Feynman Path Integral: Formulation of Quantum Dynamics

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(Date: September 22, 2016)

What is the path integral in quantum mechanics?

The path integral formulation of quantum mechanics is a description of quantum theory which generalizes the action principle of classical mechanics. It replaces the classical notion of a single, unique trajectory for a system with a sum, or functional integral, over an infinity of possible trajectories to compute a quantum amplitude. The basic idea of the path integral formulation can be traced back to Norbert Wiener, who introduced the Wiener integral for solving problems in diffusion and Brownian motion. This idea was extended to the use of the Lagrangian in quantum mechanics by P. A. M. Dirac in his 1933 paper. The complete method was developed in 1948 by Richard Feynman. This formulation has proven crucial to the subsequent development of theoretical physics, because it is manifestly symmetric between time and space. Unlike previous methods, the path-integral allows a physicist to easily change coordinates between very different canonical descriptions of the same quantum system.

((The idea of the path integral by Richard P. Feynman))

R.P. Feynman, The development of the space-time view of quantum electrodynamics (Nobel Lecture, December 11, 1965).
http://www.nobelprize.org/nobel_prizes/physics/laureates/1965/feynman-lecture.html

Feynman explained how to get the idea of the path integral in his talk of the Nobel Lecture. The detail is as follows. The sentence is a little revised because of typo.

I went to a beer party in the Nassau Tavern in Princeton. There was a gentleman, newly arrived from Europe (Herbert Jehle) who came and sat next to me. Europeans are much more serious than we are in America because they think that a good place to discuss intellectual matters is a beer party. So, he sat by me and asked, «what are you doing» and so on, and I said, «I'm drinking beer.» Then I realized that he wanted to know what work I was doing and I told him I was struggling with this problem, and I simply turned to him and said, ((listen, do you know any way of doing quantum mechanics, starting with action - where the action integral comes into the quantum mechanics?» «No», he said, «but Dirac has a paper in which the Lagrangian, at least, comes into quantum mechanics. I will show it to you tomorrow»

Next day we went to the Princeton Library, they have little rooms on the side to discuss things, and he showed me this paper. What Dirac said was the following: There is in quantum mechanics a very important quantity which carries the wave function from one time to another, besides the differential equation but equivalent to it, a kind of a kernel, which we might call $K(x',x)$,which carries the wave function $\psi(x)$ known at time *t,* to the wave function $\psi(x')$ at time, $t+\varepsilon$. Dirac points out that this function K was *analogous* to the quantity in classical mechanics that you would calculate if you took the exponential of $i\varepsilon/\hbar$, multiplied by the Lagrangian $L(\dot{x},x)$ imagining that these two positions *x, x'* corresponded t and $t+\varepsilon$. In other words, $K(x',x)$ is analogous to $\exp[i\frac{\varepsilon}{\hbar}L(\frac{x'-x}{\varepsilon},x)]$,

$$K(x',x) \approx \exp[i\frac{\varepsilon}{\hbar}L(\frac{x'-x}{\varepsilon},x)]. \quad (1)$$

Professor Jehle showed me this, I read it, he explained it to me, and I said, «what does he mean, they are analogous; what does that mean, *analogous?* What is the use of that?» He said, «you Americans ! You always want to find a use for everything!» I said, that I thought that Dirac must mean that they were equal. «No», he explained, «he doesn't mean they are equal.» «Well», I said, «let's see what happens if we make them equal.»

So I simply put them equal, taking the simplest example where the Lagrangian is $\frac{1}{2}M\dot{x}^2 - V(x)$, but soon found I had to put a constant of proportionality A in, suitably adjusted. When I substituted $\exp(i\varepsilon L/\hbar)$ for K to get

$$\psi(x',t+\varepsilon) = \int A\exp[i\frac{\varepsilon}{\hbar}L(\frac{x'-x}{\varepsilon},x)]\psi(x,t)dx, \quad (2)$$

and just calculated things out by Taylor series expansion, out came the Schrödinger equation. So, I turned to Professor Jehle, not really understanding, and said, «well, you see Professor Dirac meant that they were proportional.» Professor Jehle's eyes were bugging out-he had taken out a little notebook and was rapidly copying it down from the blackboard, and said, «no, no, this is an important discovery. You Americans are always trying to find out how something can be used. That's a good way to discover things!» So, I thought I was finding out what Dirac meant, but, as a matter of fact, had made the discovery that what Dirac thought was analogous, was, in fact, equal. I had then, at least, the connection between the Lagrangian and quantum mechanics, but still with wave functions and infinitesimal times.

It must have been a day or so later when I was lying in bed thinking about these things, that I imagined what would happen if I wanted to calculate the wave function at a finite interval later. I would put one of these factors $\exp(i\varepsilon L/\hbar)$ in here, and that would give me the wave functions the next moment, $t+\varepsilon$ and then I could substitute that back into (2) to get another factor of $\exp(i\varepsilon L/\hbar)$ and give me the wave function the next moment, $t + 2\varepsilon$, and so on and so on. In that way I found myself thinking of a large number of integrals, one after the other in sequence. In the integrand was the product of the exponentials, which, of course, was the exponential of the sum of terms like $\varepsilon L/\hbar$. Now, L is the Lagrangian and ε is like the time interval dt, so that if you took a sum of such terms, that's exactly like an integral. That's like Riemann's formula for the integral $\int Ldt$, you just take the value at each point and add them together. We are to take the limit as $\varepsilon \to 0$, of course. Therefore, the connection between the wave function of one instant and the wave function of another instant a finite time later could be obtained by an infinite number of integrals, (because ε goes to zero, of course) of exponential $(iS/\hbar)$ where S is the action expression (3),

$$S = \int L(\dot{x}, x)dt \,. \tag{3}$$

At last, I had succeeded in representing quantum mechanics directly in terms of the action *S*. This led later on to the idea of the amplitude for a path; that for each possible way that the particle can go from one point to another in space-time, there's an amplitude. That amplitude is an exponential of $i/\hbar$ times the action for the path. Amplitudes from various paths superpose by addition. This then is another, a third way, of describing quantum mechanics, which looks quite different than that of Schrödinger or Heisenberg, but which is equivalent to them.

1. Introduction

The time evolution of the quantum state in the Schrodinger picture is given by

$$|\psi(t)\rangle = \hat{U}(t,t')|\psi(t')\rangle ,$$

or

$$\langle x|\psi(t)\rangle = \langle x|\hat{U}(t,t')|\psi(t')\rangle = \int dx' \langle x|\hat{U}(t,t')|x'\rangle\langle x'|\psi(t')\rangle ,$$

in the $|x\rangle$ representation, where $K(x, t; x', t')$ is referred to the propagator (kernel) and given by

$$K(x,t;x',t') = \langle x|\hat{U}(t,t')|x'\rangle = \langle x|\exp[-\frac{i}{\hbar}\hat{H}(t-t')]|x'\rangle .$$

Note that here we assume that the Hamiltonian $\hat{H}$ is independent of time t. Then we get the form

$$\langle x|\psi(t)\rangle = \int dx' K(x,t;x',t')\langle x'|\psi(t')\rangle .$$

For the free particle, the propagator is described by

$$K(x,t;x',t') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\exp[\frac{im(x-x')^2}{2\hbar(t-t')}] .$$

(which will be derived later)

((Note))
Propagator as a transition amplitude

$$K(x,t;x',t') = \langle x|\exp[-\frac{i}{\hbar}\hat{H}(t-t')]|x'\rangle$$
$$= \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)\exp(\frac{i}{\hbar}\hat{H}t')|x'\rangle$$
$$= \langle x,t|x',t'\rangle$$

Here we define

$$|x,t\rangle = \exp(\frac{i}{\hbar}\hat{H}t)|x\rangle, \qquad \langle x,t| = \langle x|\exp(-\frac{i}{\hbar}\hat{H}t).$$

We note that

$$\langle x,t|a\rangle = \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)|a\rangle = \exp(-\frac{i}{\hbar}E_a t)\langle x|a\rangle,$$

where

$$\hat{H}|a\rangle = E_a|a\rangle .$$

((**Heisenberg picture**))
The physical meaning of the ket $|x,t\rangle$:
The operator in the Heisenberg's picture is given by

$$\hat{x}_H = \exp(\frac{i}{\hbar}\hat{H}t)\hat{x}\exp(-\frac{i}{\hbar}\hat{H}t),$$

$$\hat{x}_H|x,t\rangle = \exp(\frac{i}{\hbar}\hat{H}t)\hat{x}\exp(-\frac{i}{\hbar}\hat{H}t)\exp(\frac{i}{\hbar}\hat{H}t)|x\rangle$$
$$= \exp(\frac{i}{\hbar}\hat{H}t)\hat{x}|x\rangle$$
$$= \exp(\frac{i}{\hbar}\hat{H}t)x|x\rangle$$
$$= x\exp(\frac{i}{\hbar}\hat{H}t)|x\rangle = x|x,t\rangle$$

This means that $|x,t\rangle$ is the eigenket of the Heisenberg operator $\hat{x}_H$ with the eigenvalue *x*.

We note that

$$|\psi_S(t)\rangle = \exp(-\frac{i}{\hbar}\hat{H}t)|\psi_H\rangle.$$

Then we get

$$\langle x|\psi_S(t)\rangle = \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)|\psi_H\rangle = \langle x,t|\psi_H\rangle .$$

This implies that

$$|x,t\rangle = |x,t\rangle_H, \qquad |x\rangle = |x\rangle_S.$$

where S means Schrödinger picture and H means Heisenberg picture.

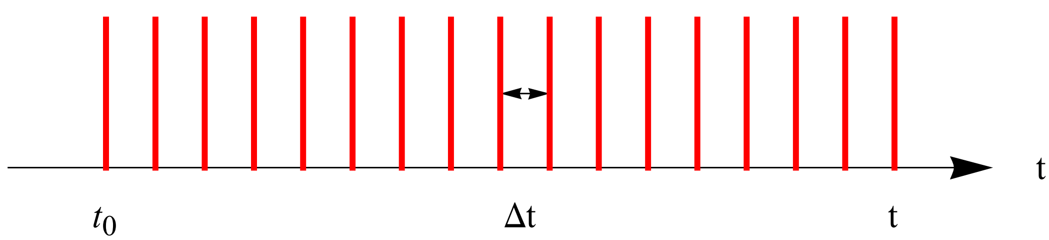
2. Propagator

We are now ready to evaluate the transition amplitude for a finite time interval

$$K(x,t;x',t') = \langle x,t|x',t'\rangle$$
$$= \langle x|\exp[-\frac{i}{\hbar}\hat{H}\Delta t)]\exp[-\frac{i}{\hbar}\hat{H}\Delta t)].....\exp[-\frac{i}{\hbar}\hat{H}\Delta t)]|x'\rangle$$

where

$$\Delta t = \frac{t-t'}{N} \text{ (in the limit of } N\to\infty)$$



where $t_0 = t'$ in this figure.

We next insert complete sets of position states (closure relation)

$$K(x,t;x',t') = \langle x,t|x',t'\rangle$$
$$= \int dx_1 \int dx_2 .... \int dx_{N-2} \int dx_{N-1} \int \langle x|\exp(-\frac{i}{\hbar}\hat{H}\Delta t)|x_{N-1}\rangle$$
$$\times \langle x_{N-1}|\exp(-\frac{i}{\hbar}\hat{H}\Delta t)|x_{N-2}\rangle ...... \langle x_3|\exp(-\frac{i}{\hbar}\hat{H}\Delta t)|x_2\rangle$$
$$\times \langle x_2|\exp(-\frac{i}{\hbar}\hat{H}\Delta t)|x_1\rangle \langle x_1|\exp(-\frac{i}{\hbar}\hat{H}\Delta t)|x'\rangle$$

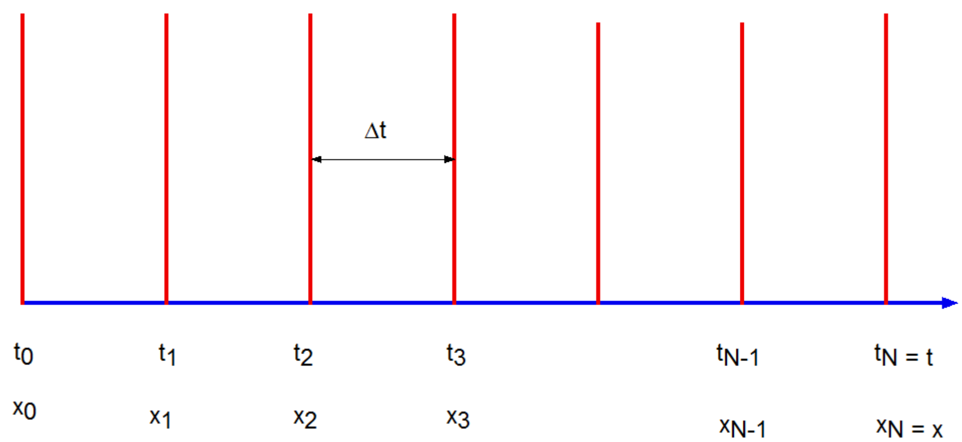
This expression says that the amplitude is the integral of the amplitude of all *N*-legged paths.

((Note))

$$(x',t'), (x_1,t_1), (x_2,t_2), (x_3,t_3), (x_4,t_4),$$
$$.....(x_{N-4},t_{N-4}), (x_{N-3},t_{N-3}), (x_{N-2},t_{N-2}), (x_{N-1},t_{N-1}), (x,t)$$

with

$$t' = t_0 < t_1 < t_2 < t_3 < t_4 < .... < t_{N-3} < t_{N-2} < t_{N-1} < t = t_N$$



We define

$$x' = x_0, \qquad t' = t_0,$$
$$x = x_N, \qquad t = t_N.$$

We need to calculate the propagator for one sub-interval

$$\langle x_i | \exp[-\frac{i}{\hbar}\hat{H}\Delta t) | x_{i-1} \rangle,$$

where $i = 1, 2, \ldots, N$, and

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}),$$

Then we have

$$
\begin{aligned}
\langle x_i | \exp(-\frac{i}{\hbar}\hat{H}\Delta t) | x_{i-1}\rangle &= \int dp_i \langle x_i | p_i\rangle\langle p_i | \exp(-\frac{i}{\hbar}\Delta t\hat{H}) | x_{i-1}\rangle \\
&\approx \int dp_i \langle x_i | p_i\rangle\langle p_i | \hat{1} - \frac{i}{\hbar}\Delta t\hat{H} | x_{i-1}\rangle + O((\Delta t)^2) \\
&= \int dp_i \langle x_i | p_i\rangle\langle p_i | \hat{1} - \frac{i}{\hbar}\Delta t(\frac{\hat{p}^2}{2m} + V(\hat{x})) | x_{i-1}\rangle + O((\Delta t)^2) \\
&= \int dp_i \langle x_i | p_i\rangle[\langle p_i | \hat{1} - \frac{i}{\hbar}\Delta t(\frac{\hat{p}^2}{2m}) | x_{i-1}\rangle + \langle p_i | -\frac{i}{\hbar}\Delta t V(\hat{x}) | x_{i-1}\rangle] + O((\Delta t)^2) \\
&= \int dp_i \langle x_i | p_i\rangle[\langle p_i | \hat{1} - \frac{i}{\hbar}\Delta t(\frac{p_i^2}{2m}) | x_{i-1}\rangle + \langle p_i | -\frac{i}{\hbar}\Delta t V(x_{i-1}) | x_{i-1}\rangle] + O((\Delta t)^2) \\
&= \int dp_i \langle x_i | p_i\rangle\langle p_i | \hat{1} - \frac{i}{\hbar}\Delta t[\frac{p_i^2}{2m} + V(x_{i-1})] | x_{i-1}\rangle + O((\Delta t)^2)
\end{aligned}
$$

where p_i (i = 1, 2, 3, …, N),

or

$$
\begin{aligned}
\langle x_i | \exp(-\frac{i}{\hbar}\hat{H}\Delta t) | x_{i-1}\rangle &\approx \int dp_i \langle x_i | p_i\rangle\langle p_i | x_{i-1}\rangle[1 - \frac{i}{\hbar}\Delta t(\frac{\hat{p}_i^2}{2m} + V(x_{i-1}))] \\
&= \frac{1}{2\pi\hbar}\int dp_i \exp[\frac{i}{\hbar} p_i (x_i - x_{i-1})][1 - \frac{i}{\hbar}\Delta t E(p_i, x_{i-1})] \\
&\approx \frac{1}{2\pi\hbar}\int dp_i \exp[\frac{i}{\hbar} p_i (x_i - x_{i-1})]\exp[-\frac{i}{\hbar}\Delta t E(p_i, x_{i-1})] \\
&\approx \frac{1}{2\pi\hbar}\int dp_i \exp[\frac{i}{\hbar}\{p_i \frac{(x_i - x_{i-1})}{\Delta t}\Delta t - E(p_i, x_{i-1})\Delta t\}] \\
&\approx \frac{1}{2\pi\hbar}\int dp_i \exp[\frac{i}{\hbar}\{p_i \frac{(x_i - x_{i-1})}{\Delta t} - E(p_i, x_{i-1})\}\Delta t]
\end{aligned}
$$

where

$$
E(p_i, x_{i-1}) = \frac{p_i^2}{2m} + V(x_{i-1}) .
$$

Then we have

$$
\begin{aligned}
K(x,t;x',t') &= \langle x,t | x',t'\rangle \\
&= \lim_{N\to\infty}\int dx_1 \int dx_2 ....\int dx_{N-1}\int \frac{dp_1}{2\pi\hbar}\int \frac{dp_2}{2\pi\hbar} ....\int \frac{dp_{N-1}}{2\pi\hbar}\int \frac{dp_N}{2\pi\hbar} \\
&\quad \times \exp[\frac{i}{\hbar}\sum_{i=1}^{N}\{p_i \frac{(x_i - x_{i-1})}{\Delta t} - (\frac{p_i^2}{2m} + V(x_{i-1}))\}\Delta t]
\end{aligned}
$$

We note that

$$\int \frac{dp_i}{2\pi\hbar} \exp[\frac{i}{\hbar}\{p_i \frac{(x_i - x_{i-1})}{\Delta t} - \frac{p_i^{\;2}}{2m}\}\Delta t\} = \int \frac{dp_i}{2\pi\hbar} \exp[\frac{i}{\hbar}\{p_i (x_i - x_{i-1}) - i\frac{p_i^{\;2}}{2m\hbar}\Delta t\}$$
$$= \sqrt{\frac{m}{2\pi\hbar i\Delta t}} \exp[\frac{im\Delta t}{2\hbar}(\frac{x_i - x_{i-1}}{\Delta t})^2]$$

((**Mathematica**))

```
Clear["Global`*"]; f1 = 1/(2 π ℏ) Exp[ⅈ/ℏ p x - ⅈ p^2/(2 m ℏ) Δt];
Integrate[f1, {p, -∞, ∞}] //
 Simplify[#, {ℏ > 0, m > 0, Im[Δt] < 0}] &
```

$$\frac{e^{\frac{i m x^2}{2 \Delta t \hbar}}}{\sqrt{2\pi}\sqrt{\frac{i \Delta t \hbar}{m}}}$$

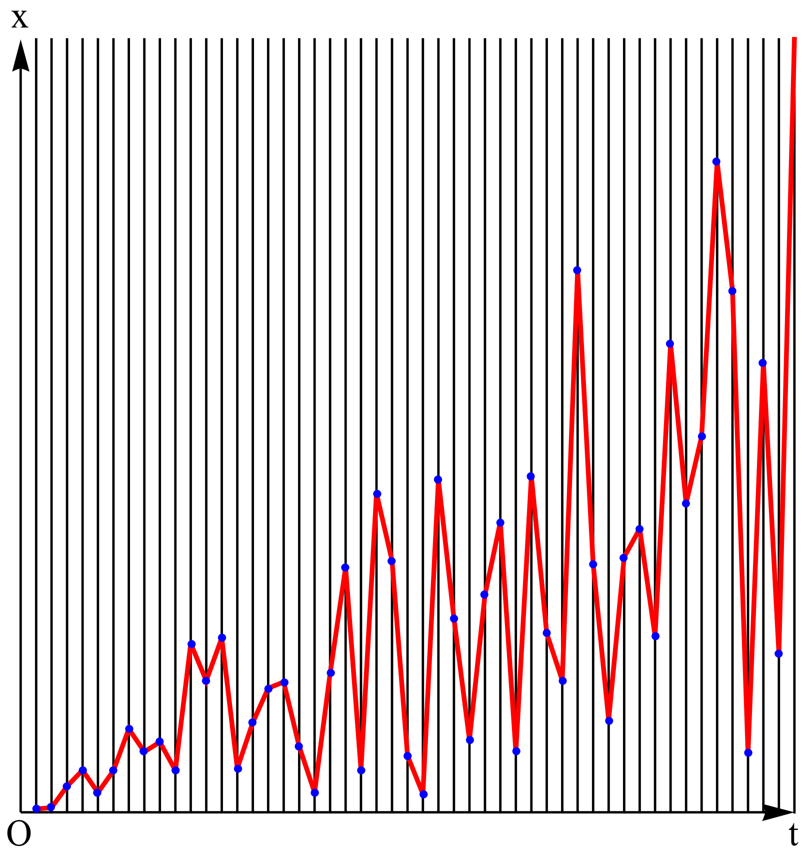
Then we have

$$K(x,t;x',t') = \lim_{N\to\infty} \int dx_1 \int dx_2 ....\int dx_{N-1} (\frac{m}{2\pi\hbar i\Delta t})^{N/2}$$
$$\times \exp[\frac{i}{\hbar}\Delta t \sum_{i=1}^{N} \{\frac{m}{2}(\frac{x_i - x_{i-1}}{\Delta t})^2 - V(x_{i-1})\}]$$

Notice that as $N \to \infty$ and therefore $\Delta t \to 0$, the argument of the exponent becomes the standard definition of a Riemann integral

$$\lim_{\substack{N\to\infty \\ \Delta t\to 0}} \frac{i}{\hbar}\Delta t \sum_{i=1}^{N} \{\frac{m}{2}(\frac{x_i - x_{i-1}}{\Delta t})^2 - V(x_{i-1})\} = \frac{i}{\hbar}\int_{t'}^{t} dt L(x, \dot{x}),$$

where L is the Lagrangian (which is described by the difference between the kinetic energy and the potential energy)



$$L(x,\dot{x}) = \frac{1}{2}m(\dot{x})^2 - V(x)\,.$$

It is convenient to express the remaining infinite number of position integrals using the shorthand notation

$$\int D[x(t)] = \lim_{N\to\infty}\int dx_1 \int dx_2 \ldots\ldots \int dx_{N-1} (\frac{m}{2\pi\hbar i\Delta t})^{N/2}\,.$$

Thus we have

$$K(x,t;x',t') = \langle x,t \,|\, x',t'\rangle = \int D[x(t)]\exp\{\frac{i}{\hbar}S[x(t)]\},$$

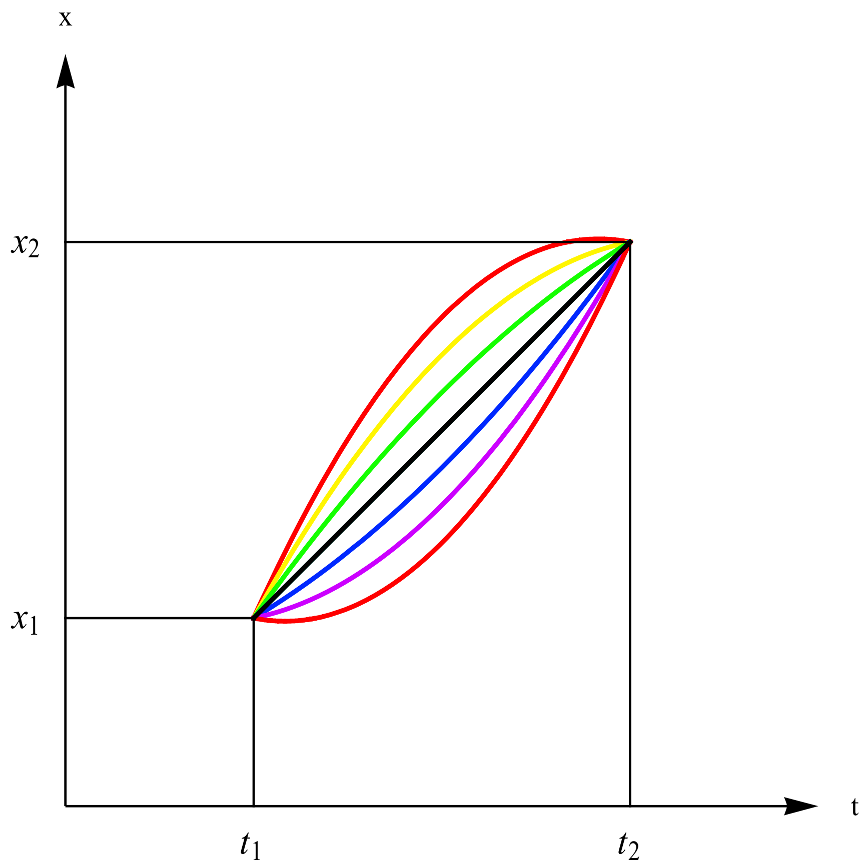
where

$$S[x(t)] = \int_{t'}^{t} dt L(x,\dot{x})\,.$$

The unit of S is [erg sec].

When two points at (t_i, x_i) and (t_f, x_f) are fixed as shown the figure below, for convenience, we use

$$S[x(t)] = \int_{t_i}^{t_f} dt L(x, \dot{x}) .$$

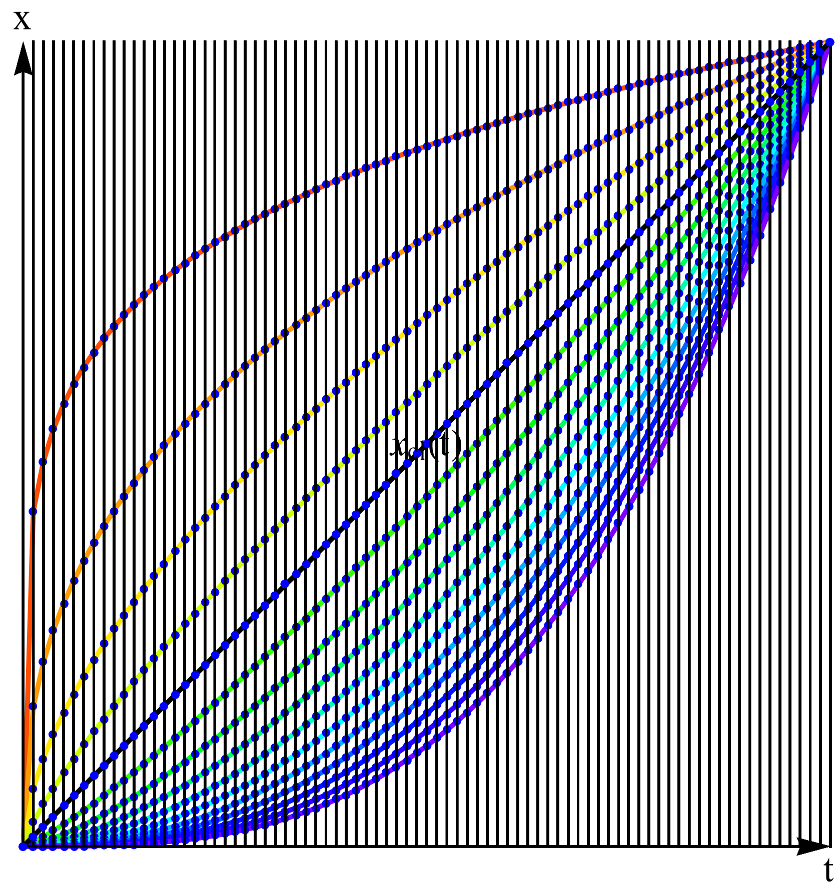


This expression is known as Feynman's path integral (configuration space path integral). $S[x(t)]$ is the value of the action evaluated for a particular path taken by the particle. If one want to know the quantum mechanical amplitude for a point particle at x', at time t' to reach a position x, at time t, one integrate over all possible paths connecting the points with a weight factor given by the classical action for each path. This formulation is completely equivalent to the usual formulation of quantum mechanics.

The expression for $K(x,t;x',t') = \langle x,t | x',t' \rangle$ may be written, in some loose sense, as

$$\langle x_N = x, t_N = t | x_0 = x', t_0 = t' \rangle \approx \sum_{(all)\, path} \exp[\frac{iS(N,0)}{\hbar}]$$
$$= \exp(\frac{iS_{path-1}}{\hbar}) + \exp(\frac{iS_{path-2}}{\hbar}) + \cdots + \exp(\frac{iS_{path-n}}{\hbar}) + \cdots$$

where the sum is to be taken over an innumerably infinite sets of paths.



(a) **Classical case**.

Suppose that $\hbar \to 0$ (classical case), the weight factor $\exp[iS/\hbar]$ oscillates very violently. So there is a tendency for cancellation among various contribution from neighboring paths. The classical path (in the limit of $\hbar \to 0$) is the path of least action, for which the action is an extremum. The constructive interference occurs in a very narrow strip containing the classical path. This is nothing but the derivation of Euler-Lagrange equation from the classical action. Thus the classical trajectory dominates the path integral in the small $\hbar$ limit.

In the classical approximation ($S >> \hbar$)

$$\langle x_N = x, t_N = t | x_0 = x', t_0 = t' \rangle = \text{"smooth function"} \exp(\frac{iS_{cl}}{\hbar}). \qquad (1)$$

But at an atomic level, S may be compared with $\hbar$, and then all trajectory must be added in $\langle x_N = x, t_N = t | x_0 = x', t_0 = t' \rangle$ in detail. No particular trajectory is of overwhelming importance, and of course Eq.(1) is not necessarily a good approximation.

(b) Quantum case.

What about the case for the finite value of $S/\hbar$ (corresponding to the quantum case)? The phase $\exp[iS/\hbar]$ does not vary very much as we deviate slightly from the classical path. As a result, as long as we stay near the classical path, constructive interference between neighboring paths is possible. The path integral is an infinite-slit experiment. Because one cannot specify which path the particle choose, even when one know what the initial and final positions are. The trajectory can deviate from the classical trajectory if the difference in the action is roughly within $\hbar$.

((Note))

R.P. Feynman and A.R. Hibbs, Quantum Mechanics and Path Integrals (extended edition) Dover 2005.

3. Free particle propagator

In this case, there is no potential energy.

$$K(x,t;x',t') = \lim_{N\to\infty}\int dx_1\int dx_2.......\int dx_{N-1}(\frac{m}{2\pi\hbar i\Delta t})^{N/2}\exp[\frac{i}{\hbar}\Delta t\sum_{i=1}^{N}\{\frac{m}{2}(\frac{x_i - x_{i-1}}{\Delta t})^2\}],$$

or

$$K(x,t;x',t') = \lim_{N\to\infty}\int dx_1\int dx_2.......\int dx_{N-1}$$

$$(\frac{m}{2\pi\hbar i\Delta t})^{N/2}\exp[\frac{-m}{2\hbar i\Delta t}\{(x_1 - x')^2 + (x_2 - x_1)^2 + (x_3 - x_2)^2 + ... + (x - x_{N-1})^2\}]$$

We need to calculate the integrals,

$$f_1 = (\frac{m}{2\pi\hbar i\Delta t})^{2/2}\int_{-\infty}^{\infty} dx_1\exp[\frac{-m}{2\hbar i\Delta t}\{(x_1 - x')^2 + (x_2 - x_1)^2]$$
$$= \frac{1}{\sqrt{4\pi}}(\frac{m}{\hbar i\Delta t})^{1/2}\exp[\frac{-m}{4\hbar i\Delta t}(x_2 - x')^2]$$

$$g_1 = f_1(\frac{m}{2\pi\hbar i\Delta t})^{1/2}\exp[\frac{-m}{2\hbar i\Delta t}(x_3 - x_2)^2]$$

$$f_2 = \int_{-\infty}^{\infty} g_1 dx_2 = \frac{1}{\sqrt{6\pi}}(\frac{m}{\hbar i\Delta t})^{1/2}\exp[\frac{-m}{6\hbar i\Delta t}(x_3 - x')^2]$$

$$g_2 = f_2(\frac{m}{2\pi\hbar i\Delta t})^{1/2}\exp[\frac{-m}{2\hbar i\Delta t}(x_4 - x_3)^2]$$

$$f_3 = \int_{-\infty}^{\infty} g_2 dx_3 = \frac{1}{\sqrt{8\pi}} (\frac{m}{\hbar i \Delta t})^{1/2} \exp[\frac{-m}{8\hbar i \Delta t}(x_4 - x')^2]$$

....

$$K(x,t;x',t') = \lim_{N\to\infty} (\frac{m}{2\pi\hbar N i \Delta t})^{1/2} \exp[\frac{-m(x-x')^2}{2\hbar i N \Delta t}],$$

or

$$K(x,t;x',t') = (\frac{m}{2\pi\hbar i (t-t')})^{1/2} \exp[\frac{-m(x-x')^2}{2\hbar i (t-t')}],$$

where we use $t - t' = N\Delta t$ in the last part.

((**Mathematica**))

Free particle propagator;
$\epsilon = \Delta t$

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
```

$$\text{h1} = \left((\text{x1} - \text{x}')^2 + (\text{x2} - \text{x1})^2\right) \text{ // Expand;}$$

$$\text{f0}[\text{x1\_}] := \left(\frac{2\pi i \hbar \epsilon}{m}\right)^{-\frac{2}{2}} \text{Exp}\left[\frac{-m}{2 i \hbar \epsilon} \text{h1}\right];$$

$$\text{f1} = \text{Integrate}[\text{f0}[\text{x1}], \{\text{x1}, -\infty, \infty\}] \text{ // } \text{Simplify}\left[\#, \text{Im}\left[\frac{m}{\epsilon \hbar}\right] > 0\right] \&$$

$$\frac{e^{\frac{i m (\text{x2}-\text{x}')^2}{4 \epsilon \hbar}} \sqrt{-\frac{i m}{\epsilon \hbar}}}{2 \sqrt{\pi}}$$

$$\text{g1} = \text{f1} \left(\frac{2\pi i \hbar \epsilon}{m}\right)^{-\frac{1}{2}} \text{Exp}\left[\frac{-m}{2 i \hbar \epsilon} (\text{x3} - \text{x2})^2\right] \text{ // Simplify;}$$

$$\text{f2} = \int_{-\infty}^{\infty} \text{g1}\, d\text{x2} \text{ // } \text{Simplify}\left[\#, \text{Im}\left[\frac{m}{\epsilon \hbar}\right] > 0\right] \&$$

$$\frac{e^{\frac{i m (\text{x3}-\text{x}')^2}{6 \epsilon \hbar}}}{\sqrt{6 \pi} \sqrt{\frac{i \epsilon \hbar}{m}}}$$

$$\text{g2} = \text{f2} \left(\frac{2\pi i \hbar \epsilon}{m}\right)^{-\frac{1}{2}} \text{Exp}\left[\frac{-m}{2 i \hbar \epsilon} (\text{x4} - \text{x3})^2\right] \text{ // Simplify;}$$

$$\text{f3} = \int_{-\infty}^{\infty} \text{g2}\, d\text{x3} \text{ // } \text{Simplify}\left[\#, \text{Im}\left[\frac{m}{\epsilon \hbar}\right] > 0\right] \&$$

$$\frac{e^{\frac{i m (\text{x4}-\text{x}')^2}{8 \epsilon \hbar}} \sqrt{-\frac{i m}{\epsilon \hbar}}}{2 \sqrt{2 \pi}}$$

$$\text{g3} = \text{f3} \left(\frac{2\pi i \hbar \epsilon}{m}\right)^{-\frac{1}{2}} \text{Exp}\left[\frac{-m}{2 i \hbar \epsilon} (\text{x5} - \text{x4})^2\right] \text{ // Simplify;}$$

$$\text{f4} = \int_{-\infty}^{\infty} \text{g3}\, d\text{x4} \text{ // } \text{Simplify}\left[\#, \text{Im}\left[\frac{m}{\epsilon \hbar}\right] > 0\right] \&$$

$$\frac{e^{\frac{i m (\text{x5}-\text{x}')^2}{10 \epsilon \hbar}}}{\sqrt{10 \pi} \sqrt{\frac{i \epsilon \hbar}{m}}}$$

4. Gaussian path integral

The simplest path integral corresponds to the vase where the dynamical variables appear at the most up to quadratic order in the Lagrangian (the free particle, simple harmonics are examples of such systems). The the probability amplitude associated with the transition from the points (x_i, t_i) to (x_f, t_f) is the sum over all paths with the action as a phase angle, namely,

$$K(x_f, t_f; x_i, t_i) = \exp[\frac{i}{\hbar} S_{cl}] F(t_f, t_i),$$

where S_{cl} is the classical action associated with each path,

$$S_{cl} = \int_{t_i}^{t_f} dt L(x_{cl}, \dot{x}_{cl}, t),$$

with the Lagrangian $L(x, \dot{x}, t)$ described by the Gaussian form,

$$L(x, \dot{x}, t) = a(t)\dot{x}^2 + b(t)\dot{x}x + c(t)x^2 + d(t)\dot{x} + e(t)x + f(t)$$

If the Lagrangian has no explicit time dependence, then we get

$$F(t_f, t_i) = F(t_f - t_i).$$

For simplicity, we use this theorem without proof.

$$K(x_f, t_f; x_i, t_i) = \exp[\frac{i}{\hbar} S_{cl}] F(t_f - t_i).$$

((**Proof**)) R.P. Feynman and A.R. Hibbs, Quantum Mechanics and Path Integrals.

Let $x_{cl}(t)$ be the classical path between the specified end points. This is the path which is an extremun for the action *S*. We can represent $x(t)$ in terms of $x_{cl}(t)$ and a new function $y(t)$;

$$x(t) = x_{cl}(t) + y(t),$$

where $y(t_i) = y(t_f) = 0$. At each t, the variables $x(t)$ and $y(t)$ differ by the constant . $x_{cl}(t)$ (Of course, this is a different constant for each value of *t*). Thus, clearly,

$$dx_i = dy_i,$$

for each specific point t_i in the subdivision of time. In general, we may say that

$$Dx(t) = Dy(t) \,.$$

The integral for the action can be written as

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

with

$$L(\dot{x}, x, t) = a(t)\dot{x}^2 + b(t)\dot{x}x + c(t)x^2 + d(t)\dot{x} + e(t)x + f(t).$$

We expand $L(\dot{x}, x, t)$ in a Taylor expansion around $x_{cl}, \dot{x}_{cl}$. This series terminates after the second term because of the Gaussian form of Lagrangian. Then

$$L(\dot{x}, x, t) = L(\dot{x}_{cl}, x_{cl}, t) + \frac{\partial L}{\partial x}|_{x_{cl}} \; y + \frac{\partial L}{\partial \dot{x}}|_{\dot{x}_{cl}} \; \dot{y} + \frac{1}{2}(\frac{\partial^2 L}{\partial x^2} y^2 + \frac{\partial^2 L}{\partial x \partial \dot{x}} y\dot{y} + \frac{\partial^2 L}{\partial \dot{x}^2} \dot{y}^2)|_{x_{cl}, \dot{x}_{cl}} \,.$$

From here we obtain the action

$$\begin{aligned} S[t_f, t_i] &= S_{cl}[t_f, t_i] + \int_{t_i}^{t_f} dt(\frac{\partial L}{\partial x}|_{x_{cl}} \; y + \frac{\partial L}{\partial \dot{x}}|_{x_{cl}} \; \dot{y}) \\ &+ \frac{1}{2}\int_{t_i}^{t_f} dt(\frac{\partial^2 L}{\partial \dot{x}^2} y^2 + \frac{\partial^2 L}{\partial \dot{x} \partial x} \dot{y}y + \frac{\partial^2 L}{\partial x^2} y^2)|_{x_{cl}, \dot{x}_{cl}} \\ &= S_{cl}[t_f, t_i] + \int_{t_i}^{t_f} dt(\frac{\partial L}{\partial x}|_{x_{cl}} \; y + \frac{\partial L}{\partial \dot{x}}|_{x_{cl}} \; \dot{y}) \\ &+ \int_{t_i}^{t_f} dt[a(t)\dot{y}^2 + b(t)y\dot{y} + c(t)y^2] \end{aligned}$$

The integration by parts and use of the Lagrange equation makes the second term on the right-hand side vanish. So we are left with

$$S[t_f, t_i] = S_{cl}[t_f, t_i] + \int_{t_i}^{t_f} dt[a(t)\dot{y}^2 + b(t)y\dot{y} + c(t)y^2] \,.$$

Then we can write

$$S[x(t)] = S_{cl}[t_f, t_i] + \int_{t_i}^{t_f} [a(t)\dot{y}^2 + b(t)\dot{y}y + c(t)y^2]dt \,.$$

The integral over paths does not depend on the classical path, so the kernel can be written as

$$K(x_f, t_f; x_i, t_i) = \exp[\frac{i}{\hbar} S_{cl}] \int_{y=0}^{y=0} \exp\{\frac{i}{\hbar} \int_{t_i}^{t_f} [a(t)\dot{y}^2 + b(t)\dot{y}y + c(t)y^2]dt\} Dy(t)$$

$$= F(t_f, t_i) \exp[\frac{i}{\hbar} S_{cl}]$$

where

$$F(t_f, t_i) = \int_{y=0}^{y=0} \exp\{\frac{i}{\hbar} \int_{t_i}^{t_f} [a(t)\dot{y}^2 + b(t)\dot{y}y + c(t)y^2]dt\} Dy(t) \,.$$

It is defined hat $F(t_f, t_i)$ is the integral over all paths from $y = 0$ back to $y = 0$ during the interval $(t_f - t_i)$.

((**Note**))

If the Lagrangian is given by the simple form

$$L(x, \dot{x}, t) = a(t)\dot{x}^2 + b(t)\dot{x}x + c(t)x^2$$

then $F(t_f, t_i)$ can be expressed by

$$F(t_f, t_i) = K(x_f = 0, t_f; x_i = 0, t_i) \,.$$

4. Evaluation of $F(t_f, t_i)$ for the free particle

We now calculate $F(t_f = t, t_i = t')$ for the free particles, where the Lagrangian is given by the form,

$$L(\dot{x}, x, t) = \frac{1}{2} m\dot{x}^2 \,.$$

Then we have

$$F(t_f, t_i) = \int_{y=0}^{y=0} \exp\{\frac{i}{\hbar} \int_{t_i}^{t_f} \frac{m}{2} \dot{y}^2 dt\} Dy(t) \,.$$

Replacing the variable *y* by *x*, we get

$$F(t_f,t_i)=\int_{x=0}^{x=0}\exp\{\frac{i}{\hbar}\int_{t_i}^{t_f}\frac{m}{2}\dot{x}^2dt\}Dx(t)$$

In this case, formally $F(t_f,t_i)$ is equal to the propagator $K(x_f=0,t_f;x_i=0,t_i)$,

$$\begin{aligned}F(t_f,t_i)&=K(x_f=0,t_f;x_i=0,t_i)\\&=\lim_{N\to\infty}\int dx_1\int dx_2.......\int dx_{N-1}\\&\quad(\frac{m}{2\pi\hbar i\Delta t})^{N/2}\exp[\frac{-m}{2\hbar i\Delta t}\{x_1{}^2+(x_2-x_1)^2+(x_3-x_2)^2+....+(x_{N-1}-x_{N-2})^2+x_{N-1}{}^2\}]\end{aligned}$$

where we put $x_i=x'=0$, and $x_f=x=0$, and $\Delta t=\frac{t_f-t_i}{N}=\frac{t-t'}{N}$.

How can we solve the integral? We use the eigenvalue problem (Gottfried and Yan). Before that we discuss the eigenvalue problem related to this problem.

Suppose that the matrix *A* (*n* x *n*) under the basis $\{|b_i\rangle\}$, is given by

$$\hat{A}=\begin{pmatrix}A_{11}&A_{12}&A_{13}&.&.&.&A_{1n}\\A_{21}&A_{22}&A_{23}&.&.&.&A_{2n}\\A_{31}&A_{32}&A_{33}&.&.&.&A_{3n}\\.&.&.&.&.&.&.\\.&.&.&.&.&.&.\\.&.&.&.&.&.&.\\A_{n1}&A_{n2}&A_{n3}&.&.&.&A_{nn}\end{pmatrix}.$$

where *n* = *N*-1. We also a ket $|\psi\rangle$ under the basis of $\{|b_i\rangle\}$ is given by

$$|\psi\rangle=\begin{pmatrix}x_1\\x_2\\x_3\\.\\.\\.\\x_n\end{pmatrix}.$$

Now we calculate the average $\langle\psi|\hat{A}|\psi\rangle$ as

$$\langle\psi|\hat{A}|\psi\rangle = \begin{pmatrix} x_1 & x_2 & x_3 & . & . & . & x_n \end{pmatrix}^* \begin{pmatrix} A_{11} & A_{12} & A_{13} & . & . & . & A_{1n} \\ A_{21} & A_{22} & A_{23} & . & . & . & A_{2n} \\ A_{31} & A_{32} & A_{33} & . & . & . & A_{3n} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ A_{n1} & A_{n2} & A_{n3} & . & . & . & A_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ . \\ . \\ . \\ x_n \end{pmatrix}$$

$$= \left(\boldsymbol{X}^T\right)^* \boldsymbol{AX}$$

$$= \sum_{i,j} x_i^{\,*} A_{1j} x_j$$

where

$$\boldsymbol{X} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ . \\ . \\ . \\ x_n \end{pmatrix}, \qquad \boldsymbol{X}^T = \begin{pmatrix} x_1 & x_2 & x_3 & . & . & . & x_n \end{pmatrix}.$$

We introduce the new basis $\{|a_i\rangle\}$ such that

$$\hat{A}|a_i\rangle = a_i|a_i\rangle, \qquad \text{(Eigen value problem)}$$

where $|a_i\rangle$ is the eigenket of $\hat{A}$ with the eigenvalue a_i. Suppose that $|\psi\rangle$ can be expressed under the basis of $\{|a_i\rangle\}$,

$$|\psi\rangle = \sum_i \eta_i |a_i\rangle.$$

Then we have

$$\langle\psi|\hat{A}|\psi\rangle = \begin{pmatrix}\eta_1 & \eta_2 & \eta_3 & . & . & . & \eta_n\end{pmatrix}^* \begin{pmatrix} a_1 & 0 & 0 & . & . & . & 0 \\ 0 & a_2 & 0 & . & . & . & 0 \\ 0 & 0 & a_3 & . & . & . & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & . & a_n \end{pmatrix} \begin{pmatrix}\eta_1 \\ \eta_2 \\ \eta_3 \\ . \\ . \\ . \\ \eta_n\end{pmatrix}$$

$$= \sum_i a_i \eta_i^* \eta_i$$

where

$$\boldsymbol{\eta} = \begin{pmatrix}\eta_1 \\ \eta_2 \\ \eta_3 \\ . \\ . \\ . \\ \eta_n\end{pmatrix}, \qquad \boldsymbol{\eta}^T = \begin{pmatrix}\eta_1 & \eta_2 & \eta_3 & . & . & . & \eta_n\end{pmatrix}.$$

We introduce the unitary operator $\hat{U}$;

$$|a_i\rangle = \hat{U}|b_i\rangle,$$

where

$$\langle b_j|a_i\rangle = \langle b_j|\hat{U}|b_i\rangle.$$

The eigenvalue problem can be rewritten as

$$\hat{A}\left(\hat{U}|b_i\rangle\right) = a_i\left(\hat{U}|b_i\rangle\right),$$

or

$$\hat{U}^+\hat{A}\hat{U}|b_i\rangle = a_i|b_i\rangle,$$

or

$$\langle b_j|\hat{U}^+\hat{A}\hat{U}|b_i\rangle = a_i\delta_{ij}.$$

We note that

$$|\psi\rangle = \sum_j \eta_j |a_j\rangle = \sum_i x_i |b_i\rangle,$$

where

$$\eta_j = \sum_i x_i \langle a_j | b_i \rangle = \sum_i \langle a_j | b_i \rangle x_i = \sum_i (U^+)_{ji} x_i ,$$

or

$$\eta = \hat{U}^+ X = \hat{U}^T X .$$

Note that each element of matrix $\hat{U}$ is real; $\hat{U}^+ = \hat{U}^T$. Then we have

$$X = \hat{U}\eta ,$$

since $\hat{U}^+\hat{U} = \hat{1}$. We now evaluate the following integral;

$$F(t_f, t_i) = \lim_{N\to\infty} \int dx_1 \int dx_2 ....\int dx_{N-1}$$
$$(\frac{m}{2\pi\hbar i\Delta t})^{N/2} \exp[\frac{-m}{2\hbar i\Delta t}\{x_1^{\ 2} + (x_2 - x_1)^2 + (x_3 - x_2)^2 + ... + (x_{N-1} - x_{N-2})^2 + x_{N-1}^{\ 2}\}]$$

We note that

$$\begin{aligned} f &= x_1^{\ 2} + (x_2 - x_1)^2 + (x_3 - x_2)^2 + ... + (x_{N-1} - x_{N-2})^2 + x_{N-1}^{\ 2} \\ &= 2(x_1^{\ 2} + x_2^{\ 2} + ... + x_{N-1}^{\ 2}) - 2(x_1 x_2 + x_2 x_3 + ... + x_{N-2} x_{N-1}) \end{aligned}$$

Using the matrix, f can be rewritten as

$$f = X^+ \hat{A} X = (\hat{U}\eta)^+ A\hat{U}\eta = \eta^+ \hat{U}^+ \hat{A}\hat{U}\eta = \eta^T (\hat{U}^+ \hat{A}\hat{U})\eta ,$$

with

$$X=\begin{pmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ . \\ x_{N-1} \end{pmatrix}, \qquad A=\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & . & 0 \\ -1 & 2 & -1 & 0 & 0 & . & . \\ 0 & -1 & 2 & -1 & 0 & . & . \\ 0 & 0 & -1 & 2 & -1 & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & 2 & -1 \\ . & . & . & . & . & -1 & 2 \end{pmatrix}.$$

We solve the eigenvalue problems to determine the eigenvalues and the unitary operator, such that

$$\hat{U}^{+}\hat{A}\hat{U}=\begin{pmatrix} \lambda_1 & 0 & 0 & 0 & . & . & 0 \\ 0 & \lambda_2 & 0 & 0 & . & . & 0 \\ 0 & 0 & \lambda_3 & 0 & . & . & 0 \\ 0 & 0 & 0 & \lambda_4 & . & . & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & . & . & \lambda_n \end{pmatrix},$$

where λ_i is the eigenvalue of A. Then we have

$$f=\begin{pmatrix} \eta_1 & \eta_1 & \eta_1 & \eta_1 & . & . & \eta_{N-1} \end{pmatrix}\begin{pmatrix} \lambda_1 & 0 & 0 & 0 & . & . & 0 \\ 0 & \lambda_2 & 0 & 0 & . & . & 0 \\ 0 & 0 & \lambda_3 & 0 & . & . & 0 \\ 0 & 0 & 0 & \lambda_4 & . & . & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & . & . & \lambda_n \end{pmatrix}\begin{pmatrix} \eta_1 \\ \eta_2 \\ . \\ . \\ . \\ . \\ \eta_{N-1} \end{pmatrix}$$

$$=\sum_{i=1}^{N-1}\lambda_i\eta_i^{\,2}$$

The Jacobian determinant is obtained as

$$\frac{\partial(x_1,x_2,...,x_{N-1})}{\partial(\eta_1,\eta_2,...,\eta_{N-1})}=\det U=1\,.$$

Then we have the integral

$$
\begin{aligned}
F(t_f, t_i) &= F(t, t') \\
&= \lim_{N\to\infty} \int d\eta_1 \int d\eta_2 ....\int d\eta_{N-1} (\frac{m}{2\pi\hbar i\Delta t})^{N/2} \exp[\frac{-m}{2\hbar i\Delta t}\{\lambda_1\eta_1{}^2 + \lambda_2\eta_2{}^2 + ... + \lambda_{N-1}\eta_{N-1}{}^2\}] \\
&= (\frac{m}{2\pi\hbar i\Delta t})^{N/2} \sqrt{\frac{2\pi\hbar i\Delta t}{m\lambda_1}} \sqrt{\frac{2\pi\hbar i\Delta t}{m\lambda_2}} ... \sqrt{\frac{2\pi\hbar i\Delta t}{m\lambda_{N-1}}} \\
&= (\frac{m}{2\pi\hbar i\Delta t})^{N/2} (\frac{m}{2\pi\hbar i\Delta t})^{-(N-1)/2} \frac{1}{\sqrt{\lambda_1\lambda_2....\lambda_{N-1}.}} \\
&= \sqrt{\frac{m}{2\pi\hbar i\Delta t(\det A)}} \\
&= \sqrt{\frac{m}{2\pi\hbar iN\Delta t}} \\
&= \sqrt{\frac{m}{2\pi\hbar i(t-t')}}
\end{aligned}
$$

where

$$\det A = \lambda_1\lambda_2\lambda_3...\lambda_{N-1} = N$$

((**Mathematica**)) **Example** ($N = 6$).
The matrix A (5 x 5): $N - 1 = 5$

$$
A = \begin{pmatrix} 2 & 1 & 0 & 0 & 0 \\ -1 & 2 & 1 & 0 & 0 \\ 0 & -1 & 2 & 1 & 0 \\ 0 & 0 & -1 & 2 & 1 \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix}
$$

The eigenvalues of A:

$$\lambda_1 = 2 + \sqrt{3}\,,\ \lambda_2 = 3\,,\ \lambda_3 = 2\,,\ \lambda_4 = 1\,,\ \lambda_5 = 2 - \sqrt{3}\,.$$

The unitary operator

$$\hat{U} =$$

$$
\begin{pmatrix}
\frac{1}{2\sqrt{3}} & \frac{1}{2} & \frac{1}{\sqrt{3}} & -\frac{1}{2} & \frac{1}{2\sqrt{3}} \\
-\frac{1}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & \frac{1}{2} \\
\frac{1}{\sqrt{3}} & 0 & -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} \\
-\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2\sqrt{3}} & -\frac{1}{2} & \frac{1}{\sqrt{3}} & \frac{1}{2} & \frac{1}{2\sqrt{3}}
\end{pmatrix}
$$

$$f = \sum_{i=1}^{N-1} \lambda_i \eta_i^{\,2} .$$

$$\hat{U}^{+}\hat{A}\hat{U} = \begin{pmatrix}
\lambda_1 & 0 & 0 & 0 & 0 \\
0 & \lambda_2 & 0 & 0 & 0 \\
0 & 0 & \lambda_3 & 0 & 0 \\
0 & 0 & 0 & \lambda_4 & 0 \\
0 & 0 & 0 & 0 & \lambda_5
\end{pmatrix}.$$

$$\det A = N = 6 .$$

```
Clear["Global`*"];
```

$$A1 = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix};$$

```
eq1 = Eigensystem[A1]
```

$$\left\{\left\{2+\sqrt{3},\ 3,\ 2,\ 1,\ 2-\sqrt{3}\right\},\ \left\{\left\{1,\ -\sqrt{3},\ 2,\ -\sqrt{3},\ 1\right\},\ \{-1,\ 1,\ 0,\ -1,\ 1\},\ \{1,\ 0,\ -1,\ 0,\ 1\},\ \{-1,\ -1,\ 0,\ 1,\ 1\},\ \left\{1,\ \sqrt{3},\ 2,\ \sqrt{3},\ 1\right\}\right\}\right\}$$

```
χ1 = Normalize[eq1[[2, 1]]] // Simplify
```

$$\left\{\frac{1}{2\sqrt{3}},\ -\frac{1}{2},\ \frac{1}{\sqrt{3}},\ -\frac{1}{2},\ \frac{1}{2\sqrt{3}}\right\}$$

```
χ2 = -Normalize[eq1[[2, 2]]] // Simplify
```

$$\left\{\frac{1}{2},\ -\frac{1}{2},\ 0,\ \frac{1}{2},\ -\frac{1}{2}\right\}$$

```
χ3 = Normalize[eq1[[2, 3]]] // Simplify
```

$$\left\{\frac{1}{\sqrt{3}}, 0, -\frac{1}{\sqrt{3}}, 0, \frac{1}{\sqrt{3}}\right\}$$

```
χ4 = Normalize[eq1[[2, 4]]] // Simplify
```

$$\left\{-\frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, \frac{1}{2}\right\}$$

```
χ5 = Normalize[eq1[[2, 5]]] // Simplify
```

$$\left\{\frac{1}{2\sqrt{3}}, \frac{1}{2}, \frac{1}{\sqrt{3}}, \frac{1}{2}, \frac{1}{2\sqrt{3}}\right\}$$

```
UT = {χ1, χ2, χ3, χ4, χ5}; U = Transpose[UT];
UH = UT;
U // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2\sqrt{3}} & \frac{1}{2} & \frac{1}{\sqrt{3}} & -\frac{1}{2} & \frac{1}{2\sqrt{3}} \\ -\frac{1}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{\sqrt{3}} & 0 & -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} \\ -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2\sqrt{3}} & -\frac{1}{2} & \frac{1}{\sqrt{3}} & \frac{1}{2} & \frac{1}{2\sqrt{3}} \end{pmatrix}$$

```
UH.U // Simplify; UH.U // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\eta = \begin{pmatrix} \eta 1 \\ \eta 2 \\ \eta 3 \\ \eta 4 \\ \eta 5 \end{pmatrix};$$

```
s1 = UH.A1.U // Simplify; s1 // MatrixForm
```

$$\begin{pmatrix} 2+\sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2-\sqrt{3} \end{pmatrix}$$

```
f1 = Transpose[η].s1.η // FullSimplify
```

$$\left\{\left\{\left(2+\sqrt{3}\right)\eta 1^2 + 3\,\eta 2^2 + 2\,\eta 3^2 + \eta 4^2 - \left(-2+\sqrt{3}\right)\eta 5^2\right\}\right\}$$

```
Det[A1]
```

6

```
K1 = eq1[[1, 1]] eq1[[1, 2]] eq1[[1, 3]] eq1[[1, 4]]
    eq1[[1, 5]] // Simplify
```

6

6. Equivalence with Schrodinger equation

The Schrödinger equation is given by

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle.$$

For an infinitesimal time interval ε, we can write

$$\left|\psi(\varepsilon)\right\rangle - \left|\psi(0)\right\rangle = -\frac{i\varepsilon}{\hbar}\hat{H}\left|\psi(0)\right\rangle,$$

from the definition of the derivative, or

$$\begin{aligned}\left\langle x\middle|\psi(\varepsilon)\right\rangle - \left\langle x\middle|\psi(0)\right\rangle &= -\frac{i\varepsilon}{\hbar}\left\langle x\middle|\hat{H}\middle|\psi(0)\right\rangle \\ &= -\frac{i\varepsilon}{\hbar}[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)]\left\langle x\middle|\psi(0)\right\rangle\end{aligned}$$

or

$$\begin{aligned}\psi(x,\varepsilon) - \psi(x,0) &= -\frac{i\varepsilon}{\hbar}\left\langle x\middle|\hat{H}\middle|\psi(0)\right\rangle \\ &= -\frac{i\varepsilon}{\hbar}[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)]\psi(x,0)\end{aligned}$$

in the $\left|x\right\rangle$ representation.

We now show that the path integral also predicts this behavior for the wave function. To this end, we start with

$$\left\langle x\middle|\psi(\varepsilon)\right\rangle = \int_{-\infty}^{\infty} dx' K(x,\varepsilon;x',0)\left\langle x'\middle|\psi(0)\right\rangle,$$

or

$$\psi(x,\varepsilon) = \int_{-\infty}^{\infty} dx' K(x,\varepsilon;x',0)\psi(x',0),$$

where

$$\begin{aligned}K(x,\varepsilon;x',0) &= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\exp[\frac{i\varepsilon}{\hbar}L(\frac{x-x'}{\varepsilon},\frac{x+x'}{2})] \\ &= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\exp[\frac{i\varepsilon}{\hbar}\{\frac{1}{2}m\frac{(x-x')^2}{\varepsilon^2} - V(\frac{x+x'}{2})\}]\end{aligned}$$

Then we get

$$\psi(x,\varepsilon) = \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\int_{-\infty}^{\infty} dx' \exp[\frac{i\varepsilon}{\hbar}\{\frac{1}{2}m\frac{(x-x')^2}{\varepsilon^2} - V(\frac{x+x'}{2})\}]\psi(x',0).$$

We now define

$$x' - x = \eta .$$

Then we have

$$\psi(x,\varepsilon) = \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \int_{-\infty}^{\infty} d\eta \exp[\frac{im\eta^2}{2\hbar\varepsilon} - \frac{i\varepsilon}{\hbar} V(x + \frac{\eta}{2})]\psi(x+\eta,0) .$$

The dominant contribution comes from the small limit of η. Using the Taylor expansion in the limit of $\eta \to 0$

$$\varepsilon V(x + \frac{\eta}{2}) = \varepsilon V(x) ,$$

$$\psi(x+\eta,0) \approx \psi(x,0) + \eta \frac{\partial \psi(x,0)}{\partial x} + \frac{\eta^2}{2} \frac{\partial^2 \psi(x,0)}{\partial x^2} ,$$

we get

$$\begin{aligned}
\psi(x,\varepsilon) &= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \int_{-\infty}^{\infty} d\eta \exp(\frac{im\eta^2}{2\hbar\varepsilon})[1 - \frac{i\varepsilon}{\hbar} V(x)][\psi(x,0) + \eta \frac{\partial \psi(x,0)}{\partial x} + \frac{\eta^2}{2} \frac{\partial^2 \psi(x,0)}{\partial x^2}] \\
&= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \int_{-\infty}^{\infty} d\eta \exp(\frac{im\eta^2}{2\hbar\varepsilon})[\psi(x,0) + \eta \frac{\partial \psi(x,0)}{\partial x} + \frac{\eta^2}{2} \frac{\partial^2 \psi(x,0)}{\partial x^2} - \frac{i\varepsilon}{\hbar} V(x)] \\
&= [1 - \frac{i\varepsilon}{\hbar} V(x) + \frac{i\varepsilon\hbar^2}{2m} \frac{\partial^2}{\partial x^2}]\psi(x,0)
\end{aligned}$$

Thus we have

$$\psi(x,\varepsilon) - \psi(x,0) = -\frac{i\varepsilon}{\hbar}[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)]\psi(x,0) ,$$

which is the same as that derived from the Schrödinger equation. The path integral formalism leads to the Schrodinger equation for infinitesimal intervals. Since any finite interval can be thought of a series of successive infinitesimal intervals the equivalence would still be true.

((**Note**))

$$\int_{-\infty}^{\infty} d\eta \exp(\frac{im\eta^2}{2\hbar\varepsilon}) = \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{1/2} , \qquad \int_{-\infty}^{\infty} \eta^2 d\eta \exp(\frac{im\eta^2}{2\hbar\varepsilon}) = \frac{i\hbar\varepsilon}{m}\left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{1/2} .$$

((**Mathematica**))

```
Clear["Global`"];

Integral[n_] :=
  Integrate[η^n Exp[(ⅈ m η^2)/(2 ℏ ϵ)], {η, -∞, ∞}] //
   Simplify[#, Im[m/(ϵ ℏ)] > 0] &;

K1 = Table[{n, Integral[n]}, {n, 0, 4}];
K1 // TableForm
```

0	$\dfrac{\sqrt{2\pi}}{\sqrt{-\frac{i m}{\epsilon \hbar}}}$
1	0
2	$\dfrac{\sqrt{2\pi}}{\left(-\frac{i m}{\epsilon \hbar}\right)^{3/2}}$
3	0
4	$\dfrac{3\sqrt{2\pi}}{\left(-\frac{i m}{\epsilon \hbar}\right)^{5/2}}$

7. Motion of free particle; Feynman path integral

The Lagrangian of the free particle is given by

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

Lagrange equation for the classical path;

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \left(\frac{\partial L}{\partial x}\right) = 0 ,$$

or

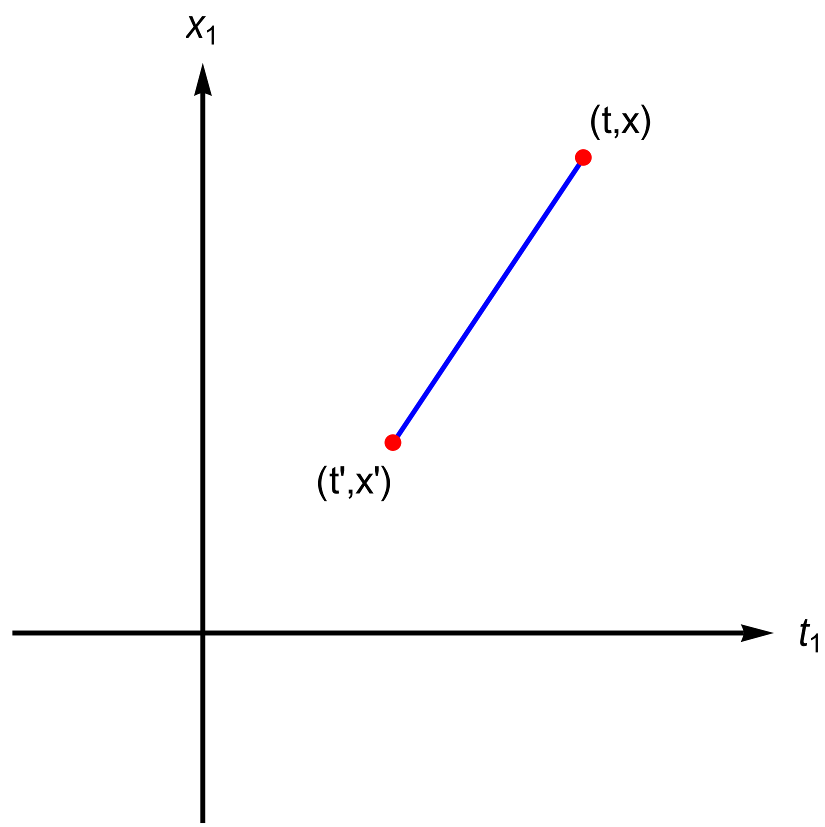
$$\dot{x} = a ,$$

or

$$x = at + b .$$

This line passes through (t', x'), (t, x);

$$x_1 - x' = \frac{x - x'}{t - t'}(t_1 - t'),$$



Then we have

$$x_1 = x' + \frac{x - x'}{t - t'}(t_1 - t'),$$

and

$$L(t_1) = \frac{1}{2}m\left(\frac{dx_1}{dt_1}\right)^2 = \frac{1}{2}m\left(\frac{x - x'}{t - t'}\right)^2 .$$

which is independent of t_1. Consequently, we have

$$S_{cl} = \int_{t'}^{t} L(t_1)dt_1 = \frac{m}{2}\int_{t'}^{t}\left(\frac{x - x'}{t - t'}\right)^2 dt_1 = \frac{m}{2}\left(\frac{x - x'}{t - t'}\right)^2\int_{t'}^{t} dt_1 = \frac{m}{2}\frac{(x - x')^2}{t - t'},$$

and

$$K(x,t,x',t') = A\exp[\frac{i}{\hbar}S_{cl}] = A\exp[\frac{-m(x-x')^2}{2\hbar i(t-t')}].$$

((Approach from the classical limit))

To find A, we use the fact that as $t-t'\to 0$, K must tend to $\delta(x-x')$,

$$\begin{aligned}\delta(x-x') &= \lim_{\Delta\to 0}\frac{1}{(\pi\Delta^2)^{1/2}}\exp[-\frac{(x-x')^2}{\Delta^2}] \\ &= \lim_{\sigma\to 0}\frac{1}{\sqrt{2\pi}\sigma}\exp[-\frac{(x-x')^2}{2\sigma^2}]\end{aligned}.$$

where

$$\sigma = \frac{\Delta}{\sqrt{2}},$$

$$f(x,x',\sigma) = \frac{1}{\sqrt{2\pi}\sigma}\exp[-\frac{(x-x')^2}{2\sigma^2}].$$ (Gaussian distribution).

So we get

$$\Delta = \sqrt{\frac{2\hbar i(t-t')}{m}},$$

$$A = \frac{1}{(\pi\Delta^2)^{1/2}} = \sqrt{\frac{m}{2\pi\hbar i(t-t')}},$$

or

$$K(x,t,x',t') = \sqrt{\frac{m}{2\pi\hbar i(t-t')}}\exp[\frac{-m(x-x')^2}{2\hbar i(t-t')}].$$

Note that

$$F_{freep-article}(t-t') = \sqrt{\frac{m}{2\pi\hbar i(t-t')}}.$$

((**Evaluation of** $S/\hbar$))
From the above discussion, S can be evaluated as

$$S = \frac{m}{2}\frac{(\Delta x)^2}{\Delta t} = \frac{m(\Delta x)}{2}\frac{\Delta x}{\Delta t} = \frac{mv}{2}\Delta x = \frac{p}{2}\Delta x = \frac{h}{2\lambda}\Delta x ,$$

or

$$\frac{S}{\hbar} = \frac{mv}{2\hbar}\Delta x = \frac{1}{2}\frac{p}{\hbar}\Delta x = \frac{1}{2}k\Delta x .$$

where p is the momentum,

$$p = \hbar k .$$

Suppose that m is the mass of electron and the velocity v is equal to $c/137$. We make a plot of $\frac{S}{\hbar}$ (radian) as a function of Δx (cm).

((**Mathematica**))

NIST Physics constant : cgs units

```
Clear["Global`*"];

rule1 = {c → 2.99792 × 10^10, ℏ → 1.054571628 10^-27,
   me → 9.10938215 10^-28};

K1 = (me c)/(2 ℏ) /. rule1

1.2948 × 10^10

K1 / 137

9.4511 × 10^7
```

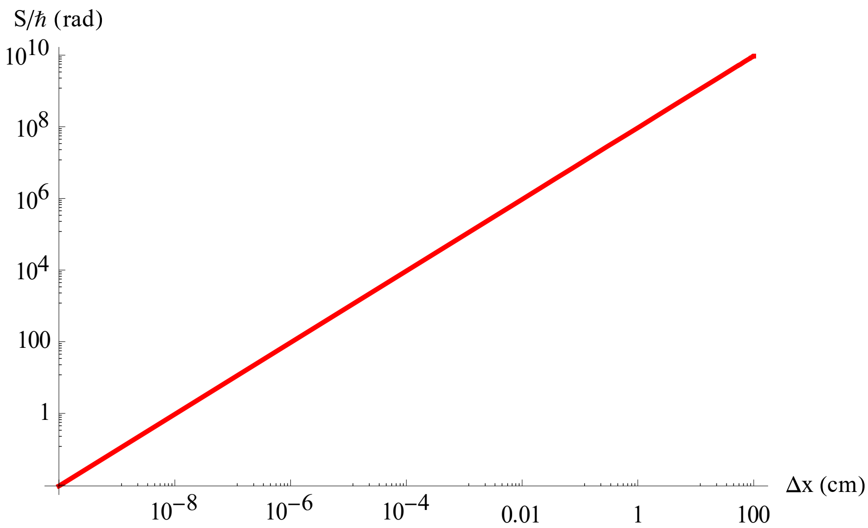
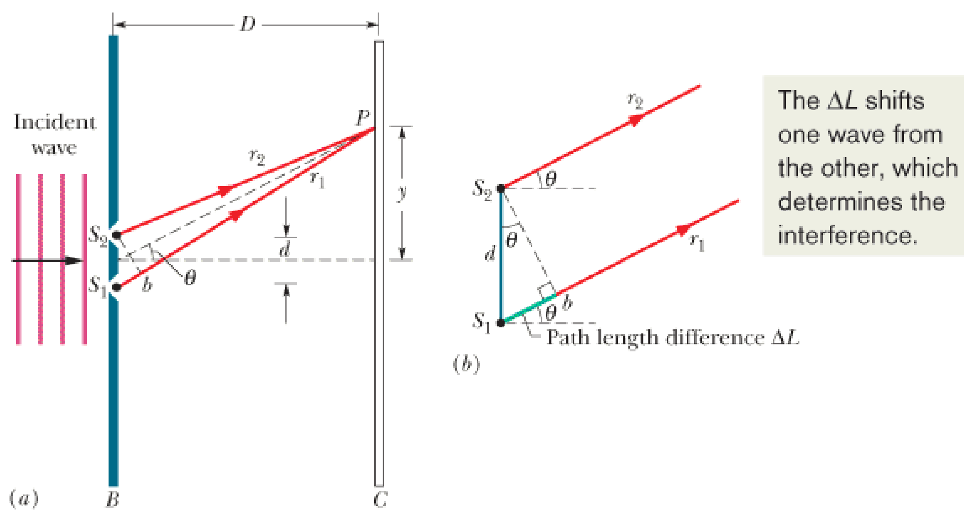


Fig. $\dfrac{S}{\hbar}$ (radian) as a function of Δx (cm), where $v = c/137$. m is the mass of electron.

8. Evaluation of S for the 1D system (example 8-1, Towmsend, 2nd edition)



We consider the Young's double slit;

$$S = \frac{mx^2}{2(\Delta t)} = \frac{m}{2}\frac{x}{t}x = \frac{1}{2}px = \frac{1}{2}\frac{h}{\lambda}x = \frac{\pi\hbar}{\lambda}x\,.$$

The phase difference between two paths is evaluated as

$$\frac{\Delta S}{\hbar} = \frac{1}{2}\frac{p}{\hbar}\Delta x = \frac{1}{2}k\Delta x = \frac{\pi}{\lambda}\Delta x\,,$$

If $\frac{\Delta S}{\hbar}$ is comparable to π, the interference effect can be observed.Such a condition is satisfied when

$$\Delta x \approx \lambda .$$

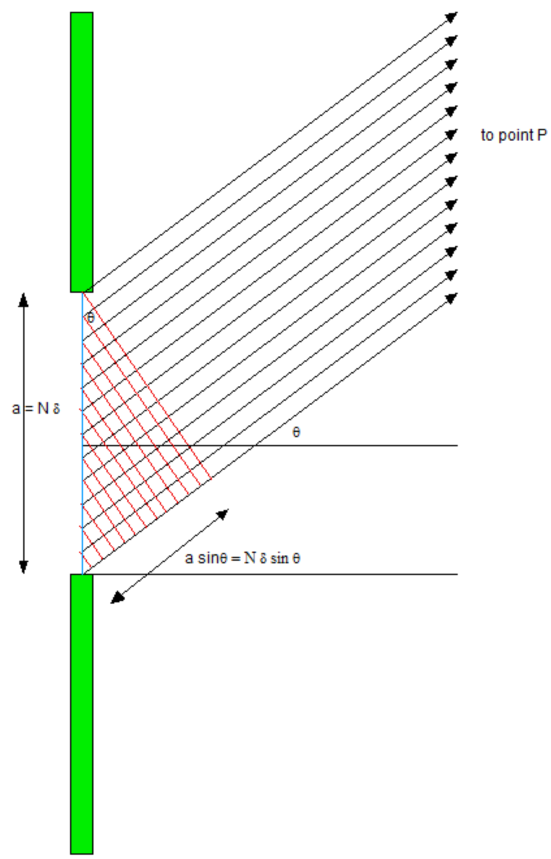
((**Note**))

In classical physics, the phase difference is given by

$$\Delta\phi = \frac{2\pi}{\lambda}\Delta x .$$

9. Single slit experiment

Imagine the slit divided into many narrow zones, width Δy (= $\delta = a/N$). Treat each as a secondary source of light contributing electric field amplitude $\Delta \boldsymbol{E}$ to the field at P.



We consider a linear array of N coherent point oscillators, which are each identical, even to their polarization. For the moment, we consider the oscillators to have no intrinsic phase difference. The rays shown are all almost parallel, meeting at some very distant point P. If the spatial extent of the array is comparatively small, the separate wave amplitudes arriving at P will be essentially equal, having traveled nearly equal distances, that is

$$E_0(r_1) = E_0(r_2) = ... = E_0(r_N) = E_0(r) = \frac{E_0}{N}$$

The sum of the interfering spherical wavelets yields an electric field at P, given by the real part of

$$\begin{aligned} E &= \mathrm{Re}[E_0(r)e^{i(kr_1-\omega t)} + E_0(r)e^{i(kr_2-\omega t)} + ... + E_0(r)e^{i(kr_N-\omega t)}] \\ &= \mathrm{Re}[E_0(r)e^{i(kr_1-\omega t)}[1 + e^{ik(r_2-r_1)} + e^{ik(r_3-r_1)} + ... + e^{ik(r_N-r_1))}]] \end{aligned}$$

((**Note**))
When the distances r_1 and r_2 from sources 1 and 2 to the field point P are large compared with the separation δ, then these two rays from the sources to the point P are nearly *parallel*. The path difference $r_2 - r_1$ is essentially equal to $\delta \sin\theta$.
Here we note that the phase difference between adjacent zone is

$$\begin{aligned} &k(r_2 - r_1) = \varphi = k\delta \sin\theta = k(\frac{a}{N}\sin\theta) \\ &k(r_3 - r_2) = \varphi \\ &k(r_4 - r_3) = \varphi \\ &------------------------ \\ &k(r_N - r_{N-1}) = \varphi \end{aligned}$$

where k is the wavenumber, $k = \dfrac{2\pi}{\lambda}$. It follows that

$$\begin{aligned} &k(r_2 - r_1) = \varphi \\ &k(r_3 - r_1) = 2\varphi \\ &k(r_4 - r_1) = 3\varphi \\ &------------------------ \\ &(r_N - r_1) = (N-1)\varphi \end{aligned}$$

Thus the field at the point P may be written as

$$E = \mathrm{Re}[E_0(r)e^{i(kr_1-\omega t)}[1 + e^{i\varphi} + e^{i2\varphi} + ... + e^{i(N-1)\varphi}]]$$

We now calculate the complex number given by

$$
\begin{aligned}
Z &= 1 + e^{i\varphi} + e^{i2\varphi} + ... + e^{i(N-1)\varphi} \\
&= \frac{1 - e^{iN\varphi}}{1 - e^{i\varphi}} \\
&= \frac{e^{iN\varphi/2}(e^{iN\varphi/2} - e^{-iN\varphi/2})}{e^{i\varphi/2}(e^{i\varphi/2} - e^{-i\varphi/2})} \\
&= e^{i(N-1)\varphi/2} \frac{\sin(\frac{N\varphi}{2})}{\sin(\frac{\varphi}{2})}
\end{aligned}
$$

If we define D to be the distance from the center of the line of oscillators to the point P, that is

$$
kD = \frac{1}{2}(N-1)k\delta \sin\theta + kr_1 = \frac{1}{2}(N-1)\varphi + kr_1
$$

$$
k(D - r_1) = \frac{1}{2}(N-1)\varphi
$$

Then we have the form for E as

$$
E = \mathrm{Re}[E_0(r)e^{i(kD-\omega t)} \frac{\sin(\frac{N\varphi}{2})}{\sin(\frac{\varphi}{2})}] = \mathrm{Re}[\widetilde{E}e^{-i\omega t}]
$$

The intensity distribution within the diffraction pattern due to N coherent, identical, distant point sources in a linear array is equal to

$$
I = \langle S \rangle = \frac{c\varepsilon_0}{2}\left|\widetilde{E}\right|^2
$$

$$
I = I_0 \frac{\sin^2(\frac{N\varphi}{2})}{\sin^2(\frac{\varphi}{2})} = I_0 \frac{\sin^2(\frac{\beta}{2})}{\sin^2(\frac{\beta}{2N})} = I_m \frac{\sin^2(\frac{\beta}{2})}{\left(\frac{\beta}{2}\right)^2}
$$

in the limit of $N \to \infty$, where

$$
\sin^2(\frac{\beta}{2N}) = \left(\frac{\beta}{2N}\right)^2
$$

$$
I_0 = \frac{c\varepsilon_0}{2}[E_0(r)]^2
$$

$$I_m = I_0 N^2 = \frac{c\varepsilon_0}{2}[NE_0(r)]^2 = \frac{c\varepsilon_0}{2} E_0{}^2$$

$$\beta = N\varphi = Nk\delta\sin\theta = ka\sin\theta$$

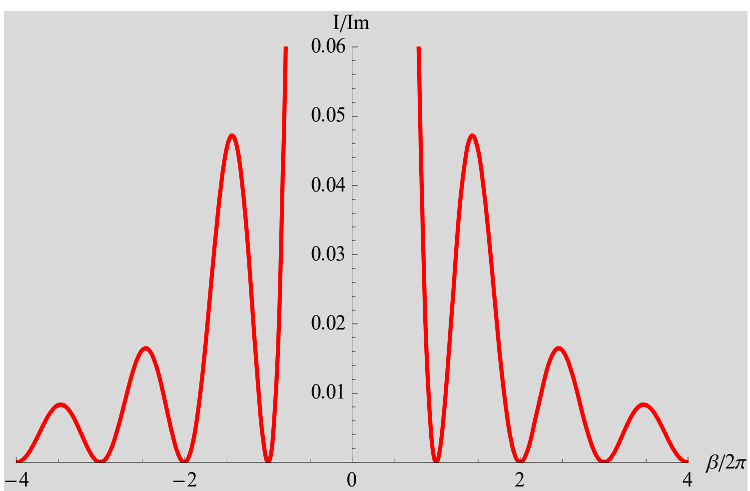
$$\varphi = k\delta\sin\theta$$

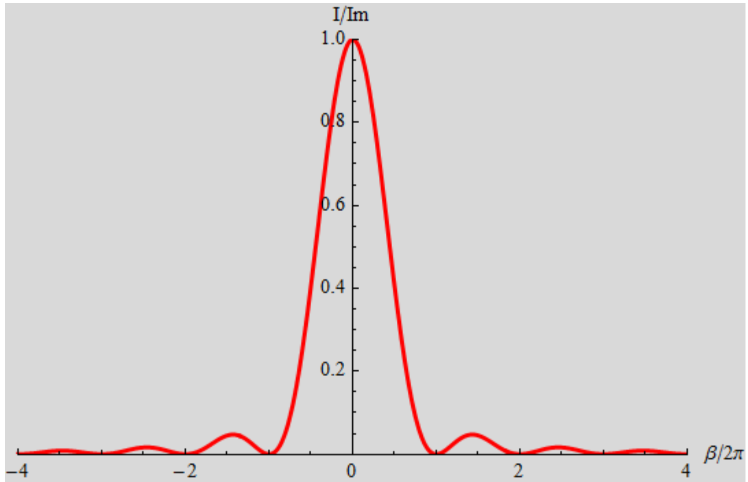
where $a = N\delta$. We make a plot of the relative intensity I/I_{m} as a function of β.

$$\frac{I}{I_m} = \frac{\sin^2(\frac{\beta}{2})}{\left(\frac{\beta}{2}\right)^2}$$

Note that

$$\int_{-\infty}^{\infty} \frac{\sin^2(\frac{\beta}{2})}{\left(\frac{\beta}{2}\right)^2} d\beta = 2\pi$$





The numerator undergoes rapid fluctuations, while the denominator varies relatively slowly. The combined expression gives rise to a series of sharp principal peaks separated by small subsidiary maxima. The principal minimum occur in directions in direction θ_m such that

$$\frac{\beta}{2} = \frac{ka}{2}\sin\theta = m\pi$$

$$a\sin\theta_m = \frac{1}{k}2m\pi = \frac{\lambda}{2\pi}2m\pi = m\lambda$$

10. Phasor diagram

(i) The system with two paths

The phasor diagram can be used for the calculation of the double slits (Young) interference. We consider the sum of the vectors given by $\overrightarrow{OS}$ and $\overrightarrow{ST}$. The magnitudes of these vectors is the same. The angle between $\overrightarrow{OS}$ and $\overrightarrow{ST}$ is ϕ (the phase difference).

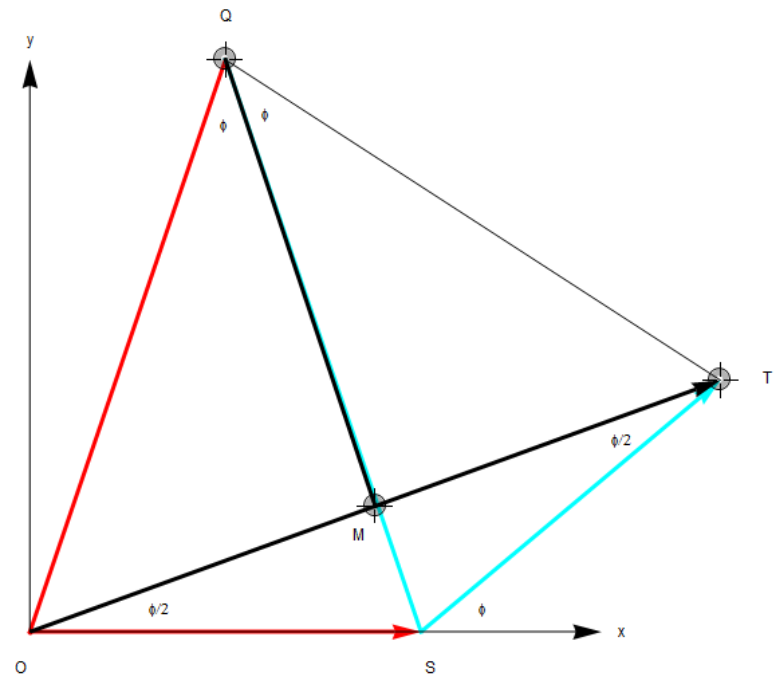


Fig. Phasor diagram for the double slit.

In this figure, $\overline{QO} = \overline{QS} = \overline{QT} = R$. $\angle SOM = \angle STM = \phi / 2$. Then we have

$$\overline{OT} = 2\overline{OM} = 2\overline{OS}\cos\frac{\phi}{2} = 2A\cos\frac{\phi}{2}.$$

The resultant intensity is proportional to $\left(\overline{OT}\right)^2$,

$$I \propto \left(\overline{OT}\right)^2 = 4A^2\cos^2\frac{\phi}{2} = 2A^2(1+\cos\phi).$$

Note that the radius R is related to $\overline{OS}$ $(= A)$ through a relation

$$A = 2R\sin\frac{\phi}{2}.$$

When $A = 1$ (in the present case), we have the intensity I as

$$I = 4\cos^2\frac{\phi}{2}$$

The intensity has a maximum ($I = 4$) at $\phi = 2\pi n$ and a minimum ($I = 0$) at

$$\phi = 2\pi(n + 1/2).$$

(ii) The system with 6 paths.

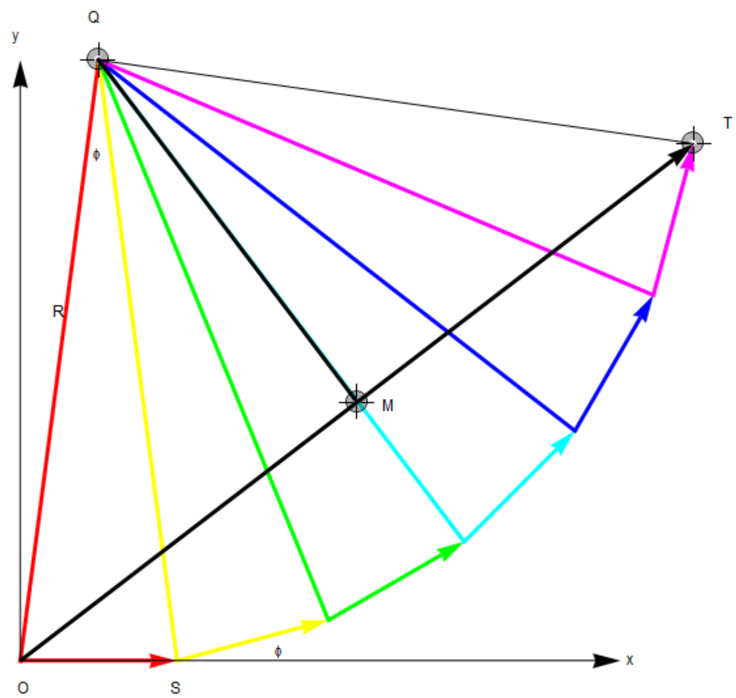


Fig. The resultant amplitude of N = 6 equally spaced sources with net successive phase difference φ. $\beta = N\,\varphi = 6\,\varphi$.

(iii) The system with 36 paths (comparable to single slit)

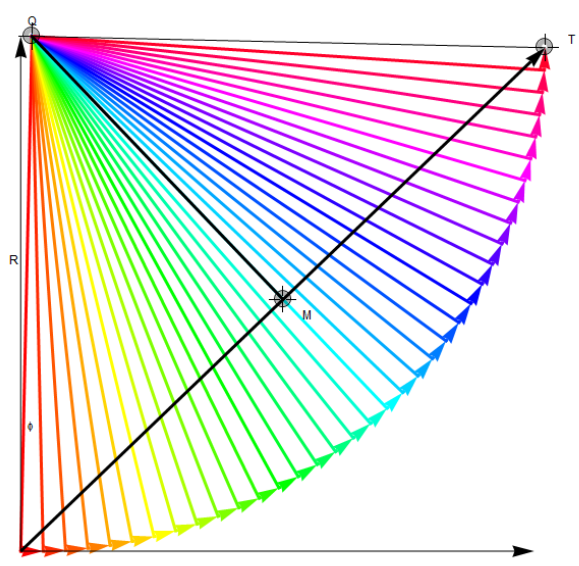
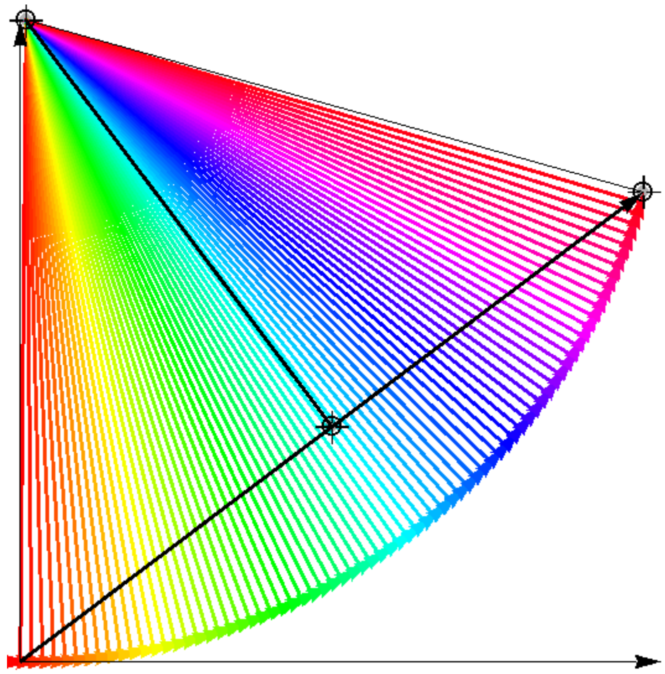


Fig. The resultant amplitude of N = 36 equally spaced sources with net successive phase difference φ.

(iv) Single slit in the limit of $N \to \infty$

We now consider the system with a very large N. We may imagine dividing the slit into N narrow strips. In the limit of large N, there is an infinite number of infinitesimally narrow strips. Then the curve trail of phasors become an arc of a circle, with arc length equal to the length E_0. The center C of this arc is found by constructing perpendiculars at O and T.



The radius of arc is given by

$$E_0 = R\beta = R(N\varphi).$$

in the limit of large N, where R is the side of the isosceles triangular lattice with the vertex angle φ, and β is given by

$$\beta = N\varphi = ka\sin\theta,$$

with the value β being kept constant. Then the amplitude E_p of the resultant electric field at P is equal to the chord $\overline{OT}$, which is equal to

$$E_P = 2R\sin\frac{\beta}{2} = 2\frac{E_0}{\beta}\sin\frac{\beta}{2} = E_0\frac{\sin\frac{\beta}{2}}{\frac{\beta}{2}}.$$

Then the intensity I for the single slits with finite width a is given by

$$I = I_m \left(\frac{\sin\frac{\beta}{2}}{\frac{\beta}{2}}\right)^2 .$$

where I_m is the intensity in the straight-ahead direction where $\beta = 0$.

The phase difference φ is given by $\beta = ka\sin\theta = 2\pi\frac{a}{\lambda}\sin\theta = 2\pi p\sin\theta$. We make a plot of I/I_m as a function of θ, where $p = a/\lambda$ is changed as a parameter.

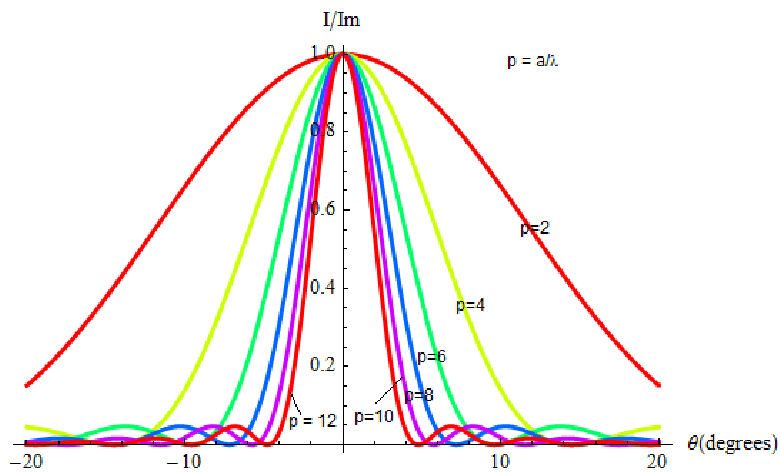


Fig. The relative intensity in single-slit diffraction for various values of the ratio $p = a/\lambda$. The wider the slit is the narrower is the central diffraction maximum.

11. Gravity: Feynman path integral

((Calculation from the classical limit))

$$L = \frac{m}{2}\dot{x}^2 - mgx ,$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \left(\frac{\partial L}{\partial x}\right),$$

$$\ddot{x} = -g ,$$

$$x_1 = -\frac{g}{2}t_1^{\ 2} + At_1 + B ,$$

Initial conditions:

$x_1 = x$ and $t_1 = t$,

$$x = -\frac{g}{2}t^2 + At + B\ .$$

and $x_1 = x'$ and $t_1 = t'$

$$x' = -\frac{g}{2}t'^2 + At' + B\ ,$$

A and *B* are determined from the above two equations.

$$x_1 = \frac{-(t'-t_1)[g(t-t')(t-t_1)+2x]+2(t-t_1)x'}{2(t-t')}\ ,$$

$$\dot{x}_1 = \frac{dx_1}{dt_1} = \frac{g(t-t')(t+t'-2t_1)+2(x-x')}{2(t-t')}\ .$$

Then we get the expression of the Lagrangian

$$L(x_1, \dot{x}_1, t_1) = \frac{m}{2}\dot{x}_1^{\ 2} - mgx_1\ .$$

The Hamilton's principle function is

$$S_{cl}(x,t,x',t') = \int_{t'}^{t} L(x_1, \dot{x}_1, t_1)dt_1$$
$$= -\frac{m[g^2(t-t')^4 - 12(x-x')^2 + 12g(t-t')^2(x+x')]}{24(t-t')}$$

$$K(x,t;x',t') = A\exp[\frac{i}{\hbar}S_{cl}(x,t:x',t')]\ .$$

((Classical limit))

When $x \to x'$ and $t \to t'+T$, we have

$$S_{cl}(x,t:x',t') = -\frac{1}{24}mg^2T^3 - x'gmT\ ,$$

and

$$K(x,t;x',t') = A\exp(-\frac{i}{24\hbar}mg^2T^3 - \frac{ix'mgT}{\hbar})$$
$$= A_1\exp(-\frac{ix'mgT}{\hbar})$$

where T is the time during which a particle passes through the system.

$$A_1 = A\exp(-\frac{i}{24\hbar}mg^2T^3).$$

((**Mathematica**))

```
Clear["Global`*"]; eq1 = x == -1/2 g t^2 + A t + B;

eq2 = x0 == -1/2 g t0^2 + A t0 + B;

rule1 = Solve[{eq1, eq2}, {A, B}] // Flatten;

x1 = (-1/2 g t1^2 + A t1 + B) /. rule1 // FullSimplify
```

$$\frac{-(t0-t1)\,(g\,(t-t0)\,(t-t1)+2\,x)+2\,(t-t1)\,x0}{2\,(t-t0)}$$

```
v1 = D[x1, t1] // Simplify
```

$$\frac{g\,(t-t0)\,(t+t0-2\,t1)+2\,(x-x0)}{2\,(t-t0)}$$

```
L1 = m/2 v1^2 - m g x1 // FullSimplify
```

$$\frac{1}{8\,(t-t0)^2}\,m\left((g\,(t-t0)\,(t+t0-2\,t1)+2\,(x-x0))^2 - 4\,g\,(t-t0)\,(-(t0-t1)\,(g\,(t-t0)\,(t-t1)+2\,x)+2\,(t-t1)\,x0)\right)$$

```
K1 = ∫_t0^t L1 ⅆt1 // FullSimplify
```

$$-\frac{m\left(g^2\,(t-t0)^4-12\,(x-x0)^2+12\,g\,(t-t0)^2\,(x+x0)\right)}{24\,(t-t0)}$$

```
rule1 = {x → x0, t → t0 + T}; K2 = K1 /. rule1 // Simplify
```

$$-\frac{1}{24}\,g\,m\,T\,\left(g\,T^2+24\,x0\right)$$

12. Simple harmonics: Feynman path integral

((**Classical limit**))

$$L = \frac{m}{2}\dot{x}^2 - \frac{1}{2}m\omega_0{}^2 x^2 ,$$

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{x}}) = (\frac{\partial L}{\partial x}) ,$$

$$\ddot{x} = -\omega_0{}^2 x ,$$

$$x_1 = A\cos(\omega_0 t_1) + B\sin(\omega_0 t_1) .$$

Initial conditions:

$x_1 = x$ and $t_1 = t,$

$$x = A\cos\omega_0 t + B\sin\omega_0 t ,$$

and

$x_1 = x'$ and $t_1 = t',$

$$x' = A\cos\omega_0 t' + B\sin\omega_0 t' .$$

A and B are determined from the above two equations.

$$x_1 = \frac{x'\sin[\omega_0(t-t_1)] - x\sin[\omega_0(t'-t_1)]}{\sin[\omega_0(t-t')]} ,$$

$$\dot{x}_1 = \frac{dx_1}{dt_1} = \frac{-x'\omega_0\cos[\omega_0(t-t_1)] + x\omega_0\cos[\omega_0(t'-t_1)]}{\sin[\omega_0(t-t')]} .$$

Then we get the expression of the Lagrangian

$$L(x_1, \dot{x}_1, t_1) = \frac{m}{2}\dot{x}_1{}^2 - \frac{1}{2}m\omega_0{}^2 x_1{}^2$$
$$= \frac{m\omega_0{}^2}{2\sin^2[\omega_0(t-t')]}[-2xx'\cos[\omega_0(t+t'-2t_1)$$
$$+ x'^2\cos[2\omega_0(t-t_1)] + x^2\cos[\omega_0(t'-t_1)])$$

The Hamilton's principle function is

$$S_{cl}(x,t,x',t') = \int_{t'}^{t} L(x_1,\dot{x}_1,t_1)dt_1$$
$$= \frac{m\omega_0}{2\sin(\omega_0(t-t')}[(x^2+x'^2)\cos(\omega_0(t-t'))-2xx']$$

$$K(x,t;x',t') = A\exp[\frac{i}{\hbar}S_{cl}(x,t:x',t')],$$

or

$$K(x,t;x',t') = A\exp[\frac{im\omega_0}{2\hbar\sin[\omega_0(t-t')]}\{(x^2+x'^2)\cos(\omega_0(t-t'))-2xx'\}].$$

In the limit of $t-t'\rightarrow 0$, we have

$$K(x,t,x',t') = A\exp[\frac{im\omega_0}{2\hbar\sin\{\omega_0(t-t')\}}(x-x')^2].$$

To find *A*, we use the fact that as $t-t'\rightarrow 0$, *K* must tend to $\delta(x-x')$,

$$\delta(x-x') = \lim_{\Delta\rightarrow 0}\frac{1}{(\pi\Delta^2)^{1/2}}\exp[-\frac{(x-x')^2}{\Delta^2}]$$
$$= \lim_{\sigma\rightarrow 0}\frac{1}{\sqrt{2\pi}\sigma}\exp[-\frac{(x-x')^2}{2\sigma^2}].$$

where

$$\sigma = \frac{\Delta}{\sqrt{2}},$$

$$f(x,x',\sigma) = \frac{1}{\sqrt{2\pi}\sigma}\exp[-\frac{(x-x')^2}{2\sigma^2}] \qquad \text{(Gaussian distribution).}$$

In other words

$$A = \frac{1}{(\pi\Delta^2)^{1/2}}, \qquad \frac{1}{\Delta^2} = \frac{m\omega_0}{2i\hbar\sin\{\omega_0(t-t')\}}.$$

So we get

$$\Delta = \sqrt{\frac{2i\hbar \sin\{\omega_0(t-t')\}}{m\omega_0}}, \qquad A = \frac{1}{(\pi\Delta^2)^{1/2}} = \sqrt{\frac{m\omega_0}{2\pi\hbar i \sin\{\omega_0(t-t')\}}}$$

or

$$K(x,t,x',t') = \sqrt{\frac{m\omega_0}{2\pi\hbar i \sin\{\omega_0(t-t')\}}} \times \exp[\frac{im\omega_0}{2\hbar \sin[\omega_0(t-t')]}[(x^2+x'^2)\cos\{\omega_0(t-t')\} - 2xx']]$$

Note that

$$K(x=0,t,x'=0,t') = \sqrt{\frac{m\omega_0}{2\pi\hbar i \sin\{\omega_0(t-t')\}}} = F(t-t')$$

and

$$K(x,t,x',t') = F(t-t')\exp[\frac{i}{\hbar}S_{cl}(x,t;x't')].$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* := expr /. {Complex[a_, b_] :> Complex[a, -b]}

seq1 = x == A Cos[ω0 t] + B Sin[ω0 t];
seq2 = x0 == A Cos[ω0 t0] + B Sin[ω0 t0];

srule1 = Solve[{seq1, seq2}, {A, B}] // Simplify // Flatten;

x1 = A Cos[t1 ω0] + B Sin[t1 ω0] /. srule1 // Simplify;
v1 = D[x1, t1] // Simplify;

L1 = m/2 v1^2 - m/2 ω0^2 x1^2 // Simplify;

∫_t0^t L1 ⅆt1 // FullSimplify

1/2 m ω0 (-2 x x0 + (x^2 + x0^2) Cos[(t - t0) ω0]) Csc[(t - t0) ω0]
```

If the initial state of a harmonic oscillator is given by the displaced ground state wave function

$$\psi(x,0) = \exp[-\frac{m\omega_0}{2\hbar}(x-x_0)^2].$$

When

$$\xi = \beta x,$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

Then we have

$$\psi(\xi,0) = \frac{1}{\pi^{1/4}} \exp[-\frac{1}{2}(\xi-\xi_0)^2],$$

and

$$\begin{aligned}
\psi(\xi,t) &= \int_{-\infty}^{\infty} K(\xi,t;\xi',0)\psi(\xi',0)d\xi' \\
&= \frac{1}{\pi^{1/4}} \exp(-\frac{i\omega_0 t}{2}) \exp[-\frac{\sin(\omega_0 t)}{2} e^{-i\omega_0 t}\{(\xi^2+\xi_0{}^2)\cot(\omega_0 t) + i\xi^2 \\
&\quad -2\xi\xi_0 \frac{1}{\sin(\omega_0 t)}\}] \\
&= \frac{1}{\pi^{1/4}} \exp(-\frac{i\omega_0 t}{2}) \exp[-\frac{1}{2} e^{-i\omega_0 t}\{(\xi^2+\xi_0{}^2)\cos(\omega_0 t) + i\xi^2 \sin(\omega_0 t) \\
&\quad -2\xi\xi_0\}] \\
&= \frac{1}{\pi^{1/4}} \exp(-\frac{i\omega_0 t}{2}) \exp[-\frac{1}{2} e^{-i\omega_0 t}\{(\xi^2 e^{i\omega_0 t} + \xi_0{}^2(\frac{e^{i\omega_0 t}+e^{-i\omega_0 t}}{2}) \\
&\quad -2\xi\xi_0\}] \\
&= \frac{1}{\pi^{1/4}} \exp[-\frac{i\omega_0 t}{2} - \frac{1}{2}\{\xi^2 - 2\xi_0\xi e^{-i\omega_0 t} + \frac{1}{2}\xi_0{}^2(1+e^{-2i\omega_0 t})\}]
\end{aligned}$$

or

$$\begin{aligned}
\psi(\xi,t) &= \frac{1}{\pi^{1/4}} \exp[-\frac{i\omega_0 t}{2} - \frac{1}{2}\{\xi^2 - 2\xi_0\xi(\cos\omega_0 t - i\sin\omega_0 t) \\
&\quad + \frac{1}{2}\xi_0{}^2(1+\cos 2\omega_0 t - i\sin 2\omega_0 t)\}] \\
&= \frac{1}{\pi^{1/4}} \exp[-\frac{1}{2}(\xi - \xi_0\cos\omega_0 t)^2 - i(\frac{\omega_0 t}{2} + \xi_0\xi\sin\omega_0 t - \frac{1}{4}\xi_0{}^2\sin 2\omega_0 t)]
\end{aligned}$$

Finally we have

$$|\psi(\xi,t)|^2 = \frac{1}{\pi^{1/2}}\exp[-(\xi-\xi_0\cos(\omega_0 t))^2]$$

((**Mathematica**))

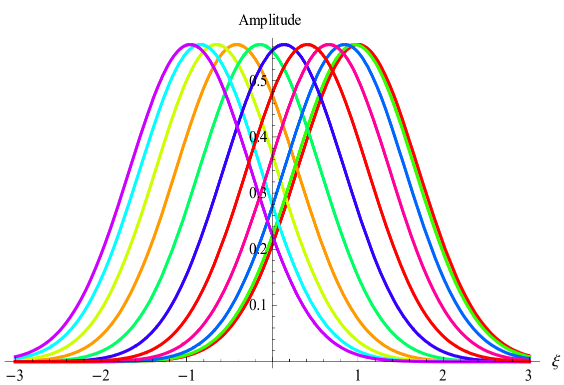
```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

KSH[ξ_, t_, ξ1_] := Sqrt[1/(2 π ⅈ Sin[ω0 t])] Exp[ⅈ/(2 Sin[ω0 t]) ((ξ^2 + ξ1^2) Cos[ω0 t] - 2 ξ ξ1)];

φ0[ξ_] := π^(-1/4) Exp[-(ξ - ξ0)^2/2];

f1 = ∫_{-∞}^{∞} KSH[ξ, t, ξ1] φ0[ξ1] ⅆξ1 // FullSimplify[#, {Im[Cot[t ω0]] > -1, ω0 t > 0}] &
```

$$\frac{e^{-\frac{(\xi^2+\xi0^2)\,\mathrm{Cot}[t\,\omega0]+i\,\xi\,(\xi+2\,i\,\xi0\,\mathrm{Csc}[t\,\omega0])}{2\,(i+\mathrm{Cot}[t\,\omega0])}}\sqrt{-i\,\mathrm{Csc}[t\,\omega0]}}{\pi^{1/4}\sqrt{1-i\,\mathrm{Cot}[t\,\omega0]}}$$

```
Amp1 = f1* f1 // FullSimplify
```

$$\frac{e^{-(\xi-\xi0\,\mathrm{Cos}[t\,\omega0])^2}}{\sqrt{\pi}}$$

```
rule1 = {ω0 → 1, ξ0 → 1}; H1 = Amp1 /. rule1;

Plot[Evaluate[Table[H1, {t, 0, 20, 2}], {ξ, -3, 3}],
 PlotStyle → Table[{Thick, Hue[0.1 i]}, {i, 0, 10}], AxesLabel → {"ξ", "Amplitude"}]
```



13. Gaussian wave packet propagation (quantum mechanics)

$$\langle x|\psi(t)\rangle = \langle x|\hat{U}(t,t')|\psi(t')\rangle = \int dx'\langle x|\hat{U}(t,t')|x'\rangle\langle x'|\psi(t')\rangle,$$

$$K(x,t;x',t') = \langle x|\hat{U}(t,t')|x'\rangle = \langle x|\exp[-\frac{i}{\hbar}\hat{H}(t-t')]|x'\rangle,$$

or

$$\langle x|\psi(t)\rangle = \int dx' K(x,t;x',t')\langle x'|\psi(t')\rangle.$$

$K(x, t; x', t')$ is referred to the propagator (kernel)

For the free particle, the propagator is given by

$$K(x,t;x',t') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\exp[\frac{im(x-x')^2}{2\hbar(t-t')}].$$

Let's give a proof for this in the momentum space.

$\hat{H}$ is the Hamiltonian of the free particle.

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx},$$

$$\hat{H}|k\rangle = E_k|k\rangle,$$

with

$$E_k = \frac{\hbar^2 k^2}{2m}, \qquad \omega_k = \frac{E_k}{\hbar},$$

$$\begin{aligned}
K(x,t;x',t') &= \langle x|\exp[-\frac{i}{\hbar}\hat{H}(t-t'))|x'\rangle \\
&= \int dk\langle x|k\rangle\langle k|\exp[-\frac{i}{\hbar}\hat{H}(t-t'))|x'\rangle \\
&= \int dk\langle x|k\rangle\langle k|\exp[-\frac{i\hbar k^2}{2m}(t-t'))|x'\rangle \\
&= \int dk\frac{1}{2\pi}\exp[ik(x-x')-\frac{i\hbar k^2}{2m}(t-t')]
\end{aligned}$$

Note that

$$\exp[ik(x-x')-\frac{i\hbar k^2}{2m}(t-t')] = \exp[-\frac{i\hbar(t-t')}{2m}\{k-\frac{m(x-x')}{\hbar(t-t')}\}^2 - \frac{m(x-x')^2}{2i\hbar(t-t')}],$$

and

$$\int_{-\infty}^{\infty} dk\exp(-i\alpha k^2) = \sqrt{\frac{\pi}{i\alpha}},$$

or

$$K(x,t;x',t') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\exp[\frac{im(x-x')^2}{2\hbar(t-t')}].$$

((Quantum mechanical treatment))

Probability amplitude that a particle initially at *x*' propagates to *x* in the interval *t-t*'. This expression is generalized to that for the three dimension.

$$K(\boldsymbol{r},t;\boldsymbol{r}',t') = [\frac{m}{2\pi i\hbar(t-t')}]^{3/2}\exp[\frac{im|\boldsymbol{r}-\boldsymbol{r}'|^2}{2\hbar(t-t')}].$$

We now consider the wave function:

$$\langle x|\psi(t=0)\rangle = \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\exp(ik_0x - \frac{x^2}{4\sigma_x{}^2}).$$

where the probability

$$P = |\langle x|\psi(t=0)\rangle|^2 = \frac{1}{\sqrt{2\pi}\sigma_x}\exp(-\frac{x^2}{2\sigma_x{}^2}),$$

has the form of Gaussian distribution with the standard deviation σ_x. The Fourier transform is given by

$$\begin{aligned}\langle k|\psi(t=0)\rangle &= \int dx\langle k|x\rangle\langle x|\psi(t=0)\rangle \\ &= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\frac{1}{\sqrt{2\pi}}\int dx\exp(-ikx)\exp(ik_0x - \frac{x^2}{4\sigma_x{}^2}) \\ &= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\frac{1}{\sqrt{2\pi}}2\sigma_x\sqrt{\pi}\exp[-\sigma_x{}^2(k-k_0)^2] \\ &= \left(\frac{2}{\pi}\right)^{1/4}\sqrt{\sigma_x}\exp[-\sigma_x{}^2(k-k_0)^2]\end{aligned}$$

or

$$\left|\langle k|\psi(t=0)\rangle\right|^2 = \sqrt{\frac{2}{\pi}}\sigma_x \exp[-2\sigma_x{}^2(k-k_0)^2]$$

$$= \frac{1}{\sqrt{2\pi}}\frac{1}{\left(\dfrac{1}{2\sigma_x}\right)}\exp[-\frac{(k-k_0)^2}{2\left(\dfrac{1}{2\sigma_x}\right)^2}].$$

$$= \frac{1}{\sqrt{2\pi}\sigma_k}\exp[-\frac{(k-k_0)^2}{2\sigma_k{}^2}]$$

which is the Gaussian distribution with the standard deviation $\sigma_k = \left(\dfrac{1}{2\sigma_x}\right)$.

Then we get the wave function at time t,

$$\langle x|\psi(t)\rangle = \int dx' K(x,t;x',0)\langle x'|\psi(0)\rangle$$

$$= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\sqrt{\frac{m}{2\pi i\hbar t}}\int dx' \exp[ik_0x' - \frac{x'^2}{4\sigma_x{}^2} + \frac{im(x-x')^2}{2\hbar t}]$$

$$= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\sqrt{\frac{m}{2\pi i\hbar t}}2\sqrt{\pi}\frac{1}{\sqrt{\dfrac{1}{\sigma_x{}^2} - \dfrac{2im}{t\hbar}}}\exp[-\frac{mx(x-4ik_0\sigma_x{}^2) + 2ik_0{}^2t\hbar\sigma_x{}^2}{4m\sigma_x{}^2 + 2it\hbar}]$$

$$= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\frac{1}{\sqrt{1+\dfrac{it\hbar}{2m\sigma_x{}^2}}}\exp[-\frac{x(x-4ik_0\sigma_x{}^2) + 2ik_0{}^2\dfrac{t\hbar}{m}\sigma_x{}^2}{4\sigma_x{}^2(1+\dfrac{it\hbar}{2m\sigma_x{}^2})}]$$

$$= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\frac{1}{\sqrt{1+\dfrac{it\hbar}{2m\sigma_x{}^2}}}\exp[-\frac{\{x(x-4ik_0\sigma_x{}^2) + 2ik_0{}^2\dfrac{t\hbar}{m}\sigma_x{}^2\}(1-\dfrac{it\hbar}{2m\sigma_x{}^2})}{4\sigma_x{}^2(1+\dfrac{it\hbar}{2m\sigma_x{}^2})(1-\dfrac{it\hbar}{2m\sigma_x{}^2})}]$$

$$= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\frac{1}{\sqrt{1+\dfrac{it\hbar}{2m\sigma_x{}^2}}}\exp[-\frac{(x-\dfrac{\hbar k_0 t}{m})^2}{4\sigma_x{}^2(1+\dfrac{t^2\hbar^2}{4m^2\sigma_x{}^4})} - i\frac{m(8k_0mx\sigma_x{}^4 + t(x^2-4k_0{}^2\sigma_x{}^4)\hbar)}{8m^2\sigma_x{}^4(1+\dfrac{t^2\hbar^2}{4m^2\sigma_x{}^4})}]$$

Since

$$\left|\frac{1}{\sqrt{1+\dfrac{it\hbar}{2m\sigma_x{}^2}}}\right| = \frac{1}{\sqrt{1+\dfrac{t^2\hbar^2}{4m^2\sigma_x{}^4}}}$$

the probability is obtained as

$$\left|\langle x|\psi(t)\rangle\right|^2 = \frac{1}{\sqrt{2\pi}\sigma_x\sqrt{1+\frac{t^2\hbar^2}{4m^2\sigma_x{}^4}}}\exp[-\frac{(x-\frac{\hbar k_0 t}{m})^2}{2\sigma_x{}^2(1+\frac{t^2\hbar^2}{4m^2\sigma_x{}^4})}].$$

which has the form of Gaussian distribution with the standard deviation

$$\sigma_x\sqrt{1+\frac{t^2\hbar^2}{4m^2\sigma_x{}^4}}.$$

and has a peak at

$$\langle x\rangle = \frac{\hbar k_0 t}{m}.$$

The Fourier transform:

$$\langle k|\psi(t)\rangle = \int dx\langle k|x\rangle\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi}}\int dxe^{-ikx}\langle x|\psi(t)\rangle$$

$$= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\frac{1}{\sqrt{1+\frac{it\hbar}{2m\sigma_x{}^2}}}\int dx\exp[-ikx-\frac{x(x-4ik_0\sigma_x{}^2)+2ik_0{}^2\frac{t\hbar}{m}\sigma_x{}^2}{4\sigma_x{}^2(1+\frac{it\hbar}{2m\sigma_x{}^2})}]$$

$$= \frac{1}{\sqrt{\sqrt{2\pi}\frac{1}{2\sigma_x}}}\exp[-\frac{(k-k_0)^2}{4\left(\frac{1}{2\sigma_x}\right)^2}-\frac{ik^2t\hbar}{2m}]$$

where

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}}\frac{1}{\sqrt{1+\frac{it\hbar}{2m\sigma_x{}^2}}}\exp[-\frac{x(x-4ik_0\sigma_x{}^2)+2ik_0{}^2\frac{t\hbar}{m}\sigma_x{}^2}{4\sigma_x{}^2(1+\frac{it\hbar}{2m\sigma_x{}^2})}].$$

Then the probability is obtained as

$$\left|\langle k|\psi(t)\rangle\right|^2 = \frac{1}{\sqrt{2\pi}\sigma_k}\exp[-\frac{(k-k_0)^2}{2\sigma_k^{\ 2}}].$$

where

$$\sigma_k = \frac{1}{2\sigma_x}.$$

Therefore

$$\left|\langle k|\psi(t)\rangle\right|^2 = \left|\langle k|\psi(t=0)\rangle\right|^2.$$

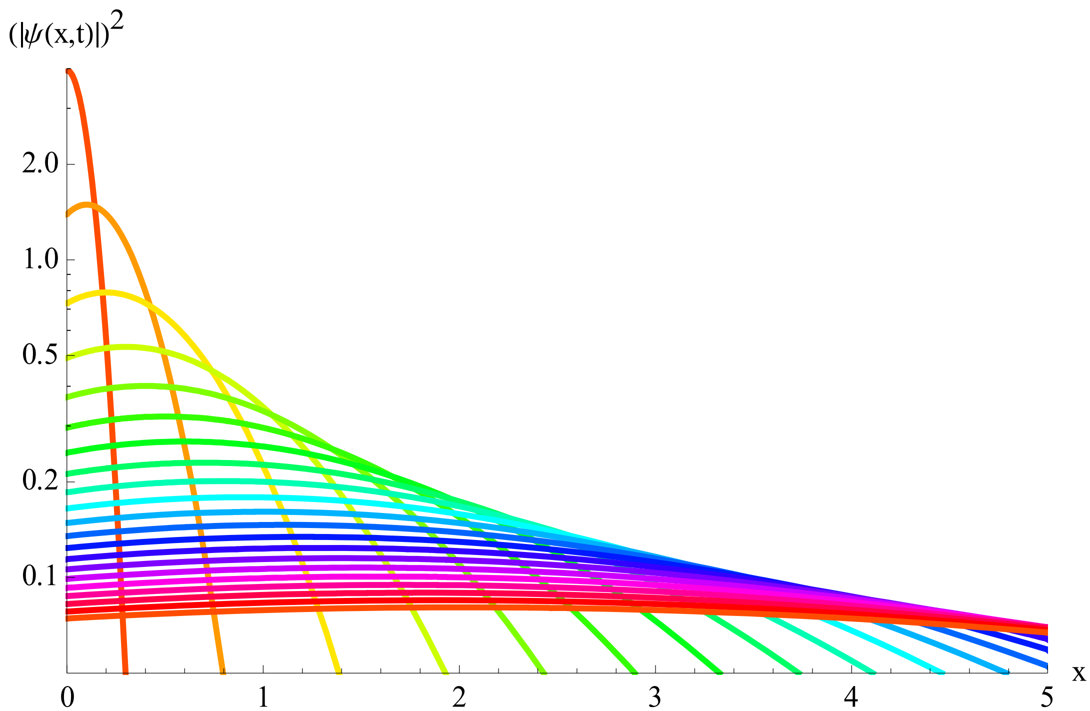


Fig. Plot of $\left|\langle x|\psi(t)\rangle\right|^2$ as a function of x where the time t is changed as a parameter.

In summary, we have

$$\left|\langle x|\psi(t)\rangle\right|^2 = \frac{1}{\sqrt{2\pi}\sigma_x\sqrt{1+\frac{t^2\hbar^2}{4m^2\sigma_x^{\ 4}}}}\exp[-\frac{(x-\frac{\hbar k_0 t}{m})^2}{2\sigma_x^{\ 2}(1+\frac{t^2\hbar^2}{4m^2\sigma_x^{\ 4}})}].$$

and

$$\left|\langle k|\psi(t)\rangle\right|^2 = \frac{1}{\sqrt{2\pi}\sigma_k}\exp[-\frac{(k-k_0)^2}{2\sigma_k{}^2}].$$

14. Wave packet for simple harmonics (quamtum mechanics)

((L.I. Schiff p.67-68))

$$\langle x|\psi(t)\rangle = \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)|\psi(t=0)\rangle$$

$$= \int \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)|x'\rangle\langle x'|\psi(t=0)\rangle dx'$$

We define the kernel $K(x,x',t)$ as

$$K(x,x',t) = \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)|x'\rangle$$

$$= \sum_n \langle x|n\rangle \exp(-\frac{i}{\hbar}E_n t)\langle n|x'\rangle$$

$$= \sum_n \exp(-\frac{i}{\hbar}E_n t)\varphi_n(x)\varphi_n^*(x')$$

Note that

$$\xi = \beta x,$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

Then we have

$$\psi(x,t) = \sum_n \exp(-\frac{i}{\hbar}E_n t)\int dx'\varphi_n^*(x')\psi(x')\varphi_n(x).$$

We assume that

$$\psi(x) = \frac{\beta^{1/2}}{\pi^{1/4}}\exp[-\frac{1}{2}\beta^2(x-a)^2],$$

or

$$\varphi_n(\xi) = \langle \xi | n \rangle = \frac{1}{\sqrt{\beta}} \langle x | n \rangle = \frac{1}{\sqrt{\beta}} \varphi_n(x) ,$$

or

$$\varphi(\xi) = \frac{1}{\pi^{1/4}} \exp[-\frac{1}{2}(\xi - \xi_0)^2] ,$$

with

$$\xi_0 = \beta x_0 .$$

We need to calculate the integral defined by

$$\begin{aligned}
I &= \int dx' \varphi_n^*(x') \psi(x') \\
&= \int dx' \varphi_n^*(x') \frac{\beta^{1/2}}{\pi^{1/4}} \exp[-\frac{1}{2}\beta^2 (x'-a)^2] \\
&= \int \frac{d\xi}{\beta} \beta^{1/2} \varphi_n^*(\xi) \frac{\beta^{1/2}}{\pi^{1/4}} \exp[-\frac{1}{2}(\xi - \xi_0)^2] \\
&= \frac{1}{\pi^{1/4}} \int d\xi \varphi_n^*(\xi) \exp[-\frac{1}{2}(\xi - \xi_0)^2]
\end{aligned}$$

Here

$$\varphi_n(\xi) = (\sqrt{\pi} 2^n n!)^{-\frac{1}{2}} e^{-\frac{\xi^2}{2}} H_n(\xi).$$

Then we get

$$I = \frac{1}{\pi^{1/4}} (\sqrt{\pi} 2^n n!)^{-\frac{1}{2}} \int d\xi \exp(-\frac{\xi^2}{2}) H_n(\xi) \exp[-\frac{1}{2}(\xi - \xi_0)^2]) .$$

Here we use the generating function:

$$\exp(2s\xi - s^2) = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(\xi).$$

Note that

$$\int_{-\infty}^{\infty} d\xi \exp(2s\xi - s^2)\exp(-\frac{\xi^2}{2})\exp[-\frac{1}{2}(\xi-\xi_0)^2] = \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} d\xi \frac{s^n}{n!}H_n(\xi)\exp(-\frac{\xi^2}{2})\exp[-\frac{1}{2}(\xi-\xi_0)^2]$$

$$= \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} d\xi \frac{s^n}{n!}H_n(\xi)\exp[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^{\ 2})]$$

The left-hand side is

$$\int_{-\infty}^{\infty} d\xi \exp(2s\xi - s^2)\exp[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^{\ 2})] = \pi^{1/2}\exp(s\xi_0 - \frac{\xi_0^{\ 2}}{4})$$

$$= \pi^{1/2}\exp(-\frac{\xi_0^{\ 2}}{4})\sum_{n=0}^{\infty}\frac{s^n\xi_0^{\ n}}{n!}$$

Thus we have

$$\pi^{1/2}\exp(-\frac{\xi_0^{\ 2}}{4})\sum_{n=0}^{\infty}\frac{s^n\xi_0^{\ n}}{n!} = \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} d\xi \frac{s^n}{n!}H_n(\xi)\exp[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^{\ 2})].$$

or

$$\pi^{1/2}\exp(-\frac{\xi_0^{\ 2}}{4})\xi_0^{\ n} = \int_{-\infty}^{\infty} d\xi H_n(\xi)\exp[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^{\ 2})].$$

Then

$$I = (\sqrt{\pi}2^n n!)^{-\frac{1}{2}}\exp(-\frac{\xi_0^{\ 2}}{4})\xi_0^{\ n},$$

and

$$\psi(x,t) = \sum_n \exp(-\frac{i}{\hbar}E_n t)(2^n n!)^{-\frac{1}{2}}\exp(-\frac{\xi_0^{\ 2}}{4})\xi_0^{\ n}\varphi_n(x).$$

Since

$$E_n = \hbar\omega_0(n+\frac{1}{2}),$$

or

$$\exp(-\frac{i}{\hbar}E_n t) = \exp(-\frac{i}{2}\omega_0 t - in\omega_0 t),$$

and

$$\psi(\xi,t) = \frac{1}{\sqrt{\beta}}\psi(x,t),$$

we get

$$\psi(\xi,t) = \sum_{n=0}^{\infty}(2^n n!)^{-\frac{1}{2}} \exp(-\frac{\xi_0^{\,2}}{4})(\xi_0 e^{-i\omega_0 t})^n \exp(-\frac{i}{2}\omega_0 t)\varphi_n(\xi),$$

or

$$\psi(\xi,t) = \frac{1}{\pi^{1/4}}\sum_{n=0}^{\infty}(2^n n!)^{-1} \exp(-\frac{\xi_0^{\,2}}{4})(\xi_0 e^{-i\omega_0 t})^n \exp(-\frac{i}{2}\omega_0 t)e^{-\frac{\xi^2}{2}}H_n(\xi)$$

$$== \frac{1}{\pi^{1/4}}\exp(-\frac{\xi_0^{\,2}}{4} - \frac{i}{2}\omega_0 t - -\frac{\xi^2}{2})\sum_{n=0}^{\infty}\frac{1}{n!}(\frac{\xi_0 e^{-i\omega_0 t}}{2})^n H_n(\xi)$$

Using the generating function

$$\sum_{n=0}^{\infty}\frac{1}{n!}(\frac{\xi_0 e^{-i\omega_0 t}}{2})^n H_n(\xi) = \exp[-\frac{1}{4}\xi_0^{\,2} e^{-2in\omega_0 t} + \xi_0 e^{-i\omega_0 t}\xi],$$

we have the final form

$$\psi(\xi,t) = \frac{1}{\pi^{1/4}}\exp(-\frac{\xi_0^{\,2}}{4} - \frac{\xi^2}{2} - \frac{i}{2}\omega_0 t - \frac{1}{4}\xi_0^{\,2} e^{-2i\omega_0 t} + \xi_0\xi e^{-i\omega_0 t})$$

$$= \frac{1}{\pi^{1/4}}\exp[-\frac{\xi_0^{\,2}}{4} - \frac{\xi^2}{2} - \frac{i}{2}\omega_0 t - \frac{1}{4}\xi_0^{\,2}(\cos 2\omega_0 t - i\sin 2\omega_0 t)$$
$$+ \xi_0\xi(\cos\omega_0 t - i\sin\omega_0 t)]$$

OR

$$\left|\psi(\xi,t)\right|^2 = \frac{1}{\pi^{1/2}}\exp[-\frac{\xi_0^{\,2}}{2} - \xi^2 - \frac{1}{2}\xi_0^{\,2}\cos 2\omega_0 t + 2\xi_0\xi\cos\omega_0 t]$$

or

$$\left|\psi(\xi,t)\right|^2 = \frac{1}{\pi^{1/2}}\exp[-(\xi - \xi_0\cos\omega_0 t)^2]$$

$\left|\psi(\xi,t)\right|^2$ represents a wave packet that oscillates without change of shape about $\xi = 0$ with amplitude ξ_0 and angular frequency ω_0.

15. Mathematica

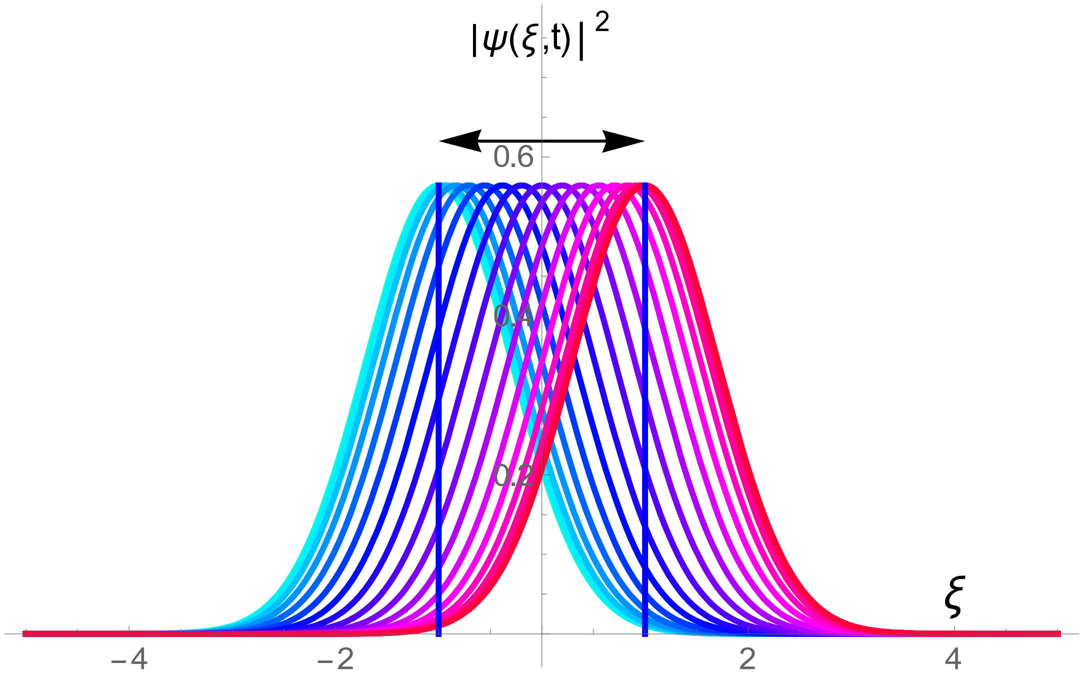
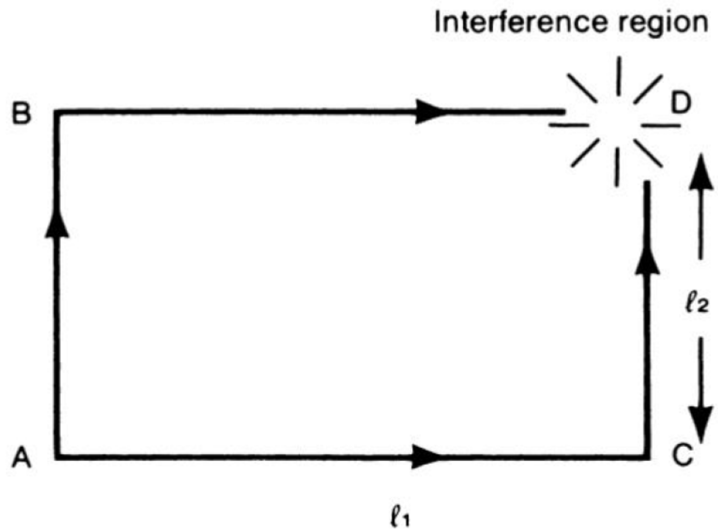


Fig. The time dependence of $|\psi(\xi,t)|^2 = \frac{1}{\pi^{1/2}}\exp[-(\xi-\xi_0\cos\omega_0 t)^2]$, where ξ_0=1. $T = 2\pi/\omega_0$. The peak shifts from ξ = 0 at t = 0 to ξ = 0 at t = T/4, ξ = ξ_0 at t = T/2, ξ = - ξ_0 at t = 3T/4, and ξ = 0 at t = T.

16. Neutron interferometry

Suppose that the interferometry initially lies in a horizontal plane so that there are no gravitational effects. We then rotate the plane formed by the two paths by angle δ about the segment AC. The segment BD is now higher than the segment AC by $l_2 \sin\delta$.



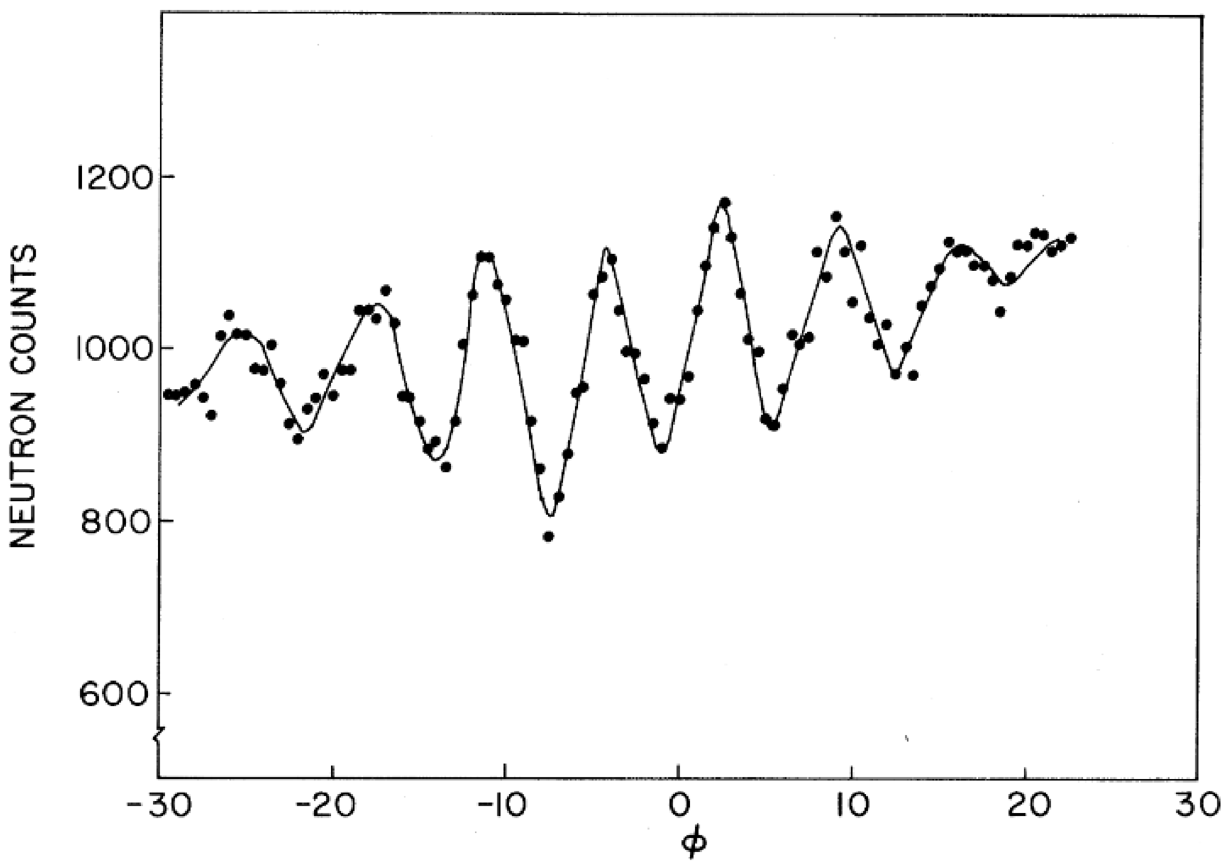


Fig. Dependence of gravity-induced phase on angle of rotation δ. From R. Colella, A. W. Overhauser, and S. A. Werner, Phys.. Rev. Lett. **34** (1975) 1472.

From the previous discussion we have the propagator for the gravity

$$K(x,t;x_0,t_0) = A\exp(\frac{i}{\hbar}S_{cl})$$
$$= \exp(-\frac{i}{24\hbar}mg^2T^3 - \frac{ix_0 mgT}{\hbar})$$
$$= A_1\exp(-\frac{ix_0 mgT}{\hbar})$$

For the path ABD and path ACD, we have

$$\psi = \exp[\frac{i}{\hbar}S(ABD)] + \exp[\frac{i}{\hbar}S(ACD)] = \exp[\frac{i}{\hbar}S(ACD)]\{1+\exp(i\Delta\phi)\}.$$

The phase difference between the path ABD and the path ACD is given by

$$\Delta\varphi = \frac{S(ABD)-S(ACD)}{\hbar} = -\frac{1}{\hbar}mgl_2T\sin\delta = -\frac{1}{\hbar}\frac{m^2gl_1l_2}{p}\sin\delta,$$

or

$$\Delta\varphi = -\frac{1}{\hbar}\frac{m^2gl_1l_2}{\frac{2\pi\hbar}{\lambda}}\sin\delta = -\frac{m^2gl_1l_2\lambda}{2\pi\hbar^2}\sin\delta = -\varepsilon\sin\delta.$$

where p is the momentum

$$p = mv.$$

T is related to l_1 (the distance over the horizontal line) as

$$T = \frac{l_1}{v} = \frac{ml_1}{p} = \frac{ml_1}{\frac{2\pi\hbar}{\lambda}} = \frac{ml_1\lambda}{2\pi\hbar}.$$

The Probability is

$$|\psi|^2 = 4\cos^2(\frac{\varepsilon^2\sin\delta}{2}).$$

Note that

$$\varepsilon = \frac{m^2 g l_1 l_2 \lambda}{2\pi\hbar^2},$$

with

mg=1.025 neV/cm.

where g = 9.80446 m/s^2 at Binghamton, NY (USA). The energy of neutron is evaluated as

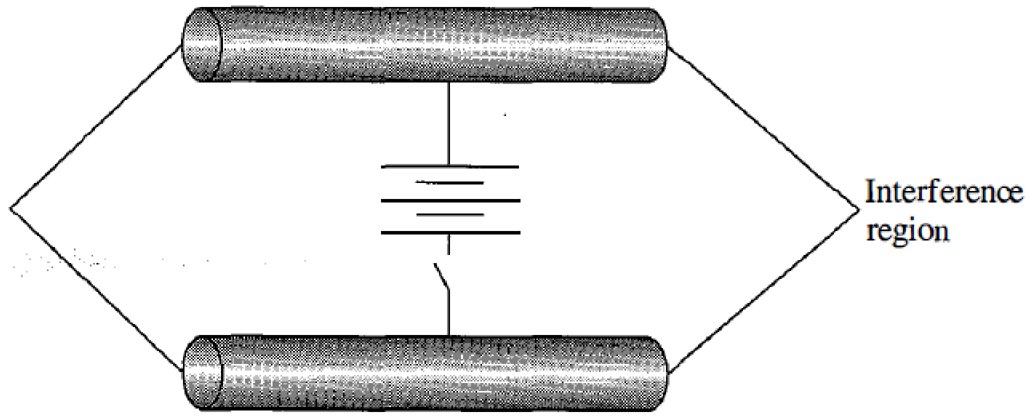
$$E = \frac{\hbar^2}{2M_n}k^2 = \frac{\hbar^2}{2M_n}\left(\frac{2\pi}{\lambda}\right)^2 = 40.63 \text{ meV}$$

for λ =1.419Å.

((**Mathematica**))

```
Clear["Global`*"];
rule1 = {ℏ → 1.054571628 10^-27, mn → 1.674927211 × 10^-24,
   qe → 4.8032068 × 10^-10, meV → 1.602176487 × 10^-15,
   A0 → 10^-8, neV → 1.602176487 × 10^-21, g → 980.446,
   λ → 1.419 A0};

(mn g)/neV //. rule1

1.02497

E1 = ℏ^2/(2 mn) ((2 π/λ)^2)/meV //. rule1

40.6266
```

17. Quantum-mechanical interference to detect a potential difference



A low-intensity beam of charged particles, each with charge q, is split into two parts. each part then enters a very long metallic tube shown above. Suppose that the length of the wave packet for each of the particles is sufficiently smaller than the length of the tube so that for a certain time interval, say from t_0 to t, the wave packet for the particle is definitely within the tubes. During this time interval, a constant electric potential V_1 is applied to the upper tube and a constant electric potential V_2 is applied to the lower tube. The rest of the time there is no voltage applied to the tubes. Here we consider how the interference pattern depends on the voltages V_1 and V_2.

Without the applied potentials, the amplitude to arrive at a particular point on the detecting screen is

$$\psi = \psi_1 + \psi_2 .$$

The intnsity is proportional to

$$I_0 = |\psi_1 + \psi_2|^2 = |\psi_1|^2 + |\psi_2|^2 + (\psi_1^* \psi_2 + \psi_1 \psi_2^*) .$$

With the potential, the Lagrangian in the path is modified as

$$L_0 \to L = L_0 - qV .$$

Thus the wave functions are modified as

$$\begin{aligned}
\Psi &= \psi_1 \exp[\frac{i}{\hbar}\int_{t_0}^{t}(-qV_1)dt] + \psi_2 \exp[\frac{i}{\hbar}\int_{t_0}^{t}(-qV_{12})dt] \\
&= \psi_1 \exp[-\frac{iqV_1}{\hbar}(t-t_0)] + \psi_2 \exp[-\frac{iqV_2}{\hbar}(t-t_0)] \\
&= \psi_1 \exp[-\frac{iqV_1}{\hbar}\Delta t] + \psi_2 \exp[-\frac{iqV_2}{\hbar}\Delta t]
\end{aligned}$$

where $\Delta t = t - t_0$. The intensity of the screen is proportional to

$$I = |\psi|^2$$
$$= \left|\psi_1 \exp[-\frac{iqV_1}{\hbar}\Delta t] + \psi_2 \exp[-\frac{iqV_2}{\hbar}\Delta t]\right|^2$$
$$= \left|\psi_1 + \psi_2 \exp[\frac{iq(V_1 - V_2)}{\hbar}\Delta t]\right|^2$$

We assume that

$$\varphi = \frac{q(V_1 - V_2)}{\hbar}.$$

Then we have

$$I = \left|\psi_1 + \psi_2 e^{i\phi}\right|^2 = |\psi_1|^2 + |\psi_2|^2 + (\psi_1{}^*\psi_2 e^{i\varphi} + \psi_1\psi_2{}^* e^{-i\varphi})$$

When $\psi_1 = \psi_2 = \psi_0$, we have

$$I = 2|\psi_0|^2(1 + \cos\phi) = 4|\psi_0|^2 \cos^2\frac{\varphi}{2}$$

The intensity depends on the phase; I becomes maximum when $\varphi = 2n\pi$ and minimum at $\phi = 2(n + \frac{1}{2})\pi$.

((**Note**)) **Method with the use of gauge transformation**

The proof for the expression can also be given using the concept of the Gauge trasnformation. The vector potential ***A*** and scalar potential ϕ are related to the magnetic field ***B*** and electric field ***E*** by

$$\boldsymbol{B} = \nabla \times \boldsymbol{A},$$

$$\boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} - \nabla\phi,$$

The gauge transformation is defined by

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\chi,$$

$$\phi' = \phi - \frac{1}{c}\frac{\partial \chi}{\partial t},$$

where c is an arbitrary function. The new wave function is related to the old wave function through

$$\psi'(\boldsymbol{r}) = \exp(\frac{iq}{\hbar c}\chi)\psi(r).$$

Suppose that $\phi' = 0$. Then $\psi'(\boldsymbol{r}) = \psi_0(\boldsymbol{r})$ is the wave function of free particle. Then we get

$$\phi = \frac{1}{c}\frac{\partial \chi}{\partial t}, \qquad \chi = c\int dt\phi .$$

The wave function $\psi(r)$ is given by

$$\begin{aligned}\psi(r) &= \exp(-\frac{iq}{\hbar c}\chi)\psi_0(\boldsymbol{r}) \\ &= \exp(-\frac{iq}{\hbar c}c\int dt\phi)\psi_0(\boldsymbol{r}) \\ &= \exp(-\frac{iq}{\hbar}\int dtV)\psi_0(\boldsymbol{r})\end{aligned}$$

When *V* is the electric potential and is independent of time *t*, we have

$$\psi(r) = \exp[-\frac{iq}{\hbar}V(t-t_0)]\psi_0(\boldsymbol{r})$$

This expression is exactly the same as that derived from the Feynman path integral.

18. Quantization of magnetic flux and Aharonov-Bohm effect

The classical Lagrangian *L* is defined by

$$L = \frac{1}{2}m\boldsymbol{v}^2 - q\phi + \frac{q}{c}\boldsymbol{v}\cdot\boldsymbol{A}.$$

in the presence of a magnetic field. In the absence of the scalar potential ($\phi = 0$), we get

$$L_{cl} = \frac{1}{2}m\boldsymbol{v}^2 + \frac{q}{c}\boldsymbol{v}\cdot\boldsymbol{A} = L_c^{(0)} - \frac{e}{c}\boldsymbol{v}\cdot\boldsymbol{A},$$

where the charge *q* = -*e* (*e*>0), ***A*** is the vector potential. The corresponding change in the action of some definite path segment going from $(\boldsymbol{r}_{n-1}, t_{n-1})$ to $(\boldsymbol{r}_{n1}, t_n)$ is then given by

$$S^{(0)}(n,n-1) \to S^{(0)}(n,n-1) - \frac{e}{c}\int_{t_{n-1}}^{t_n} dt\left(\frac{d\boldsymbol{r}}{dt}\right)\cdot \boldsymbol{A},$$

This integral can be written as

$$\frac{e}{c}\int_{t_{n-1}}^{t_n} dt\left(\frac{d\boldsymbol{r}}{dt}\right)\cdot \boldsymbol{A} = \frac{e}{c}\int_{\boldsymbol{r}_{n-1}}^{\boldsymbol{r}_n} \boldsymbol{A}\cdot d\boldsymbol{r},$$

where $d\boldsymbol{r}$ is the differential line element along the path segment.

Now we consider the Aharonov-Bohm (AB) effect. This effect can be usually explained in terms of the *gauge transformation*. Here instead we discuss the effect using the Feynman's path integral. In the best known version, electrons are aimed so as to pass through two regions that are free of electromagnetic field, but which are separated from each other by a long cylindrical solenoid (which contains magnetic field line), arriving at a detector screen behind. At no stage do the electrons encounter any non-zero field $\boldsymbol{B}$.

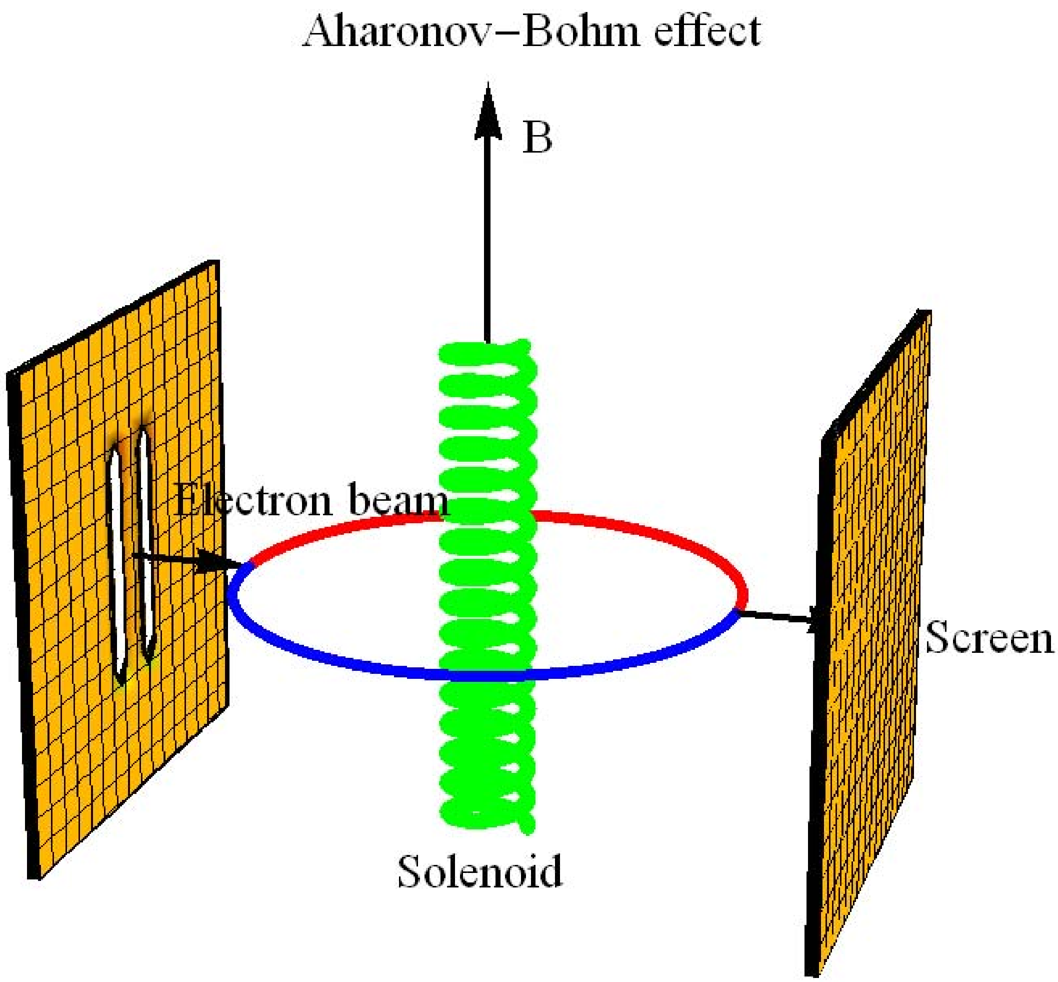


Fig. Schematic diagram of the Aharonov-Bohm experiment. Electron beams are split into two paths that go to either a collection of lines of magnetic flux (achieved by means of a long solenoid). The beams are brought together at a screen, and the resulting quantum interference pattern depends upon the magnetic flux strength- despite the fact that the electrons only encounter a zero magnetic field. Path denoted by red (counterclockwise). Path denoted by blue (clockwise)

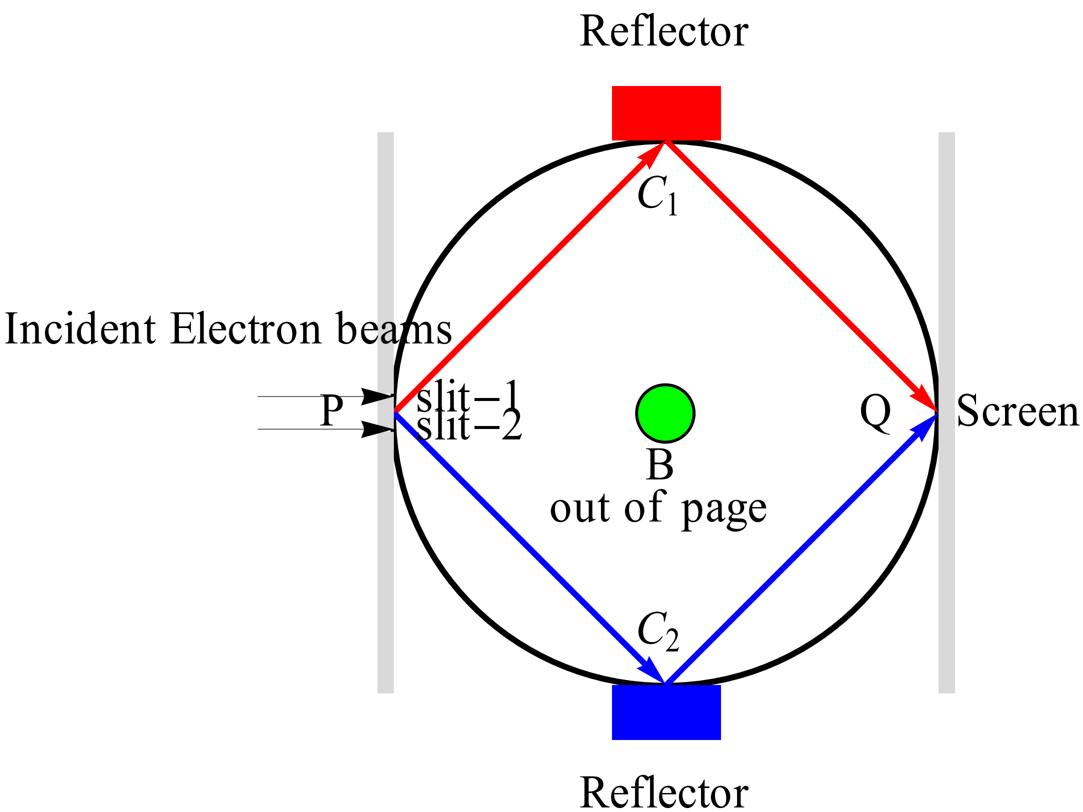


Fig. Schematic diagram of the Aharonov-Bohm experiment. Incident electron beams go into the two narrow slits (one beam denoted by blue arrow, and the other beam denoted by red arrow). The diffraction pattern is observed on the screen. The reflector plays a role of mirror for the optical experiment. The path1: slit-1 – C1 – S. The path 2: slit-2 – C2 – S.

Let ψ_{1B} be the wave function when only slit 1 is open.

$$\psi_{1,B}(\boldsymbol{r}) = \psi_{1,0}(\boldsymbol{r})\exp[-\frac{ie}{\hbar c}\int_{Path1} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})], \qquad (1)$$

The line integral runs from the source through slit 1 to $\boldsymbol{r}$ (screen) through C_1. Similarly, for the wave function when only slit 2 is open, we have

$$\psi_{1,B}(\boldsymbol{r}) = \psi_{2,0}(\boldsymbol{r})\exp[-\frac{ie}{\hbar c}\int_{Path2} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})], \qquad (2)$$

The line integral runs from the source through slit 2 to $\boldsymbol{r}$ (screen) through C_2. Superimposing Eqs.(1) and (2), we obtain

$$\psi_{B}(\boldsymbol{r}) = \psi_{1,0}(\boldsymbol{r})\exp[-\frac{ie}{\hbar c}\int_{Path1} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})] + \psi_{2,0}(\boldsymbol{r})\exp[-\frac{ie}{c\hbar}\int_{Path2} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})].$$

The relative phase of the two terms is

$$\int_{Path1} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r}) - \int_{Path2} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r}) = \oint d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r}) = \int (\nabla\times\boldsymbol{A})\cdot d\boldsymbol{a},$$

by using the Stokes' theorem, where the closed path consists of path1 and path2 along the same direction. The relative phase now can be expressed in terms of the flux of the magnetic field through the closed path,

$$\Delta\theta = \frac{e}{c\hbar}\oint \boldsymbol{A}\cdot d\boldsymbol{r} = \frac{e}{c\hbar}\int (\nabla\times\boldsymbol{A})\cdot d\boldsymbol{a} = \frac{e}{c\hbar}\int \boldsymbol{B}\cdot d\boldsymbol{a} = \frac{e}{c\hbar}\Phi .$$

where the magnetic field $\boldsymbol{B}$ is given by

$$\boldsymbol{B} = \nabla\times\boldsymbol{A}.$$

The final form is obtained as

$$\psi_B(\boldsymbol{r}) = \exp[-\frac{ie}{\hbar c}\int_{Path2} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})][\psi_{1,0}(\boldsymbol{r})\exp(-i\Delta\theta) + \psi_{2,0}(\boldsymbol{r})],$$

and Φ is the magnetic flux inside the loop. It is required that

$$\Delta\theta = 2n\pi .$$

Then we get the quantization of the magnetic flux,

$$\Phi_n = n\frac{2\pi c\hbar}{e},$$

where n is a positive integer, n = 0, 1,2,….. Note that

$$\frac{2\pi c\hbar}{e} = 4.1356675\times 10^{-7} \text{ Gauss cm}^2.$$

which is equal to $2\Phi_0$, where Φ_0 is the magnetic quantum flux,

$$\Phi_0 = \frac{2\pi c\hbar}{2e} = 2.067833758(46) \times 10^{-7} \text{ Gauss cm}^2. \quad \text{(NIST)}$$

19. Example-1: Feynman path integral

We consider the Gaussian position-space wave packet at t = 0, which is given by

$$\langle x|\psi(t=0)\rangle = \frac{1}{\sqrt{2\pi}\sigma}\exp(-\frac{x^2}{2\sigma^2}) \quad \text{(Gaussian wave packet at } t = 0\text{).}$$

The Gaussian position-space wave packet evolves in time as

$$\begin{aligned}\langle x|\psi(t)\rangle &= \int dx_0 K(x,t;x_0,0)\langle x_0|\psi(0)\rangle \\ &= \frac{1}{\sqrt{2\pi}\sigma}\sqrt{\frac{m}{2\pi i\hbar t}}\int dx_0 \exp[-\frac{x_0{}^2}{2\sigma^2}+\frac{im(x-x_0)^2}{2\hbar t}] \\ &= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\sigma^2+\frac{i\hbar t}{m}}}\exp[-\frac{x^2}{2(\sigma^2+\frac{i\hbar t}{m})}]\end{aligned} \qquad (1)$$

where

$$K(x,t;x_0,t_0=0)=(\frac{m}{2\pi i\hbar t})^{1/2}\exp[\frac{im(x-x_0)^2}{2\hbar t}] \qquad \text{(free propagator)} \qquad (2)$$

(Note) You need to show all the procedures to get the final form of $\langle x|\psi(t)\rangle$.

(a) Prove the expression for $\langle x|\psi(t)\rangle$ given by Eq.(1).

(b) Evaluate the probability given by $|\langle x|\psi(t)\rangle|^2$ for finding the wave packet at the position x and time t.

(a)
The Gaussian wave packet:

$$\langle x|\psi(t=0)\rangle = \frac{1}{\sqrt{2\pi}\sigma}\exp(-\frac{x^2}{2\sigma^2}). \qquad \text{(Gaussian)}$$

The free propagator:

$$K(x,t;x_0,t_0=0)=(\frac{m}{2\pi i\hbar t})^{1/2}\exp[\frac{im(x-x_0)^2}{2\hbar t}].$$

Then we have

$$\begin{aligned}\langle x|\psi(t)\rangle &= \int dx_0 K(x,t;x_0,0)\langle x_0|\psi(0)\rangle \\ &= \frac{1}{\sqrt{2\pi}\sigma}\left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\int dx_0 \exp[-\frac{x_0{}^2}{2\sigma^2}+\frac{im(x-x_0)^2}{2\hbar t}]\end{aligned}$$

Here we have

$$-\frac{x_0{}^2}{2\sigma^2}+\frac{im(x-x_0)^2}{2\hbar t}=-\frac{x_0{}^2}{2\sigma^2}+\frac{im(x^2-2x_0x+x_0{}^2)}{2\hbar t}$$
$$=(-\frac{1}{2\sigma^2}+\frac{im}{2\hbar t})x_0{}^2+(-\frac{imx}{\hbar t})x_0+\frac{imx^2}{2\hbar t}$$
$$=ax_0{}^2+bx_0+c$$
$$=a(x_0+\frac{b}{2a})^2-\frac{b^2-4ac}{4a}$$

where

$$a=-\frac{1}{2\sigma^2}+\frac{im}{2\hbar t},\qquad b=-\frac{imx}{\hbar t},\qquad c=\frac{imx^2}{2\hbar t}.$$

Then we get the integral

$$\int_{-\infty}^{\infty}dx_0\exp[ax_0{}^2+bx_0+c]=\int_{-\infty}^{\infty}dx_0\exp[a(x_0+\frac{b}{2a})^2+c-\frac{b^2}{4a}$$
$$=\exp(c-\frac{b^2}{4a})\int_{-\infty}^{\infty}dx_0\exp[a(x_0+\frac{b}{2a})^2$$
$$=\sqrt{\frac{\pi}{-a}}\exp(c-\frac{b^2}{4a})$$

Note that when $\mathrm{Re}(a)=-\frac{1}{2\sigma^2}<0$, the above integral can be calculated as

$$\int_{-\infty}^{\infty}dx_0\exp[a(x_0+\frac{b}{2a})^2=\frac{1}{\sqrt{-a}}\int_{-\infty}^{\infty}dy\exp(-y^2)=\sqrt{\frac{\pi}{-a}},$$

with the replacement of variable as $y=\sqrt{-a}(x_0+\frac{b}{2a})$ and $dy=dx_0\sqrt{-a}$. Thus we have

$$\langle x|\psi(t)\rangle=\frac{1}{\sqrt{2\pi}\sigma}\sqrt{\frac{m}{2\pi i\hbar t}}\sqrt{\frac{\pi}{-a}}\exp(c-\frac{b^2}{4a})$$
$$=\frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{2\pi i\hbar t}}\sqrt{\frac{\pi}{\frac{1}{2}-\frac{im\sigma^2}{2\hbar t}}}\exp[\frac{imx^2}{2\hbar t}+\frac{\left(-\frac{imx}{\hbar t}\right)^2}{4(\frac{1}{2\sigma^2}-\frac{im}{2\hbar t})}]$$

or

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m\pi}{2\pi i\hbar t(\frac{1}{2}-\frac{im\sigma^2}{2\hbar t})}}\exp[\frac{imx^2}{2\hbar t}+\frac{\left(-\frac{imx}{\hbar t}\right)^2}{4(\frac{1}{2\sigma^2}-\frac{im}{2\hbar t})}]$$

$$= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{i\hbar t-\frac{im}{2\hbar t}(2i\hbar t\sigma^2)}}\exp[\frac{imx^2}{2\hbar t}-\frac{\left(\frac{mx}{\hbar t}\right)^2}{2(\frac{\hbar t-im\sigma^2}{\sigma^2\hbar t})}]$$

$$= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m}+\sigma^2}}\exp[\frac{imx^2}{2\hbar t}+\frac{\left(\frac{mx}{\hbar t}\right)^2}{2im(\frac{\sigma^2+\frac{i\hbar t}{m}}{\sigma^2\hbar t})}]$$

$$= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m}+\sigma^2}}\exp[\frac{imx^2}{2\hbar t}+\frac{\sigma^2\hbar t}{2im}\frac{\left(\frac{mx}{\hbar t}\right)^2}{\sigma^2+\frac{i\hbar t}{m}}]$$

or

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m}+\sigma^2}}\exp(\frac{imx^2}{2\hbar t}-\frac{imx^2}{2\hbar t}\frac{\sigma^2}{\sigma^2+\frac{i\hbar t}{m}})$$

$$= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m}+\sigma^2}}\exp[\frac{imx^2}{2\hbar t}(1-\frac{\sigma^2}{\sigma^2+\frac{i\hbar t}{m}})]$$

$$= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m}+\sigma^2}}\exp[\frac{imx^2}{2\hbar t}(\frac{\frac{i\hbar t}{m}}{\sigma^2+\frac{i\hbar t}{m}})]$$

$$= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\frac{i\hbar t}{m}+\sigma^2}}\exp[-\frac{x^2}{2(\sigma^2+\frac{i\hbar t}{m})}]$$

Finally we get

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\sigma^2+\frac{i\hbar t}{m}}}\exp[-\frac{x^2}{2(\sigma^2+\frac{i\hbar t}{m})}].$$

It is clear that at $t = 0$, $\langle x|\psi(t)\rangle$ is the original Gaussian wave packet.

(b)

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\sigma^2+\frac{i\hbar t}{m}}}\exp[-\frac{x^2}{2(\sigma^4+\frac{\hbar^2t^2}{m^2})}(\sigma^2-\frac{i\hbar t}{m})]$$

$$= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\sigma^2+\frac{i\hbar t}{m}}}\exp[-\frac{\sigma^2x^2}{2(\sigma^4+\frac{\hbar^2t^2}{m^2})}]\exp[\frac{i\frac{i\hbar t}{m}x^2}{2(\sigma^4+\frac{\hbar^2t^2}{m^2})}]$$

$$= \frac{1}{\sqrt{2\pi}}\frac{1}{\left(\sigma^4+\frac{\hbar^2t^2}{m^2}\right)^{1/4}}\exp[-\frac{\sigma^2x^2}{2(\sigma^4+\frac{\hbar^2t^2}{m^2})}]e^{-i\varphi}\exp[\frac{i\frac{\hbar t}{m}x^2}{2(\sigma^4+\frac{\hbar^2t^2}{m^2})}]$$

where

$$\sigma^2+\frac{i\hbar t}{m} = \sqrt{\sigma^4+\frac{\hbar^2t^2}{m^2}}e^{i\varphi} \qquad \text{with } \varphi = \arctan(\frac{\hbar^2t^2}{m^2\sigma^2}).$$

Then we have

$$\left|\langle x|\psi(t)\rangle\right|^2 = \frac{1}{2\pi}\frac{1}{\sqrt{\sigma^4+\frac{\hbar^2t^2}{m^2}}}\exp[-\frac{\sigma^2x^2}{(\sigma^4+\frac{\hbar^2t^2}{m^2})}]$$

The height of $\left|\langle x|\psi(t)\rangle\right|^2$ is $\dfrac{1}{2\pi}\dfrac{1}{\sqrt{\sigma^4+\frac{\hbar^2t^2}{m^2}}}$.

The width is $\Delta x = \dfrac{1}{\sigma}\sqrt{\sigma^4+\dfrac{\hbar^2t^2}{m^2}}$.

20. Example-2: Feynman path integral

Suppose that the Gaussian wave packet is given by

$$\langle x|\psi(t=0)\rangle = \frac{1}{\sqrt{2\pi}\sigma}\exp(ik_0x - \frac{x^2}{2\sigma^2}). \qquad \text{(Gaussian)}$$

Here we discuss how such a Gaussian wave packet propagates along the x axis as the time changes.

The free propagator:

$$K(x,t;x_0,t_0=0) = (\frac{m}{2\pi i\hbar t})^{1/2}\exp[\frac{im(x-x_0)^2}{2\hbar t}].$$

Then we have

$$\begin{aligned}\langle x|\psi(t)\rangle &= \int dx_0 K(x,t;x_0,0)\langle x_0|\psi(0)\rangle \\ &= \frac{1}{\sqrt{2\pi}\sigma}\left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\int dx_0 \exp[-\frac{x_0^{\ 2}}{2\sigma^2} + \frac{im(x-x_0)^2}{2\hbar t} + ik_0x_0]\end{aligned}$$

Here we have

$$\begin{aligned}-\frac{x_0^{\ 2}}{2\sigma^2} + \frac{im(x-x_0)^2}{2\hbar t} + ik_0x_0 &= -\frac{x_0^{\ 2}}{2\sigma^2} + \frac{im(x^2 - 2x_0x + x_0^{\ 2})}{2\hbar t} + ik_0x_0 \\ &= (-\frac{1}{2\sigma^2} + \frac{im}{2\hbar t})x_0^{\ 2} + i(k_0 - \frac{mx}{\hbar t})x_0 + \frac{imx^2}{2\hbar t} \\ &= ax_0^{\ 2} + bx_0 + c \\ &= a(x_0 + \frac{b}{2a})^2 - \frac{b^2 - 4ac}{4a}\end{aligned}$$

where

$$a = -\frac{1}{2\sigma^2} + \frac{im}{2\hbar t}, \qquad b = i(k_0 - \frac{mx}{\hbar t}), \qquad c = \frac{imx^2}{2\hbar t}.$$

Then we get the integral

$$\int_{-\infty}^{\infty} dx_0 \exp[a{x_0}^2 + bx_0 + c] = \int_{-\infty}^{\infty} dx_0 \exp[a(x_0 + \frac{b}{2a})^2 + c - \frac{b^2}{4a}$$

$$= \exp(c - \frac{b^2}{4a}) \int_{-\infty}^{\infty} dx_0 \exp[a(x_0 + \frac{b}{2a})^2$$

$$= \sqrt{\frac{\pi}{-a}} \exp(c - \frac{b^2}{4a})$$

Note that when $\mathrm{Re}(a) = -\frac{1}{2\sigma^2} < 0$, the above integral can be calculated as

$$\int_{-\infty}^{\infty} dx_0 \exp[a(x_0 + \frac{b}{2a})^2] = \frac{1}{\sqrt{-a}} \int_{-\infty}^{\infty} dy \exp(-y^2) = \sqrt{\frac{\pi}{-a}} ,$$

with the replacement of variable as $y = \sqrt{-a}(x_0 + \frac{b}{2a})$ and $dy = dx_0\sqrt{-a}$. Thus we have

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi}\sigma} \sqrt{\frac{m}{2\pi i\hbar t}} \sqrt{\frac{\pi}{-a}} \exp(c - \frac{b^2}{4a})$$

$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{m}{2\pi i\hbar t}} \sqrt{\frac{\pi}{\frac{1}{2} - \frac{im\sigma^2}{2\hbar t}}} \exp[\frac{imx^2}{2\hbar t} + \frac{\left(ik_0 - \frac{imx}{\hbar t}\right)^2}{4(\frac{1}{2\sigma^2} - \frac{im}{2\hbar t})}]$$

or

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m\pi}{2\pi i\hbar t(\frac{1}{2}-\frac{im\sigma^2}{2\hbar t})}}\exp[\frac{imx^2}{2\hbar t}+\frac{\left(ik_0-\frac{imx}{\hbar t}\right)^2}{4(\frac{1}{2\sigma^2}-\frac{im}{2\hbar t})}]$$

$$= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{i\hbar t-\frac{im}{2\hbar t}(2i\hbar t\sigma^2)}}\exp[\frac{imx^2}{2\hbar t}-\frac{\left(\frac{mx}{\hbar t}-k_0\right)^2}{2(\frac{\hbar t-im\sigma^2}{\sigma^2\hbar t})}]$$

$$= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m}+\sigma^2}}\exp[\frac{imx^2}{2\hbar t}+\frac{\left(\frac{mx}{\hbar t}-k_0\right)^2}{2im(\frac{\sigma^2+\frac{i\hbar t}{m}}{\sigma^2\hbar t})}]$$

$$= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m}+\sigma^2}}\exp[\frac{imx^2}{2\hbar t}+\frac{\sigma^2\hbar t}{2im}\frac{\left(\frac{mx}{\hbar t}-k_0\right)^2}{\sigma^2+\frac{i\hbar t}{m}}]$$

or

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m}+\sigma^2}}\exp(\frac{imx^2}{2\hbar t}-\frac{im(x-\frac{\hbar k_0 t}{m})^2}{2\hbar t}\frac{\sigma^2(\sigma^2-\frac{i\hbar t}{m})}{\sigma^4+\frac{\hbar^2t^2}{m^2}})$$

$$= \frac{1}{\sqrt{2\pi}}\frac{1}{\left(\sigma^4+\frac{\hbar^2t^2}{m^2}\right)^{1/4}}e^{-i\varphi}$$

$$\exp(\frac{imx^2}{2\hbar t}-\frac{im(x-\frac{\hbar k_0 t}{m})^2}{2\hbar t}\frac{\sigma^4}{\sigma^4+\frac{\hbar^2t^2}{m^2}})\exp[-\frac{1}{2}\frac{\sigma^2(x-\frac{\hbar k_0 t}{m})^2}{\sigma^4+\frac{\hbar^2t^2}{m^2}}]$$

where

$$\sigma^2+\frac{i\hbar t}{m}=\sqrt{\sigma^4+\frac{\hbar^2t^2}{m^2}}e^{i\varphi} \qquad \text{with } \varphi = \arctan(\frac{\hbar^2t^2}{m^2\sigma^2}).$$

Then we have

$$|\langle x|\psi(t)\rangle|^2 = \frac{1}{2\pi}\frac{1}{\sqrt{\sigma^4 + \frac{\hbar^2 t^2}{m^2}}}\exp[-\frac{\sigma^2(x-\frac{\hbar k_0 t}{m})^2}{(\sigma^4 + \frac{\hbar^2 t^2}{m^2})}].$$

This means the center of the Gaussian wave packet moves along the x axis at the constant velocity.

(i) The height of $|\langle x|\psi(t)\rangle|^2$ is $$\frac{1}{2\pi}\frac{1}{\sqrt{\sigma^4 + \frac{\hbar^2 t^2}{m^2}}}.$$

(ii) The width is $$\Delta x = \frac{1}{\sigma}\sqrt{\sigma^4 + \frac{\hbar^2 t^2}{m^2}}.$$

(iii) The Group velocity is $$v_g = \frac{\hbar k_0}{m}.$$

21. Summary: Feynman path integral

The probability amplitude associated with the transition from the point (x_i, t_i) to (x_f, t_f) is the sum over all paths with the action as a phase angle, namely,

$$\text{Amplitude} = \sum_{\substack{All\\paths}} \exp(\frac{i}{\hbar}S),$$

where S is the action associated with each path. So we can write down

$$\begin{aligned} K(x_f, t_f; x_i, t_i) &= \langle x_f, t_f | x_i, t_i \rangle \\ &= \sum_{\substack{All\\paths}} \exp(\frac{i}{\hbar}\int_{t_i}^{t_f} dt L) \\ &= F(t_f - t_i)\exp(\frac{i}{\hbar}S_{cl}) \end{aligned}$$

where $S_{\rm cl}$ is the classical action associated with each path.

If the Lagrangian is given by the simple form

$$L(x, \dot{x}, t) = a(t)\dot{x}^2 + b(t)\dot{x}x + c(t)x^2,$$

then $F(t_f, t_i)$ can be expressed by

$$F(t_f, t_i) = K(x_f = 0, t_f; x_i = 0, t_i) .$$

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APPENDIX-I

Mathematical formula-1

$$\int_{-\infty}^{\infty} dx \exp(-ax^2 + bx + c) = \sqrt{\frac{\pi}{a}} \exp(\frac{b^2}{4a} + c)$$

for $\quad \mathrm{Re}[a] > 0$

APPENDIX-II Action in the classical mechanics

We start to discuss the calculus of variations with an action given by the form

$$S = \int_{t_i}^{t_f} L[\dot{x}, x] dt ,$$

where $\dot{x} = \dfrac{dx}{dt}$. The problem is to find has a stationary function $x_{cl}(x)$ so as to minimize the value of the action *S*. The minimization process can be accomplished by introducing a parameter ε.

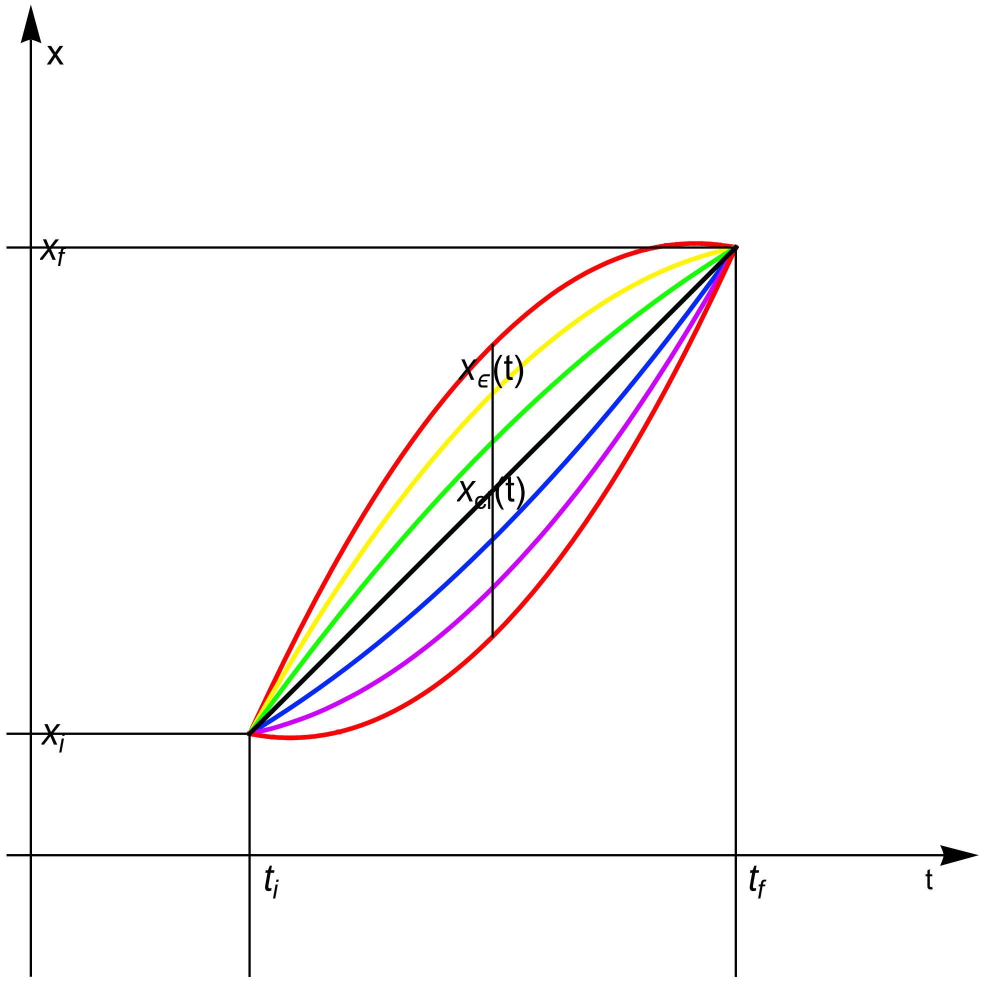

Fig.

$$x(t_i) = x_i, \qquad x(t_f) = x_f,$$

$$x_\varepsilon(t) = x_{cl}(t) + \varepsilon\eta(t),$$

where ε is a real number and

$$x_{cl}(t_i) = x_i, \qquad x_{cl}(t_f) = x_f,$$

$$\eta(t_i) = 0, \qquad \eta(t_f) = 0,$$

$$\delta x = \left(\frac{\partial x}{\partial \varepsilon}\right)_{\varepsilon=0} d\varepsilon = \eta(t)d\varepsilon ,$$

$$S[x_\varepsilon] = \int_{t_i}^{t_f} L(x_{cl}(t) + \varepsilon\eta(t), \dot{x}_{cl}(t) + \varepsilon\dot{\eta}(t))dt ,$$

has a minimum at $\varepsilon = 0$.

$$S[x_{\varepsilon=0}] = \int_{t_i}^{t_f} L[x_{cl}(t)]dt ,$$

$$\left(\frac{\partial L[x_\varepsilon]}{\partial \varepsilon}\right)_{\varepsilon=0} = 0 , \qquad \delta L = \frac{\partial L}{\partial \varepsilon}|_{\varepsilon=0} d\varepsilon ,$$

$$\begin{aligned}\frac{\partial S[x_\varepsilon]}{\partial \varepsilon} &= \int_{t_i}^{t_f} \{\frac{\partial L}{\partial x}\eta(t) + \frac{\partial L}{\partial \dot{x}}\dot{\eta}(t)\}dt \\ &= \int_{t_i}^{t_f} \frac{\partial L}{\partial x}\eta(t)dt + \frac{\partial L}{\partial \dot{x}}\eta(t)\}|_{t_i}^{t_f} - \int_{t_i}^{t_f} \frac{d}{dt}(\frac{\partial L}{\partial \dot{x}})\eta(t)dt \\ &= \int_{t_i}^{t_f} [\frac{\partial L}{\partial x} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{x}})]\eta(t)dt\end{aligned}$$

(1)

The Taylor expansion:

$$S[x_\varepsilon] = \int_{t_i}^{t_f} L(x_{cl}(t) + \varepsilon\eta(t), \dot{x}_{cl}(t) + \varepsilon\dot{\eta}(t))dt$$

((Fundamental lemma))
If

$$\int_{t_i}^{t_f} M(t)\eta(t)dt = 0$$

for all arbitrary function $\eta(t)$ continuous through the second derivative, then $M(t)$ must identically vanish in the interval $t_i \le t \le t_f$.

From this fundamental lemma of variational and Eq.(1), we have Lagrange equation

$$\frac{\partial L}{\partial x} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{x}}) = 0 . \qquad (2)$$

L can have a stationary value only if the Lagrange equation is valid.

In summary,

$$S = \int_{x_1}^{x_2} L(x, \dot{x}) dt ,$$

$$\delta S = 0 \Leftrightarrow \frac{\partial L}{\partial x} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{x}}) = 0 .$$