2$, we get

$$S = \frac{m}{2\Delta t} (y - x_0)^2 + \frac{m}{2\Delta t} (x_1 - y)^2.$$

Using the principle of cutting and pasting, we integrate out the choice of the intermediate point y to get amplitude

$$\int dy \exp \left(\frac{im}{2\Delta t \hbar} \left[(y - x_0)^2 + (x_1 - y)^2 \right] \right) = \sqrt{\frac{m}{2\pi i \hbar (t_1 - t_0)}} \exp \left(\frac{im(x_1 - x_0)^2}{2\hbar (t_1 - t_0)} \right)$$

the amplitude from going along two linear pieces, with an arbitrary choice of midpoint.¹ To handle 3 pieces, we carry out two integrations over midpoints in the same manner and find exactly the same answer.

Continuing in this manner, if we divide up an interval of time from t_0 to t_1 into pieces of duration $\Delta t = (t_1 - t_0)/N$ for a large N , we get amplitude

$$\sqrt{\frac{m}{2\pi i\hbar(t_1 - t_0)}} \exp\left(\frac{im(x_1 - x_0)^2}{2\hbar(t_1 - t_0)}\right)$$

for traveling along a piecewise linear path with breakpoints at times $t_0, t_0 + \Delta t/N, \dots, t_1$. Since this expression is independent of how many break points we use, in the limit as $N \rightarrow \infty$ we obtain, for any points x_0, t_0 and x_1, t_1 :

$$\langle x_1, t_1 | x_0, t_0 \rangle = \sqrt{\frac{m}{2\pi i\hbar(t_1 - t_0)}} \exp\left(\frac{im(x_1 - x_0)^2}{2\hbar(t_1 - t_0)}\right).$$

Therefore the probability of the particle arriving at x_1 at time t_1 , if it was at x_0 at time t_0 , is

$$\text{Prob}(x_1) = \left| \sqrt{\frac{m}{2\pi i\hbar(t_1 - t_0)}} \exp\left(\frac{im(x_1 - x_0)^2}{2\hbar(t_1 - t_0)}\right) \right|^2 = \frac{m}{2\pi(t_1 - t_0)\hbar}$$

which is independent of x_1 so it is equally likely to be anywhere. The probability that the particle is somewhere at all is

$$\int \text{Prob}(x_1) dx_1 = \infty.$$

So it isn't really a probability at all.

Exercise 1. Wave functions

Given a function $\phi_0(x)$ define

$$(1) \quad \phi(x, t) = \int \langle x, t | x_0, 0 \rangle \phi_0(x_0) dx_0$$

where the expression

$$\langle x, t | x_0, 0 \rangle$$

is the free particle amplitude computed above. Show that

- (a) The function $\phi(x, t)$ satisfies the *Schrödinger equation for the free particle*

$$\frac{\partial \phi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \phi}{\partial x^2}.$$

- (b)

$$\phi(x, t) \rightarrow \phi_0(x) \text{ in } L^2 \text{ as } t \rightarrow 0.$$

- (c)

$$\int |\phi(x, t)|^2 dx$$

is independent of t (unitary evolution).

¹The evaluation of Gaussian integrals will be discussed in section 15 on page 28.

To handle the infinity of the “probability” $\int \text{Prob } dx_1$, we must “smear” the particles, giving them their own amplitude functions, say $\phi(x, t)$, so that the probability that the electron is between x_0 and $x_0 + \Delta x$ is

$$\int_{x_0}^{x_0 + \Delta x} |\phi(x, t_0)|^2 dx$$

and allow these amplitude functions to evolve via equation 1 on the page before.

Call the function ϕ the *wave function* or *state* of the electron.

To handle the free particle in n dimensional space \mathbb{R}^n , treat it as a sum of independent contributions to the Lagrangian, which get exponentiated:

$$\langle x_1, t_1 | x_0, t_0 \rangle = \left(\frac{m}{2\pi i \hbar (t_1 - t_0)} \right)^{n/2} \exp \left(\frac{im \|x_1 - x_0\|^2}{2\hbar (t_1 - t_0)} \right).$$

Exercise 2. The free particle on the circle

- (a) Take a particle $\alpha(t)$ on a circle $\mathbb{R}/2\pi R\mathbb{Z}$, with $R > 0$, and the same free particle Lagrangian

$$L = \frac{m}{2} \left(\frac{d\alpha}{dt} \right)^2.$$

Calculate

$$\langle \alpha_1, t_1 | \alpha_0, t_0 \rangle$$

for

$$-\pi R \leq \alpha_0, \alpha_1 < \pi R.$$

Hint: you will have to sum over all “winding numbers” of a path around the circle.

- (b) Express your answer in terms of the ϑ function

$$\vartheta(z, \tau) = \sum_{N \in \mathbb{Z}} \exp(\pi i N^2 \tau + 2\pi i N z).$$

- (c) Use the functional identity

$$\vartheta(z, \tau) = \exp\left(\frac{\pi i}{4}\right) \tau^{-1/2} \exp\left(\frac{-\pi i z^2}{\tau}\right) \vartheta\left(\frac{z}{\tau}, -\frac{1}{\tau}\right)$$

to find that

$$\langle \alpha_1, t_1 | \alpha_0, t_0 \rangle = \frac{1}{2\pi R} \vartheta\left(\frac{\alpha_1 - \alpha_0}{2\pi R}, -\frac{\hbar(t_1 - t_0)}{2\pi R^2 m}\right).$$

- (d) Now show directly from the definition of ϑ that this amplitude $\langle \alpha_1, t_1 | \alpha_0, t_0 \rangle$ satisfies the same properties that you found for the free particle amplitude in the previous problem: it is a Green’s function for the same free particle Schrödinger equation, and as a Green’s function, it propagates a function $\phi(\alpha, t)$ preserving

$$\int_{\mathbb{R}/2\pi R\mathbb{Z}} d\alpha |\phi(\alpha, t)|^2$$

over all time t . (Hint: see pages 4 and 5 of Mumford [3].) Note that $\vartheta(z, \tau)$ is defined by an “oscillatory sum” for real values of τ (real τ is the boundary of the Siegel half-plane),

but still makes sense in this context as a pseudodifferential operator.

Exercise 3. Fourier series

Use Fourier transforms [or Fourier series] in the x [or α] variable to solve the free particle Schrödinger equation on the line [or the circle], expressing the answer as

$$\phi(x, t) = \int G(x, t, x_0, t_0) \phi_0(x_0) dx_0$$

so that ϕ satisfies the free Schrödinger equation, and $\phi = \phi_0$ at $t = t_0$. Compare to the amplitude coming from the path integral.

Exercise 4. Twisted sectors

Consider an s -fold covering of a circle:

$$\alpha \in \mathbb{R}/2\pi R\mathbb{Z} \mapsto \beta = s\alpha \in \mathbb{R}/2\pi R\mathbb{Z}.$$

Split each function $\phi(\alpha)$ on the covering circle into Fourier series,

$$\phi(\alpha) = \sum_{k \in \mathbb{Z}} c_k e^{ik\alpha}$$

and write it as

$$\phi(\alpha) = \sum_{r=0}^{s-1} \phi_r(\alpha)$$

where

$$\phi_r(\alpha) = \sum_{q \in \mathbb{Z}} c_{qs+r} e^{i(qs+r)\alpha}.$$

Interpret this as defining line bundles on the base circle. Show that $\phi(\alpha)$ evolves as a free particle wave function precisely if each of the functions $\phi_r(\alpha)$ evolves as in equation 1 on page 11 with the amplitudes

$$\langle \beta_1, t_1 | \beta_0, t_0 \rangle_r = \frac{1}{2\pi R} \vartheta_{\begin{bmatrix} r/s \\ 0 \end{bmatrix}}(z, \tau)$$

where

$$z = \frac{\beta_1 - \beta_0}{2\pi R} \quad \text{and} \quad \tau = -\frac{\hbar(t_1 - t_0)}{2\pi m(R/s)^2}$$

and the expression $\vartheta_{\begin{bmatrix} r/s \\ 0 \end{bmatrix}}$ means the ϑ -function with characteristics, defined by

$$\vartheta_{\begin{bmatrix} a \\ b \end{bmatrix}}(z, \tau) = \sum_{N \in \mathbb{Z}} \exp(\pi i(a + N)^2 \tau + 2\pi i(a + N)(z + b)).$$

7. EXAMPLE: THE HARMONIC OSCILLATOR

The Lagrangian is

$$L = \frac{m}{2} \left(\left(\frac{dx}{dt} \right)^2 - \omega^2 x^2 \right).$$

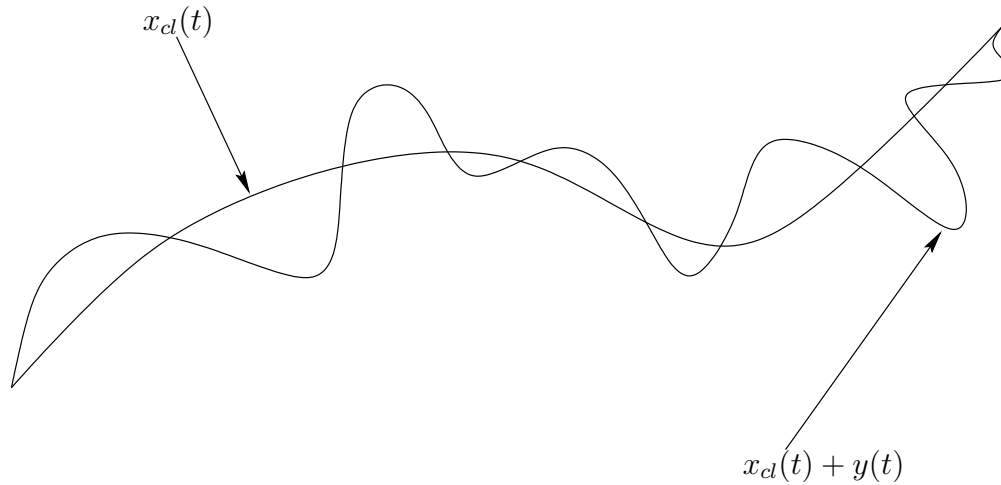


FIGURE 13. Perturbing a classical path

We will find the amplitude $\langle x_1, t_1 | x_0, t_0 \rangle$. It suffices to find $\langle x_1, T | x_0, 0 \rangle$, because the Lagrangian does not depend (directly) on time. Note that the Lagrangian is quadratic. So

$$S[x] = \int dt L(x(t), \dot{x}(t))$$

is quadratic in x .

If we take a path $x(t)$ we can split it into a classical path $x_{cl}(t)$ (satisfying the Euler–Lagrange equations) and a “perturbation” $y(t)$ with $y(0) = y(T) = 0$, as in figure 7.

Since $S[x]$ is quadratic, we can write it as $S[x, x]$ a bilinear form, and find

$$\begin{aligned} S[x] &= S[x_{cl} + y] \\ &= S[x_{cl}] + 2S[x_{cl}, y] + S[y] \end{aligned}$$

Exercise 5.

Write $S[x_{cl}, y]$ as an integral.

The Euler–Lagrange equations say perturbing a classical path has no influence on the action, to first order, so

$$S[x_{cl}, y] = 0.$$

Therefore

$$S[x] = S[x_{cl}] + S[y]$$

and the amplitude is

$$\begin{aligned}\langle x_1, T | x_0, 0 \rangle &= \int [dx] e^{iS[x]/\hbar} \\ &= \int [dy] e^{iS[x_{cl}+y]/\hbar} \\ &= \int [dy] e^{iS[x_{cl}]/\hbar} e^{iS[y]/\hbar} \\ &= e^{iS[x_{cl}]/\hbar} \int [dy] e^{iS[y]/\hbar}.\end{aligned}$$

The $[dy]$ integral is an integral over all perturbations of the classical path $x_{cl}(t)$, so these $y(t)$ must vanish at times $t = 0$ and $t = T$. Hence we have factored

$$\langle x_1, T | x_0, 0 \rangle = \underbrace{e^{iS[x_{cl}]/\hbar}}_{\text{Depends on } x_0, x_1, T} \underbrace{\langle 0, T | 0, 0 \rangle}_{\text{Depends on } T}$$

into a purely classical contribution, and a path integral.

Exercise 6. The action on classical paths

- (a) Find the Euler–Lagrange equations of the harmonic oscillator.
- (b) Find the classical path $x_{cl}(t)$ passing through x_0 at time $t = 0$ and x_1 at time $t = T$. Assume that ωT is *not* an integer.
- (c) Calculate the action $S[x_{cl}]$ along this classical path. You should get

$$\begin{aligned}S[x_{cl}] &= \int dt L(x(t), \dot{x}(t)) \\ &= \frac{m\omega}{2\sin(\omega T)} (\cos(\omega T) (x_0^2 + x_1^2) - 2x_0x_1).\end{aligned}$$

Now we expand the perturbation into eigenfunctions of the Sturm–Liouville operator. What is that?

Exercise 7. Sturm–Liouville operators

Recall that the Euler–Lagrange equations for a path $x_{cl}(t)$ with $t_0 \leq t \leq t_1$ are $S'[x_{cl}] = 0$, where

$$S'[x]y = \int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) y.$$

- (a) Show that if $S'[x_{cl}] = 0$, then for any functions $y(t), z(t)$ vanishing at $t = t_0$ and $t = t_1$:

$$S''[x_{cl}](y, z) = \int \left(\frac{\partial^2 L}{\partial x^2} z(t) + \frac{\partial^2 L}{\partial x \partial \dot{x}} \dot{z}(t) - \frac{d}{dt} \left(\frac{\partial^2 L}{\partial x \partial \dot{x}} z(t) + \frac{\partial^2 L}{\partial \dot{x}^2} \dot{z}(t) \right) \right) y(t).$$

In particular if we ask that $S''[x_{cl}](y, z) = 0$ for all y then we obtain a second ordinary differential operator in z which we write $S''[x](z)$, called the *Sturm–Liouville operator*.

- (b) Why is the Sturm–Liouville operator self-adjoint?
- (c) Show that the Sturm–Liouville operator of the harmonic oscillator is

$$S''[x] = -m \frac{d^2}{dt^2} - m\omega^2.$$

Show that the functions

$$y_k(t) = \sqrt{\frac{2}{T}} \sin\left(\frac{\pi kt}{T}\right)$$

are an orthonormal basis of its eigenfunctions, with eigenvalues

$$\lambda_k = m \left(\left(\frac{\pi k}{T} \right)^2 - \omega^2 \right).$$

So in the basis $y_k(t)$ the quadratic function S is now given by a diagonal matrix:

$$S = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \lambda_3 & \\ & & & \ddots \end{pmatrix}$$

and the path integral is a Gaussian integral:

$$\int [dy] e^{iS[y]/\hbar} = \frac{1}{\sqrt{\det\left(\frac{S''}{2\pi}\right)}}$$

(essentially; see section 15 on page 28 for more). How do we calculate the determinant? It is the product of eigenvalues:

$$\begin{aligned} \frac{1}{\sqrt{\det\left(\frac{S''}{2\pi}\right)}} &= \frac{1}{\sqrt{\prod_k \frac{\lambda_k}{2\pi}}} \\ &= \frac{1}{\sqrt{\prod_k \frac{m}{2\pi} \left(\left(\frac{\pi k}{T} \right)^2 - \omega^2 \right)}} \\ &= \frac{1}{\sqrt{\prod_k \frac{m\pi k^2}{2T^2} \underbrace{\prod_k \left(1 - \frac{\omega^2 T^2}{k^2 \pi^2} \right)}_{\text{Ahlfors [1] pg. 197}}}} \\ &= \frac{1}{F(T) \sqrt{\frac{\sin(\omega T)}{\omega T}}} \end{aligned}$$

This $F(T)$ is annoying: it has to be

$$F(T) = \sqrt{\prod_k \frac{m\pi k^2}{2T^2}}$$

which is divergent. But if we ignore it, we have

$$\langle x_1, T | x_0, 0 \rangle = \frac{e^{iS[x_c]/\hbar}}{F(T) \sqrt{\frac{\sin(\omega T)}{\omega T}}}.$$

Exercise 8. Normalizing the amplitude

Taking $\omega \rightarrow 0$ we should get the same result as the free particle. Note that $F(T)$ above is independent of ω . Use this to find $F(T)$ and to show that the final amplitude is

$$(2) \quad \langle x_1, T | x_0, 0 \rangle = \sqrt{\frac{m}{2\pi i \hbar T}} \left(\frac{\omega T}{\sin(\omega T)} \right)^{1/2} \exp \left(\frac{im}{2\hbar T} \left(\frac{(x_0^2 + x_1^2) \omega T}{\tan(\omega T)} - \frac{2x_0 x_1 \omega T}{\sin(\omega T)} \right) \right).$$

Exercise 9. The Schrödinger picture

Get Maple (or a long hand calculation) to show that this function is a Green's function for the Schrödinger equation for the harmonic oscillator, which is

$$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial x^2} + m\omega^2 x^2 \phi.$$

8. THE SCHRÖDINGER EQUATION

We have insisted (but by no means proven) that our amplitudes

$$\langle x_1, t_1 | x_0, t_0 \rangle$$

must provide a transformation of wave functions preserving probabilities, i.e. if

$$(3) \quad \phi_1(x_1) = \int dx_0 \langle x_1, t_1 | x_0, t_0 \rangle \phi_0(x_0)$$

then we require

$$\int dx_1 |\phi_1(x_1)|^2 = \int dx_0 |\phi_0(x_0)|^2.$$

This is essential to ensure that if we start with $|\phi_0|^2$ a probability density (i.e. nonnegative of unit integral), then we end up with another probability density.

Therefore equation 3 is an equation of unitary evolution. Write it as

$$U(t_0, t_1) \phi_0 = \phi_1.$$

This $U(t_0, t_1)$ is a unitary operator on complex valued functions. Therefore its inverse is its adjoint:

$$U(t_1, t_0) = U(t_0, t_1)^{-1} = U(t_0, t_1)^*.$$

In terms of integrals, this is just

$$(4) \quad \int dx_0 \langle x_1, t_1 | x_0, t_0 \rangle \langle x'_1, t_1 | x_0, t_0 \rangle^* = \delta(x_0 - x'_0)$$

(where the * here means complex conjugate of a complex number).

Differentiating and then setting $t_1 = t_0$, and defining

$$\hat{H}(t_0) = i\hbar \left. \frac{\partial}{\partial t_1} U(t_0, t_1) \right|_{t_1=t_0}$$

we find that this $\hat{H}(t_0)$ is a self-adjoint operator.² Call it the *Hamiltonian operator*. Another way to say this: the Lie algebra of the unitary group consists of the *skew-adjoint* operators. But every skew-adjoint operator is just $A = -i\hat{H}$ where \hat{H} is

²For the present, we will write hats on operators to indicate that they are self-adjoint operators.

self-adjoint. We put in the \hbar for convenience. Then we recover the unitary evolution from

$$(5) \quad \frac{\partial \phi}{\partial t} = -\frac{i}{\hbar} \hat{H}(t)\phi$$

which is the *Schrödinger equation*.³

9. AMPLITUDES AS STATES

Now suppose that we carry out an experiment, in which a particle hits a certain spot if the particle has a certain property, and doesn't hit it otherwise. (In some manner, perhaps involving many particles, all experiments have this form.) The way in which we arrange the experimental apparatus, our lab equipment, is described by a Lagrangian, say $L_{\text{experiment}}$. Therefore the probability that the particle has the property is

$$\text{Prob} = \left| \int_{\text{spot}} dx_1 \langle x_1, t_1 | x_0, t_0 \rangle_{\text{experiment}} \phi(x_0) \right|^2$$

where ϕ is the wave function of the particle at the time t_0 when the experiment started.

If the particle's wave function was a δ function at a point x_0 , this would give

$$\left| \langle x_1, t_1 | x_0, t_0 \rangle_{\text{experiment}} \right|^2.$$

So the amplitude

$$\langle x_1, t_1 | x_0, t_0 \rangle$$

as a function of x_1 is the wave function at time t_1 , so that the original wave function at time t_0 was a δ function.

On the other hand, if we want to be certain about the precise outcome of the experiment, then we want a δ function to come out, say at a point x_{target} .

$$\int dx_1 \langle x_1, t_1 | x_0, t_0 \rangle_{\text{experiment}} \phi(x_0) = \delta(x_1 - x_{\text{target}}).$$

What function ϕ should we use? From equation 4 on the preceding page, we see that we can take

$$\phi(x_0) = \langle x_{\text{target}}, t_1 | x_0, t_0 \rangle_{\text{experiment}}^*.$$

By invertibility of unitary evolution, this function is the only function we can use. Therefore the complex conjugate $\langle x_1, t_1 | x_0, t_0 \rangle_{\text{experiment}}^*$ of the amplitude is the state a particle must be in at time t_0 to have complete certainty that it will end up at x_1 at time t_1 .

Write

$$\psi(x_0) = \langle x_1, t_1 | x_0, t_0 \rangle_{\text{experiment}}^*.$$

This is the state that a particle must be in at time t_0 to have certainty of its being at x_1 at time t_1 . So each experimental outcome has associated with it a state ψ ,

$$\psi(x) = \langle x, t_1 | x_0, t_0 \rangle.$$

³For an arbitrary Lie group, instead of just a unitary group, we would prefer to call a *Lie equation*.

In this case, we will say that it is the state of being at x_1 at time t_1 . The amplitude of a particle in state $\phi(x_0)$ ending up at x_1 at time t_1 is

$$\int dx_0 \psi^*(x_0) \phi(x_0)$$

which we write as an inner product

$$\langle \psi, \phi \rangle.$$

In general, the probability of a particle represented by ϕ at time t_0 behaving a certain way at a given time t_1 is given by

$$|\langle \psi, \phi \rangle|^2$$

where ψ is the state associated to that behaviour.

10. MEASUREMENTS AND OPERATORS

The expected value of an experimental measurement (which we assume to be a real number) is the sum over all possible outcomes a of

$$a \text{Prob}(a).$$

Let us call A the quantity we are trying to measure. Then let ψ_a be the state representing $A = a$. The expected value of A for a particle in state ϕ is

$$\begin{aligned} \int da a |\langle \psi_a, \phi \rangle|^2 &= \int da a \left(\int dx \psi_a(x) \phi^*(x) \right) \left(\int dx' \psi_a^*(x') \phi(x') \right) \\ &= \int dx dx' \phi^*(x) \langle x|A|x' \rangle \phi(x') \end{aligned}$$

where we have written

$$\langle x|A|x' \rangle = \int da a \psi_a(x) \psi_a^*(x').$$

Exercise 10.

Show that

$$\langle x|A|x' \rangle^* = \langle x'|A|x \rangle.$$

Use this to show that the operator

$$\hat{A}\phi(x) = \int dx' \langle x|A|x' \rangle \phi(x')$$

is self-adjoint in the L^2 norm.

Exercise 11.

- (a) Show that the expected value of A in state $\psi_a(x)$ is a .
- (b) Show that

$$\hat{A}\psi_a(x) = a\psi_a(x).$$

These $\psi_a(x)$ are the *eigenfunctions* of the operator A , and these a values are the *eigenvalues*.

Exercise 12. Measuring position

Suppose that A is the measurement of position at time t_0 .

- (a) Show that

$$\psi_{x_0}(x) = \delta(x - x_0)$$

and that

$$\hat{A}\phi(x) = x\phi(x).$$

Consequently, we will write this operator as \hat{x} .

- (b) Find the function
- $\langle x'|\hat{x}|x\rangle$
- .

Exercise 13. Measuring momentum

- (a) Let us first return to classical mechanics. Recall from Aaron's lectures
- ⁴
- that the Hamiltonian vector field
- \vec{H}
- associated to a function
- $H(x, p)$
- (on the cotangent bundle) is

$$\vec{H} = \frac{\partial H}{\partial p} \frac{\partial}{\partial x} - \frac{\partial H}{\partial x} \frac{\partial}{\partial p}.$$

Also, the observables of classical mechanics are functions on the cotangent bundle. So observables $F(x, p)$ have “dynamics” associated to them: the flow of the vector field \vec{F} . Show that the flow of the vector field \vec{p} (i.e. taking Hamiltonian function $H(x, p) = p$) is translation in the x variables, leaving p fixed.

- (b) Suppose that we write
- \hat{p}
- for the operator

$$\hat{p}\phi(x) = -i\hbar \frac{\partial \phi}{\partial x}.$$

Show that this operator is self-adjoint.

- (c) Taking
- \hat{p}
- as Hamiltonian operator,
- $\hat{H} = \hat{p}$
- , plug it into the Schrödinger equation 5 on page 18 and integrate it to show that the associated evolution is given by

$$U(t_0, t_1)\phi(x_1) = \phi(x_1 - (t_1 - t_0)).$$

This should explain why this operator is called *momentum* and written \hat{p} : the associated evolution is through translations in the q variables.

- (d) Find the eigenfunctions and eigenvalues of
- \hat{p}
- .
-
- (e) Find the function

$$\langle x'|\hat{p}|x\rangle.$$

Exercise 14.

Calculate

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$$

Exercise 15. Momentum representation

(For now) write the Fourier transform as

$$\tilde{\phi}(p) = \int dx e^{-ixp/\hbar} \phi(x)$$

- (a) Show that the operator
- \hat{p}
- becomes the operator

$$\hat{p}\tilde{\phi}(p) = p\tilde{\phi}(p).$$

- (b) What happens to the position operator
- \hat{x}
- ?

⁴The gentle reader will pardon me for not maintaining his distinction between q and x .

- (c) What is the inverse of this Fourier transform? (Get the constants right.)
 (d) What constant c do we have to take so that

$$\int c dp \left| \tilde{\phi}(p) \right|^2 = \int dx |\phi(x)|^2?$$

11. INSERTIONS IN THE PATH INTEGRAL

The operator \hat{x} which gives the expected position of a particle applies only to wave functions at a given time t_0 like

$$\text{expected position at time } t_0 = \int dx \phi(x, t_0)^* x \phi(x, t_0).$$

If we only know the wave function at earlier and later times, say at times t_0 and t_1 , and we want its expected position at an intermediate time t_m then this is given by taking the amplitude to get to a point x_m , multiplying by x_m , and taking the amplitude to get from x_m :

$$\int dx_1 dx_0 dx_m \phi(x_1, t_1)^* \langle x_1, t_1 | x_m, t_m \rangle x_m \langle x_m, t_m | x_0, t_0 \rangle \phi(x_0, t_0)$$

which we will write as

$$\int dx_1 dx_0 \phi(x_1, t_1)^* \langle x_1, t_1 | \hat{x}(t_m) | x_0, t_0 \rangle \phi(x_0, t_0).$$

By cutting and pasting,

$$\langle x_1, t_1 | \hat{x}(t_m) | x_0, t_0 \rangle = \int [dx(t)] e^{\frac{i}{\hbar} S} \underbrace{x(t_m)}_{\text{A number!}}$$

so that expected position at an intermediate time t_m is expressed in terms of a path integral with $x(t_m)$ inserted into it. Similarly, we can calculate any operator $F(\hat{x})$ at time t_m by inserting $F(x(t_m))$ into the path integral.

Exercise 16. Momentum in the path integral

Show that expected momentum at time t_m is calculated from the wave function in the same manner as above for position, using

$$\int dp \phi(x_1, t_1)^* \langle x_1, t_1 | \hat{p}(t_m) | x_0, t_0 \rangle \phi(x_0, t_0)$$

but where the “matrix elements”

$$\langle x_1, t_1 | \hat{p}(t_m) | x_0, t_0 \rangle$$

are calculated by taking the amplitudes

$$\langle x_1, t_1 | x + y, t_m \rangle p e^{ipy/\hbar} \langle x, t_m | x_0, t_0 \rangle$$

and integrating out the intermediate position x and “jump” y , and the momentum value p . So the interpretation is that the particle moves along from x_0 to x , and then jumps to $x + y$ (see figure 11 on the following page) with a contribution $e^{ipy/\hbar}$ (which is the amplitude for a free particle to move from x to $x + y$ with momentum p), and then the particle moves from x to x_1 . We measure the momentum during the jump to be p . But the “jump” is instantaneous.

Emitter of electrons

Detector

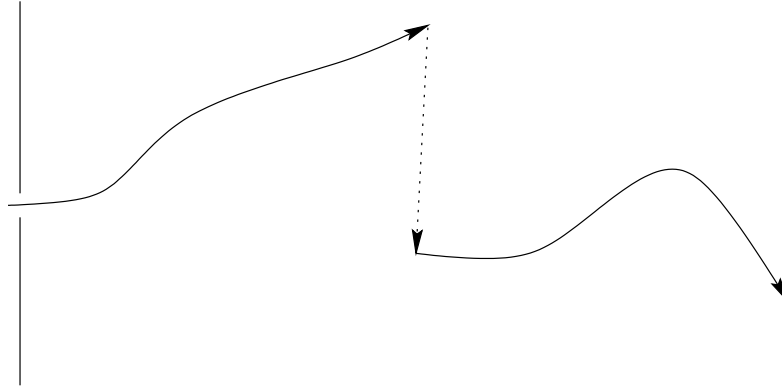


FIGURE 14. Measuring momentum with path integrals; we use paths with jumps

Taking any functions $A(x)$ and $B(x)$ we can plug them into the path at two different times

$$\int [dx] e^{\frac{i}{\hbar} S[x]} A(x(t_a)) B(x(t_b))$$

to calculate $A(\hat{x}(t_a)) B(\hat{x}(t_b))$. But this doesn't quite work: if we expand out the result in terms of amplitudes up to different times, we find that this computes $A(\hat{x}(t_a)) B(\hat{x}(t_b))$ if $t_a > t_b$ but computes $B(\hat{x}(t_b)) A(\hat{x}(t_a))$ if $t_a < t_b$. Therefore we define the *time ordered product*

$$T[A(\hat{x}(t_a)) B(\hat{x}(t_b))] = \theta(t_a - t_b) A(\hat{x}(t_a)) B(\hat{x}(t_b)) + \theta(t_b - t_a) B(\hat{x}(t_b)) A(\hat{x}(t_a))$$

where

$$\theta(t) = \begin{cases} 1 & \text{if } t > 0 \\ \frac{1}{2} & \text{if } t = 0 \\ 0 & \text{if } t < 0 \end{cases}$$

Exercise 17. Calculating Hamiltonians

We still haven't indicated how to write down the Hamiltonian operator of any quantum systems, except the free particle and the harmonic oscillator. Suppose that you have a Lagrangian L_0 and you know its Hamiltonian operator $\hat{H}_0(t)$. Make a new Lagrangian by

$$L(x, \dot{x}) = L_0(x, \dot{x}) - V(x)$$

for some function $V(x)$. Lets try to find the associated Hamiltonian $\hat{H}(t)$.

(a) First, we need to express \hat{H}_0 in terms of a path integral. Show that

$$(6) \quad \hat{H}_0(t) \phi(x) = i\hbar \left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \int \langle x, t + \varepsilon | y, t \rangle_0 \phi(y) dy.$$

where the amplitude with a zero subscript

$$\langle x, t + \varepsilon | y, t \rangle_0$$

means that it is computed with a path integral containing L_0 instead of L .

- (b) Next, we need to write amplitudes for L in terms of those for L_0 . Writing

$$\exp\left(\frac{i}{\hbar}S[x]\right) = \exp\left(\frac{i}{\hbar}S_0[x]\right) \exp\left(-\frac{i}{\hbar}\int dt V(x(t))\right),$$

expand out the second exponential factor, and derive the equation

$$\langle x, t + \varepsilon | y, t \rangle = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{-i}{\hbar}\right)^k \int_t^{t+\varepsilon} dt_1 \dots \int_t^{t+\varepsilon} dt_k \langle x, t + \varepsilon | T[V(\hat{x}(t_1)) \dots V(\hat{x}(t_k))] | y, t \rangle_0.$$

- (c) Differentiate this expression with

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0}$$

to find

$$\hat{H}(t) = \hat{H}_0(t) + V(\hat{x}).$$

- (d) If

$$L = \frac{m}{2}\dot{x}^2 - V(x)$$

show that

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

- (e) Show that this is what you get from taking the Legendre transform (see Aaron's notes) of the Lagrangian and then replacing p variables by \hat{p} operators and x variables by \hat{x} operators.

12. WHY THE HAMILTONIAN OPERATOR REPRESENTS ENERGY

We want to see that the operator \hat{H} has some relation to the Hamiltonian function H , at least in the semiclassical limit.

Exercise 18. The Hamilton–Jacobi equation

(It would have been better to see this in Aaron's lectures.) Consider the picture of classical paths as trajectories of a flow

$$\vec{H} = \frac{\partial H}{\partial p} \frac{\partial}{\partial x} - \frac{\partial H}{\partial x} \frac{\partial}{\partial p}.$$

The phase space maps to the configuration space by $(x, p) \mapsto x$. Fix a particular point of configuration space x_0 , and look at the fiber of this map above that point. In figures 12 on the next page and 12 on page 25 this fiber is a vertical line.

- (a) Fix times $t_1 > t_0$. Consider the map $p_0 \mapsto x_1$ defined by taking an initial momentum p_0 (a point of the fiber) and then following along the flow from (x_0, p_0) for time $t_1 - t_0$ to a point (x_1, p_1) . Looking at the expression of the Hamiltonian vector field above, under what conditions will it be true that for sufficiently small times $t_1 - t_0$ the map $p_0 \mapsto x_1$ is a local diffeomorphism near some fixed value of p_0 ? (Essentially the idea is that in the phase diagram, the x components of the

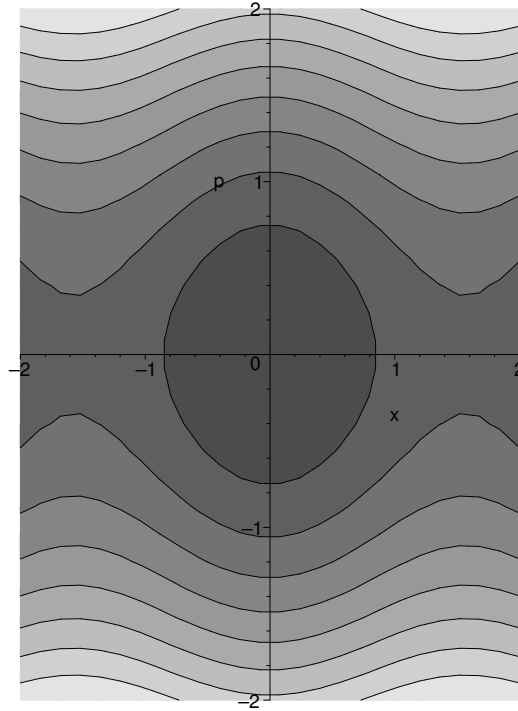


FIGURE 15. The phase flow of a classical pendulum, indicating the levels of the Hamiltonian

vector \vec{H} are all different at different points of the fiber, at least locally.) For what positions and times does this work for the harmonic oscillator?

- (b) Suppose that this map $p_0 \mapsto x_1$ is a diffeomorphism. Now consider the action $S = S(x_1, t_1)$ obtained by integrating the Lagrangian along the classical path that leaves x_0 at time t_0 and reaches x_1 at time t_1 . Consider the extended phase space with coordinates (x, p, t) , and the 1-form $\xi = p dx - H dt$ on that space. The flow on the extended phase space is given by the vector field

$$\vec{H} = \frac{\partial H}{\partial p} \frac{\partial}{\partial x} - \frac{\partial H}{\partial x} \frac{\partial}{\partial p} + \frac{\partial}{\partial t}.$$

Show that $\vec{H} \lrcorner d\xi = 0$. Now taking two points x_1 and $x_1 + \Delta x_1$ and two times t_1 and $t_1 + \Delta t_1$, consider for each $0 \leq s \leq 1$ the classical path that leaves x_0 at time t_0 and arrives at $x_1 + s\Delta x_1$ at time $t_1 + s\Delta t_1$. These paths form a rectangle in extended phase space. By using Stoke's theorem applied to ξ on this rectangle, show that

$$\Delta S = S(x_1 + \Delta x_1, t_1 + \Delta t_1) - S(x_1, t_1)$$

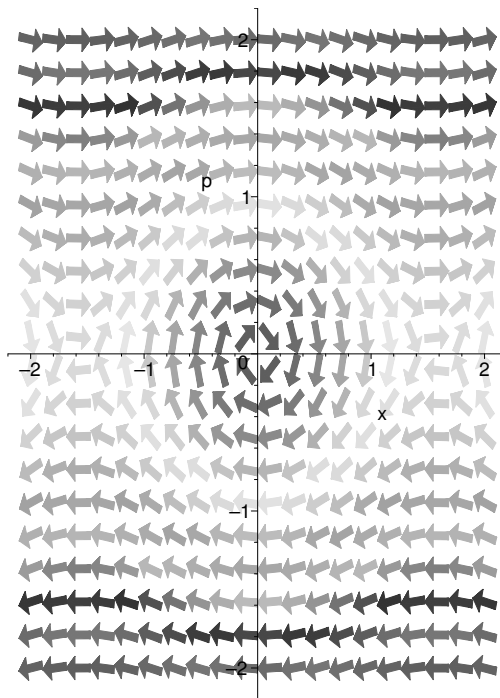


FIGURE 16. The phase flow of a classical pendulum, indicating phase velocity

is given by

$$\Delta S = p_1 \Delta x_1 - H \Delta t_1 + O\left((\Delta x_1)^2, (\Delta t_1)^2\right).$$

(c) Show that

$$dS = p dx - H dt.$$

(d) Use this to see that the function $S = S(x_1, t_1)$ satisfies the *Hamilton-Jacobi equation*

$$\frac{\partial S}{\partial t} + H\left(x, \frac{\partial S}{\partial x}, t\right) = 0.$$

This says that if you allow yourself more time Δt to get there, the classical path requires less action by about $-H\Delta t$, where H is total energy at the end of that original path.

Exercise 19.

In the semiclassical limit, i.e. for \hbar very small, we have seen that only classical paths contribute. Lets assume this.

(a) For any two points x_0, x_1 and times $t_0 < t_1$, show that in the semiclassical limit,

$$\langle x_1, t_1 | x_0, t_0 \rangle = \sum_x \exp\left(\frac{i}{\hbar} S[x]\right)$$

and that

$$\langle x_1, t_1 | \hat{H}(t_m) | x_0, t_0 \rangle = \sum_x H(x(t_m), p(t_m)) \exp\left(\frac{i}{\hbar} S[x]\right)$$

where the sum is over all classical paths $x(t)$ which satisfy

$$x(t_0) = x_0 \quad x(t_1) = x_1$$

and the momentum $p(t)$ is the momentum along that classical path. (Hint: equation 6 on page 22.) So it looks like an insertion of the classical Hamiltonian into the path integral.

It is in this sense that we say that the eigenvalues of \hat{H} represent *energy levels*.

13. FUNCTIONAL CALCULUS AND THE OPERATOR EQUATION OF MOTION

The action $S[x]$ is a functional: it eats paths and gives numbers. We differentiate it like:

$$dS[x]y = \left. \frac{d}{d\varepsilon} S[x + \varepsilon y] \right|_{\varepsilon=0}$$

where y is a perturbation of the path x .

Writing

$$S[x] = \int_{t_0}^{t_1} dt L(x(t), \dot{x}(t))$$

we find

$$dS[x]y = \left. \frac{\partial L}{\partial x} y \right|_{t=t_0}^{t=t_1} + \int_{t_0}^{t_1} dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) y(t).$$

We will also consider more general functionals, say $F[x]$.

If we take y to be a δ function:

$$y(t) = \delta(t - t_m)$$

then we will write

$$\frac{\delta F}{\delta x(t_m)} = dF[x]y.$$

For example, if $t_0 < t_m < t_1$, then

$$\frac{\delta S}{\delta x(t_m)} = \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \Big|_{t=t_m}.$$

It is this which vanishes on classical paths.

If $y(t)$ vanishes at $t = t_0$ and $t = t_1$, then since we add all paths into the path integral,

$$\int [dx] F[x] = \int [d(x+y)] F[x+y] = \int [dx] F[x+y].$$

Therefore

$$\begin{aligned} \int [dx] dF[x]y &= \lim_{\varepsilon \rightarrow 0} \frac{\int [dx] F[x + \varepsilon y] - \int [dx] F[x]}{\varepsilon} \\ &= 0. \end{aligned}$$

(Stoke's theorem). Allowing y to become a δ function,

$$\int [dx] \frac{\delta F}{\delta x(t_m)} = 0.$$

In particular if $F[x] = \exp(iS[x]/\hbar)$,

$$\begin{aligned} 0 &= \int [dx] \frac{\delta F}{\delta x(t_m)} \\ &= \int [dx] e^{iS/\hbar} \frac{\delta S}{\delta x(t_m)} \\ &= \left\langle x_1, t_1 \left| \widehat{\frac{\delta S}{\delta x(t_m)}} \right| x_0, t_0 \right\rangle \end{aligned}$$

shows that

$$\widehat{\frac{\delta S}{\delta x(t_m)}} = 0.$$

This is *Ehrenfest's theorem* or the *operator equation of motion*. For example, it says that the expected acceleration of a free particle is zero. In general it says that a particle is expected to satisfy the Euler–Lagrange equations.

Exercise 20.

Using integration by parts in the path integral, show that

$$T \left[\widehat{\frac{\delta S}{\delta x(t_A)}} \hat{x}(t_B) \right] = i\hbar \delta(t_B - t_A)$$

as operators.

14. THE FUNCTIONAL FOURIER TRANSFORM

To package all of the insertions into one object, consider a function $J(t)$ vanishing at times t_0 and t_1 and let L_J be the new Lagrangian

$$L_J = L - J(t)x(t).$$

Exercise 21.

Starting with Lagrangian

$$L = \frac{m}{2} \left(\frac{dx}{dt} \right)^2 - V(x)$$

show that this corresponds physically to adding an external force $J(t)$.

Define the *partition function*

$$Z(J) = \int [dx] \exp \left(\frac{i}{\hbar} S_J[x] \right).$$

We can expand this out into

$$\begin{aligned} Z(J) &= \int [dx] \exp \left(\frac{i}{\hbar} S[x] \right) \exp \left(-\frac{i}{\hbar} \int dt J(t)x(t) \right) \\ &= \int [dx] \exp \left(\frac{i}{\hbar} S[x] \right) \sum_{k=0}^{\infty} \frac{1}{k!} \left(-\frac{i}{\hbar} \int dt J(t)x(t) \right)^k. \end{aligned}$$

Now take functional derivatives:

$$\begin{aligned} \frac{\delta}{\delta J(t_1)} \cdots \frac{\delta}{\delta J(t_k)} \Big|_{J=0} Z(J) &= \left(\frac{-i}{\hbar}\right)^k \int [dx] \exp\left(\frac{i}{\hbar} S[x]\right) x(t_1) \cdots x(t_k) \\ &= \left(\frac{-i}{\hbar}\right)^k \langle x_1, t_1 | T[\hat{x}(t_1) \cdots \hat{x}(t_k)] | x_0, t_0 \rangle. \end{aligned}$$

This gives all possible insertions, contained in the functional $Z(J)$. By definition, $Z(J)$ is the Fourier transform of $\exp(iS[x]/\hbar)$. It might be useful to write it as $\langle x_1, t_1 | x_0, t_0 \rangle_J$ to emphasize the dependence on the initial and final points.

Physicists say that the insertions determine the partition function $Z(J)$ by Taylor expansion:

$$Z(J) = -i\hbar \sum \frac{1}{k!} \langle x_1, t_1 | T[\hat{x}(t_1) \cdots \hat{x}(t_k)] | x_0, t_0 \rangle J(t_1) \cdots J(t_k).$$

I don't know what this means, except that they clearly believe that the values of all insertions determine the partition function, although I don't see how.

Exercise 22. The free particle partition function

Calculate $Z(J)$ for the free particle. It helps to have some notation like

$$J_1(t) = \int_{t_0}^t J(u) du.$$

15. GAUSSIAN INTEGRALS

We have used some Gaussian integrals already. Define

$$I(A, b) = \int_{\mathbb{R}^n} dx e^{-\frac{1}{2} \langle Ax, x \rangle + \langle b, x \rangle}$$

where A is a positive definite symmetric matrix. To calculate it:

- (1) Change variables to $y = x - A^{-1}b$ (so that $y = 0$ is the minimum point) to get

$$I(A, b) = e^{\frac{1}{2} \langle A^{-1}b, b \rangle} I(A, 0).$$

- (2) Diagonalize A by a rotation of the y variables

$$I(A, 0) = I(\Lambda, 0)$$

where

$$\Lambda = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix}$$

is the matrix of eigenvalues of A .

- (3) Use the identity

$$e^{-\frac{1}{2} \langle \Lambda x, x \rangle} = e^{-\lambda_1 x_1^2 / 2} \cdots e^{-\lambda_n x_n^2 / 2}$$

to get

$$I(\Lambda, 0) = I(\lambda_1, 0) \cdots I(\lambda_n, 0).$$

Now we are reduced to 1-dimensional integrals.

and on $-i\mu_k$ it gives

$$\sqrt{-i\mu_k} = e^{-\pi i/4} \sqrt{\mu_k}.$$

So we get

$$\sqrt{\det\left(\frac{-iQ}{2\pi}\right)} = e^{-\pi i \text{Index}(Q)/4} \sqrt{\det\left(\frac{Q}{2\pi}\right)}.$$

Note that this index is the index of inertia (also known as the signature), not the Fredholm index. Finally:

$$\int_{\mathbb{R}^n} e^{\frac{i}{2}\langle Qx, x \rangle + \langle b, x \rangle} = e^{\pi i \text{Index}(Q)/4} \frac{e^{\frac{i}{2}\langle Q^{-1}b, b \rangle}}{\sqrt{\det\left(\frac{Q}{2\pi}\right)}}$$

Exercise 23. Large radius limit

Use Gaussian integrals to show that the amplitude

$$\langle \alpha_1, t_1 | \alpha_0, t_0 \rangle$$

of a free particle on the circle of radius R approaches the amplitude of a free particle on the line as the radius R goes to infinity. Hint: the ϑ function looks like a Riemann sum.

Exercise 24. Constant force fields

For a particle in a constant external field f , with Lagrangian

$$L = \frac{m}{2} \dot{x}^2 + fx$$

show that the amplitude for travelling between two points is

$$\langle x_1, t_1 | x_0, t_0 \rangle = \left(\frac{m}{2\pi i \hbar T} \right) \exp \left(\frac{i}{\hbar} \left[\frac{m(x_1 - x_0)^2}{2T} + \frac{1}{2} fT(x_0 + x_1) - \frac{f^2 T^3}{24m} \right] \right)$$

where $T = t_1 - t_0$. The Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} - f\hat{x}.$$

Express the eigenfunctions of \hat{H} in terms of the Airy function. Draw the eigenfunction with lowest eigenvalue and interpret the picture.

Exercise 25.

Using Fourier transforms of distributions (i.e. generalized functions) show that we can “define” the oscillatory integral

$$\int_{\mathbb{R}^n} e^{\frac{i}{2}\langle Qx, x \rangle} dx = \int f(x) dx$$

as the limit

$$\lim_{p \rightarrow 0} \tilde{f}(p)$$

of its Fourier transform, and that we obtain the expected answer.

Exercise 26.

Using a Gaussian integral, being careful about phase, show that the phase in our calculation of the amplitude $\langle x_1, T | x_0, 0 \rangle$ for the harmonic oscillator in equation 2 on page 17 is wrong. What is the right phase?

16. GAUSSIAN INTEGRALS WITH INSERTIONS

To handle insertions into the integrals, which we write like

$$\langle p(x) \rangle = \int_{\mathbb{R}^n} dx e^{\frac{i}{2}\langle Qx, x \rangle} p(x)$$

with $p(x)$ a polynomial, we just need to keep in mind

$$\frac{\partial}{\partial b} e^{bx} = x e^{bx}$$

and its multivariate generalizations. In multiindices $\alpha = (\alpha_1, \dots, \alpha_n)$ with

$$x^\alpha = x_1^{\alpha_1} \dots x_n^{\alpha_n}$$

and

$$|\alpha| = \alpha_1 + \dots + \alpha_n$$

we find

$$\frac{\partial^{|\alpha|}}{\partial b^\alpha} e^{\langle b, x \rangle} = x^\alpha e^{\langle b, x \rangle}$$

and if

$$p(x) = \sum_{\alpha} c_{\alpha} x^{\alpha}$$

then

$$p\left(\frac{\partial}{\partial b}\right) e^{\langle b, x \rangle} = p(x) e^{\langle b, x \rangle}.$$

Then

$$p\left(\frac{\partial}{\partial b}\right) \int_{\mathbb{R}^n} dx e^{\frac{i}{2}\langle Qx, x \rangle + \langle b, x \rangle} \Big|_{b=0} = \int_{\mathbb{R}^n} dx e^{\frac{i}{2}\langle Qx, x \rangle} p(x).$$

Consequently

$$\begin{aligned} \langle p(x) \rangle &= p\left(\frac{\partial}{\partial b}\right) J(Q, b) \Big|_{b=0} \\ &= \frac{\exp\left(\frac{\pi i}{4} \text{Index}(Q)\right)}{\sqrt{\det\left(\frac{Q}{2\pi}\right)}} p\left(\frac{\partial}{\partial b}\right) \exp\left(\frac{i}{2} \langle Q^{-1}b, b \rangle\right) \Big|_{b=0}. \end{aligned}$$

Expand out the exponential

$$\langle p(x) \rangle = \frac{\exp\left(\frac{\pi i}{4} \text{Index}(Q)\right)}{\sqrt{\det\left(\frac{Q}{2\pi}\right)}} p\left(\frac{\partial}{\partial b}\right) \sum_k \frac{1}{k!} \left(\frac{i}{2} \langle Q^{-1}b, b \rangle\right)^k \Big|_{b=0}.$$

In particular, since all terms are even in b , odd order terms in $p(x)$ make no contribution.

Theorem 16.1 (Wick).

$$(7) \quad \langle x^\alpha \rangle = \langle 1 \rangle i^k \sum Q_{i_1 j_1}^{-1} \dots Q_{i_k j_k}^{-1}$$

where $|\alpha| = 2k$, and the sum is over all possible pairings of indices so that

$$x^\alpha = \prod_{m=1}^k x_{i_m} x_{j_m}$$

and we include two terms into the sum in equation 7 on the page before precisely if they generate (formally) different terms. The number of terms is

$$\frac{(4k)!}{2^{2k} (2k)!}.$$

In terms of a symmetric matrix A with positive definite real part, the integral

$$\langle x^\alpha \rangle = \int_{\mathbb{R}^n} dx e^{-\frac{1}{2}\langle Ax, x \rangle} x^\alpha$$

is given by

$$\langle x^\alpha \rangle = \frac{\sum A_{i_1 j_1}^{-1} \cdots A_{i_k j_k}^{-1}}{\sqrt{\det\left(\frac{A}{2\pi}\right)}}$$

with the same type of sum.

17. PERTURBATION THEORY AND FEYNMAN DIAGRAMS

A perturbation of an insertion is something like

$$\langle p(x) \rangle_\lambda = \int_{\mathbb{R}^n} dx e^{i\left(\frac{1}{2}\langle Qx, x \rangle - \lambda V(x)\right)} p(x)$$

where $V(x)$ is a function and λ a small parameter.

Naively, expand the $\exp(-i\lambda V(x))$ in λ :

$$\begin{aligned} \langle p(x) \rangle_\lambda &= \sum_k \frac{(-i\lambda)^k}{k!} \int_{\mathbb{R}^n} dx e^{i\frac{1}{2}\langle Qx, x \rangle} V(x)^k p(x) \\ &= \sum_k \frac{(-i\lambda)^k}{k!} \langle V(x)^k p(x) \rangle \end{aligned}$$

a sum of insertions.

Exercise 27. Asymptotic series

- (a) Use this perturbative approach to expand

$$\int_{-\infty}^{\infty} e^{-x^2/2 - \lambda x^4} dx$$

into a series in λ . You should get

$$\sqrt{2\pi} \sum_{k=0}^{\infty} \left(-\frac{1}{4}\right)^k \frac{(4k)!}{k!(2k)!} \lambda^k.$$

- (b) Use Stirling's formula to estimate the coefficients of this expansion. You should get that the λ^k coefficient is approximately

$$\left(-\frac{16k}{e}\right)^k.$$

So this is a divergent series.

- (c) How could we have guessed that the series would diverge by just looking at the integral—in other words why is this not an analytic function of λ near $\lambda = 0$?

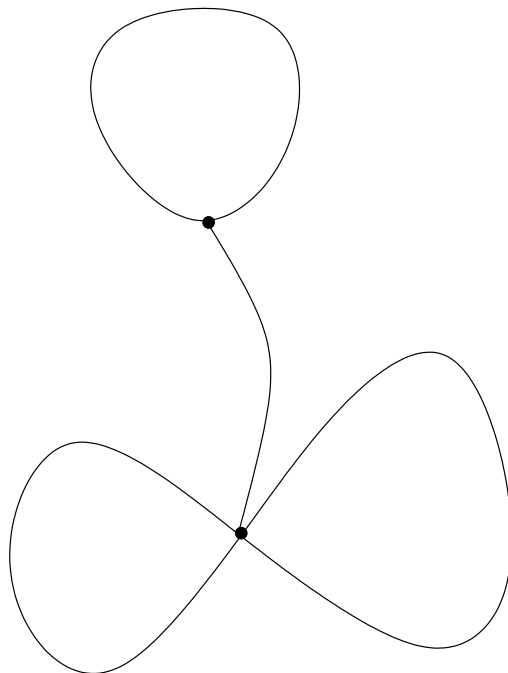


FIGURE 17. A Feynman diagram

- (d) Extra credit (i.e. I have no idea): why is the exact value of the integral

$$\frac{1}{4} \sqrt{\frac{2}{\lambda}} e^{1/32\lambda} K_{1/4} \left(\frac{1}{32\lambda} \right)$$

where $K_\nu(\zeta)$ is the modified Bessel function of the second kind, satisfying

$$\zeta^2 \frac{\partial^2 K}{\partial \zeta^2} + \zeta \frac{\partial K}{\partial \zeta} = (\zeta^2 + \nu^2) K?$$

Is it an analytic function of $1/32\lambda$? For help, you might look at Zinn-Justin [5], chapters 36 and 40.

Write

$$V(x) = \sum_{\alpha} c_{\alpha} x^{\alpha}$$

as a Taylor expansion. Then these insertions can be expanded out as insertions in monomials. The λ^k order term is calculated as follows: it is a sum of insertions involving k monomial terms from $V(x)$ and one from $p(x)$. For each $V(x)$ monomial, draw a vertex. For each linear factor in that monomial, draw an edge coming out of the vertex. Then do the same for the monomial from $p(x)$. Now to form the sum in the Wick theorem, we have to sum over all pairings of monomials, i.e. ways of joining the legs.

Traditionally, we draw the $p(x)$ monomial vertex at infinity, so just have a bunch of edges sticking out. Figure 17 shows a diagram for $p(x) = 1$. If

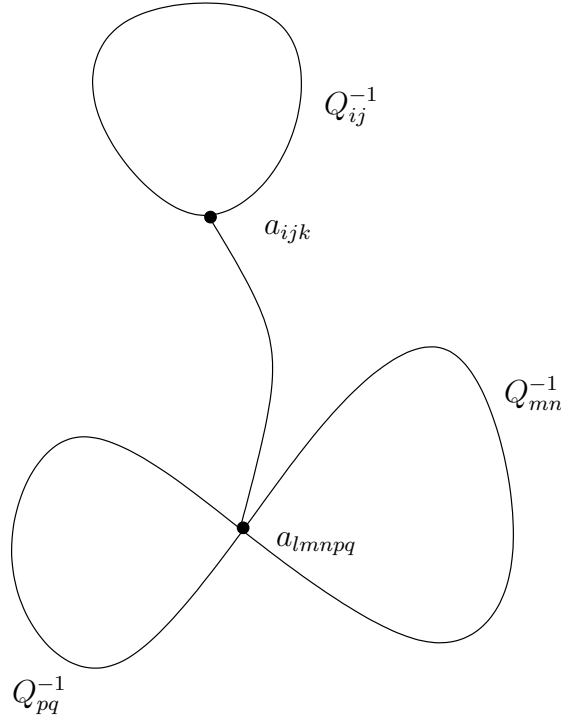


FIGURE 18. The diagram from figure 17 on the preceding page decorated by the relevant expansion terms

$$V(x) = a_0 + a_i x^i + \frac{1}{2} a_{ij} x^i x^j + \frac{1}{6} a_{ijk} x^i x^j x^k + \dots$$

then this diagram contributes the expression

$$(-i\lambda)^8 Q_{ij}^{-1} a_{ijk} Q_{pq}^{-1} a_{lmnpq} Q_{mn}^{-1}$$

which we see when it is decorated as in figure 17.

Theorem 17.1 (Wick).

$$\int_{\mathbb{R}^n} dx e^{i(\frac{1}{2}\langle Qx, x \rangle - \lambda V(x))} p(x) = \frac{\exp(\pi i \text{Index}(Q)/4)}{\sqrt{\det\left(\frac{Q}{2\pi}\right)}} \sum_k \frac{(-i\lambda)^k}{k!} \sum_{\Gamma} \frac{\text{contribution from } \Gamma}{|\text{Aut}(\Gamma)|}$$

where the sum \sum_{Γ} is over all diagrams Γ which have k edges.

18. ANSWERS TO THE EXERCISES

1. (a) Just take derivatives.
- (b) Test this on a Gaussian first; it is just a Gaussian integral. Next, use the fact that Gaussian functions are dense in L^2 .
- (c) Write

$$|\phi(x, t)|^2 = \phi(x, t)^* \phi(x, t)$$

and differentiate in time, and then plug in the Schrödinger equation.

2. Take α_0, α_1 with

$$-\pi R \leq \alpha_0, \alpha_1 < \pi R.$$

Every path $\alpha(t)$ satisfying

$$\alpha(t_j) = \alpha_j, \quad j = 0, 1$$

can be written as a classical piece and a perturbation. The classical piece is

$$\alpha_N(t) = v_N(t - t_0) + \alpha_0$$

where

$$v_N = \frac{2\pi RN + \alpha_1 - \alpha_0}{t_1 - t_0}.$$

The perturbation is any path $\beta(t)$ with

$$\beta(t_0) = \beta(t_1) = 0.$$

$$\langle \alpha_1, t_1 | \alpha_0, t_0 \rangle = \sum_{N \in \mathbb{Z}} \int [d\beta] \exp\left(\frac{i}{\hbar} \int dt L_N\right)$$

where

$$\begin{aligned} L_N &= L[\alpha_N + \beta] \\ &= \frac{m}{2} \left(\frac{d\alpha_N}{dt} + \frac{d\beta}{dt} \right)^2 \\ &= \frac{m}{2} \left(v_N^2 + 2v_N \frac{d\beta}{dt} + \left(\frac{d\beta}{dt} \right)^2 \right). \end{aligned}$$

But the term

$$2v_N \frac{d\beta}{dt}$$

contributes nothing, since it integrates to

$$2v_N (\beta(t_1) - \beta(t_0)) = 0.$$

So we take

$$L_N = \frac{m}{2} v_N^2 + \frac{m}{2} \left(\frac{d\beta}{dt} \right)^2.$$

The action is

$$\begin{aligned} S &= \int dt L_N \\ &= v_N(t_1 - t_0) + \frac{m}{2} \int \left(\frac{d\beta}{dt} \right)^2. \end{aligned}$$

The path integral is

$$\begin{aligned} \langle \alpha_1, t_1 | \alpha_0, t_0 \rangle &= \sum_{N \in \mathbb{Z}} \exp\left(\frac{i}{\hbar} \frac{m}{2} v_N^2 (t_1 - t_0)\right) \int [d\beta] \exp\left(\frac{i}{\hbar} L_{\text{line}}\right) \\ &= \int [d\beta] \exp\left(\frac{i}{\hbar} L_{\text{line}}\right) \sum_{N \in \mathbb{Z}} \exp\left(\frac{i}{\hbar} \frac{m}{2} v_N^2 (t_1 - t_0)\right). \end{aligned}$$

The remaining path integral, with Lagrangian L_{line} , is just the path integral of a free particle on the line, going from 0 to 0, which gives the contribution

$$\sqrt{\frac{m}{2\pi i\hbar(t_1 - t_0)}}.$$

Putting it together:

$$\langle \alpha_1, t_1 | \alpha_0, t_0 \rangle = \sqrt{\frac{m}{2\pi i\hbar(t_1 - t_0)}} \sum_{N \in \mathbb{Z}} \exp\left(\frac{i}{\hbar} \frac{m}{2} v_N^2 (t_1 - t_0)\right).$$

Plug in the value of v_N :

$$\begin{aligned} v_N^2 &= (2\pi RN + \alpha_1 - \alpha_0)^2 \\ &= 4\pi^2 R^2 N^2 + 4\pi RN(\alpha_1 - \alpha_0) + (\alpha_1 - \alpha_0)^2. \end{aligned}$$

This gives

$$\frac{im}{2\hbar} v_N^2 (t_1 - t_0) = \pi i N^2 \left(\frac{2\pi R^2 m}{\hbar(t_1 - t_0)}\right) + 2\pi N \frac{mR(\alpha_1 - \alpha_0)}{\hbar(t_1 - t_0)} + \frac{im(\alpha_1 - \alpha_0)^2}{2\hbar(t_1 - t_0)}.$$

Define

$$\begin{aligned} z &= \frac{mR(\alpha_1 - \alpha_0)}{\hbar(t_1 - t_0)} \\ \tau &= \frac{2\pi R^2 m}{\hbar(t_1 - t_0)}. \end{aligned}$$

The amplitude is

$$\begin{aligned} \langle \alpha_1, t_1 | \alpha_0, t_0 \rangle &= \sqrt{\frac{m}{2\pi i\hbar(t_1 - t_0)}} \sum_{N \in \mathbb{Z}} \exp(\pi i N^2 \tau + 2\pi i N z) \exp\left(\frac{im(\alpha_1 - \alpha_0)^2}{2\hbar(t_1 - t_0)}\right) \\ &= \sqrt{\frac{m}{2\pi i\hbar(t_1 - t_0)}} \exp\left(\frac{im(\alpha_1 - \alpha_0)^2}{2\hbar(t_1 - t_0)}\right) \exp(\pi i N^2 \tau + 2\pi i N z) \end{aligned}$$

Just employ the functional identity.

- (b) The proof that it is a Green's function for the Schrödinger equation is the same as for the heat equation, as in Mumford's book. The unitarity of evolution follows again from using the Schrödinger equation.
3. We leave the Fourier transform to the reader. On the circle, using the Fourier series

$$\phi(\alpha, t) = \sum c_k(t) e^{ik\alpha/R},$$

we recover the coefficients c_k from

$$c_k(t) = \frac{1}{2\pi R} \int \phi(\alpha, t) e^{-im\alpha/R} d\alpha.$$

Just differentiating, we find that the Schrödinger equation is satisfied on ϕ precisely when the coefficients c_k satisfy

$$\frac{dc_k}{dt} = -\frac{i\hbar k^2}{2mR^2} c_k.$$

The solution of this ordinary differential equation is

$$c_k(t) = \exp\left(-\frac{i\hbar k^2 t}{2mR^2}\right) c_k(0).$$

We recover ϕ :

$$\phi(\alpha, t) = \sum_k \exp\left(-\frac{i\hbar k^2 t}{2mR^2}\right) c_k(0) \exp(ikx/R).$$

Plugging in the expression for $c_k(0)$ as a Fourier coefficient of $\phi(\alpha, 0)$,

$$\phi(\alpha, t) = \sum_k \exp\left(-\frac{i\hbar k^2 t}{2mR^2} + ik\alpha/R\right) \int \phi(\alpha_0, 0) \exp(-ik\alpha_0) d\alpha_0.$$

Changing the order of integration, we find

$$\phi(\alpha_1, t_1) = \int d\alpha_0 G(\alpha_1 - \alpha_0, t_1 - t_0) \phi(\alpha_0, t_0)$$

where

$$G(\alpha, t) = \frac{1}{2\pi R} \vartheta\left(\frac{\alpha}{2\pi R}, -\frac{\hbar t}{2\pi m R^2}\right).$$

4. Up on the covering circle, the Fourier coefficients c_k evolve as

$$\frac{dc_k}{dt} = -\frac{i\hbar k^2}{2mR^2} c_k.$$

Writing $c_k = c_{qs+r}$ this gives

$$c_{qs+r}(t) = \exp\left(-\frac{i\hbar}{2m} \left(\frac{qs+r}{R}\right)^2 t\right).$$

This gives

$$\phi_r(\alpha, t) = \exp\left(\frac{ir\alpha}{R}\right) \sum_q \exp\left(-\frac{i\hbar t}{2m} \left(\frac{qs+r}{R}\right)^2 + \frac{iqs\alpha}{R}\right) c_{qs+r}(0).$$

Plugging in the Fourier integral that computes $c_{qs+r}(0)$ out of $\phi(\alpha, 0)$,

$$\phi_r(\beta_1, t_1) = \int d\alpha_0 \langle \beta_1, t_1 | \beta_0, t_0 \rangle_r \phi_r(\beta_0, t_0)$$

where

$$\langle \beta_1, t_1 | \beta_0, t_0 \rangle_r = \frac{1}{2\pi R} \sum_q \exp\left(\pi i (q+r/s)^2 \left(-\frac{\hbar t}{2m\pi(R/s)^2}\right) + 2\pi i (q+r/s) \frac{\beta_1 - \beta_0}{2\pi R}\right)$$

which is expressed in terms of the ϑ function with characteristics in the manner indicated.

5.

$$\begin{aligned} S[x_{cl}, y] &= \int dt \frac{m}{2} \left(\frac{dx}{dt} \frac{dy}{dt} - \omega^2 xy \right) \\ &= \int dt \frac{m}{2} \left(-\frac{d^2x}{dt^2} - \omega^2 x \right) y \end{aligned}$$

6. (a)

$$-\frac{d^2x}{dt^2} - \omega^2 x = 0.$$

(b)

$$x(t) = \frac{1}{\sin(\omega T)} (\sin(\omega(T-t)) x_0 + \sin(\omega t) x_1).$$

(c) Plugging in the classical path from the last part, this is a very complicated, but ultimately elementary integral.

7. (a) We have seen that

$$S'[x]y = \int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) y$$

so

$$\begin{aligned} S'[x_{cl} + \varepsilon z]y &= S'[x_{cl}]y + \varepsilon S''[x_{cl}](z, y) + \dots \\ &= \varepsilon S''[x_{cl}](z, y) + \dots \end{aligned}$$

and we just plug in $x = x_{cl} + \varepsilon z$.

(b) This is just the symmetry of second derivatives.

(c) Easy calculation. There is a complete basis of the square integrable functions, because the Sturm–Liouville operator is self-adjoint.

8. Using

$$\frac{\sin(\omega T)}{\omega T} \rightarrow 1$$

we find the action goes to the action of a free particle, and so the amplitude goes to that of the free particle precisely if

$$F(T) = \sqrt{\frac{2\pi i \hbar T}{m}}.$$

9. Plug the amplitude function into Maple and differentiate it; you see that it satisfies the Schrödinger equation (except at $T = 0$). Now convolve with a Gaussian function $\phi_0(x)$:

$$\phi(x, t) = \int dx_0 \langle x_1, t | x_0, 0 \rangle \phi_0(x_0).$$

Since this story is translation invariant, you can take a Gaussian centered at $x = 0$, and since rescaling just changes the constants, you can assume it is

$$\phi_0(x) = e^{-x^2}.$$

Get Maple to show that this is an isometry in L^2 , and that

$$\lim_{t \searrow 0} \phi(x, t) = \phi_0(x)$$

pointwise and in L^2 (by carrying out the appropriate integrals for the L^2 norm of the difference explicitly). Then density of Gaussians proves the result.

10.

$$\langle x | A | x' \rangle = \int da a \psi_a(x) \psi_a^*(x')$$

so

$$\langle x | A | x' \rangle^* = \int da a \psi_a(x)^* \psi_a(x') = \langle x' | A | x \rangle.$$

To calculate A^* ,

$$\begin{aligned}
 \langle \psi, \hat{A}\phi \rangle_{L^2} &= \int dx \psi^*(x) \hat{A}\phi(x) \\
 &= \int dx \psi^*(x) \int dx' \langle x|A|x' \rangle \phi(x') \\
 &= \int dx' \phi(x') \int dx \langle x|A|x' \rangle \psi^*(x) \\
 &= \int dx \phi(x) \int dx' \langle x'|A|x \rangle^* \psi^*(x') \\
 &= \langle \hat{A}\psi, \phi \rangle_{L^2}.
 \end{aligned}$$

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UNIVERSITY OF UTAH, SALT LAKE CITY, UTAH
E-mail address: `mckay@math.utah.edu`