Feynman Path Integral: Formulation of Quantum Dynamics

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((**Overview**))

We consider quantum superpositions of possible alternative classical trajectories, a history being a path in configuration space, taken between fixed points (*a* and *b*). The basic idea of the Feynman path integral is a perspective on the fundamental quantum mechanical principle of complex linear superposition of such entire spacetime histories. In the quantum world, instead of there being just one classical 'reality', represented by one such trajectory (one history), there is a great complex superposition of all these 'alternative realities' (superposed alternative histories). Accordingly, each history is to be assigned a complex weighting factor, which we refer to as an amplitude, if the total is normalized to modulus unity, so the squared modulus of an amplitude gives us a probability. The magic role of the Lagrangian is that it tells us what amplitude is to be assigned to each such history. If we know the Lagrangian *L*, then we can obtain the action *S*, for that history (the action being just the integral of *L* for that classical history along the path). The complex amplitude to be assigned to that particular history is then given by the deceptively simple formula amplitude

$$\exp(\frac{i}{\hbar}S) = \exp(\frac{i}{\hbar}\int_a^b L dt).$$

The total amplitude to get from *a* to *b* is the sum of these.

((**Path integral**))

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 $\exp[i\frac{\varepsilon}{\hbar}L(\frac{x'-x}{\varepsilon},x)]$,

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

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

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

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 Schrödinger picture is given by

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

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

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

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

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

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

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.

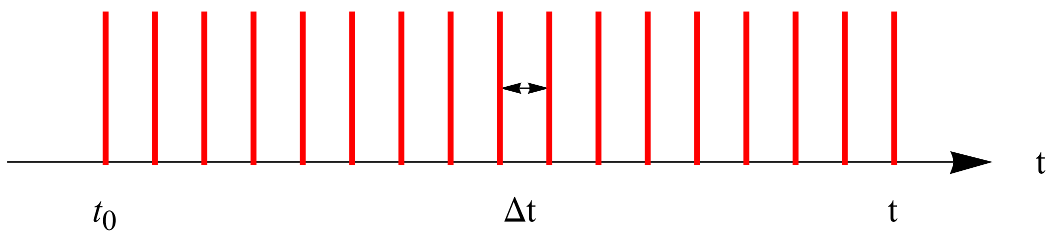
2. Propagator

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

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

where

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



where $t_0 = t'$ in this figure.

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

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

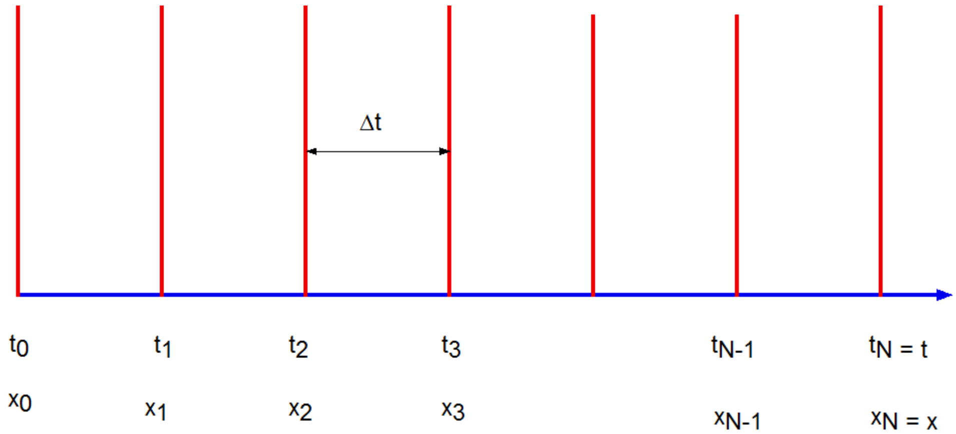
This expression says that the amplitude is the integral of the amplitude of all N-legged paths.

((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, …, N, and

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

Then we have

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

where p_i (i = 1, 2, 3, …, N), or

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

where

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

Then we have

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

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

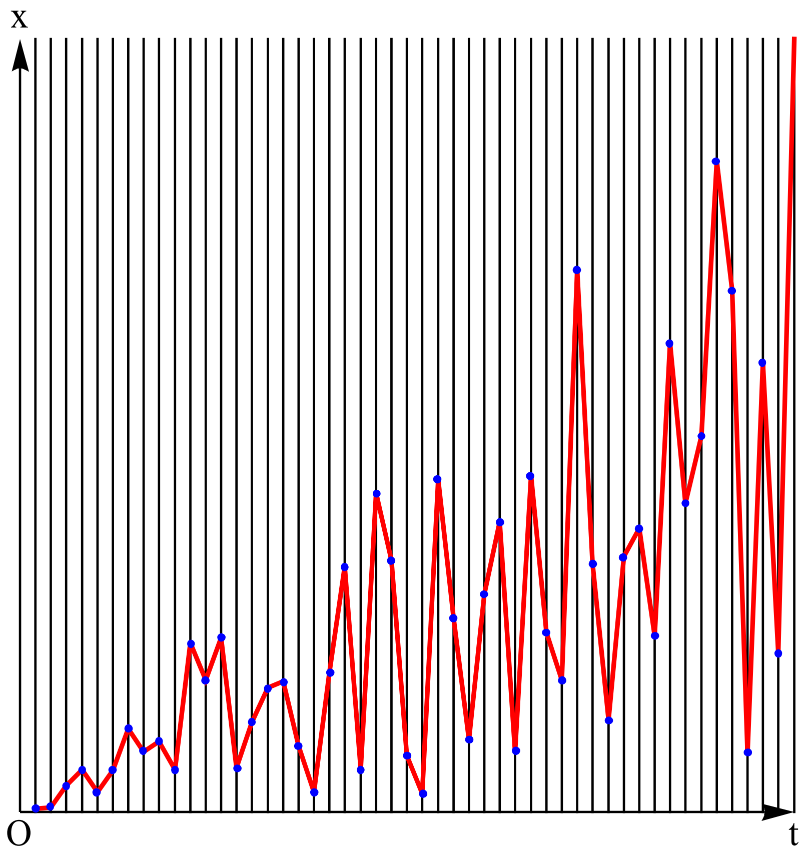
$$K(x,t;x',t') = \lim_{N\to\infty}\int dx_1 \int dx_2 ....\int dx_{N-1} (\frac{m}{2\pi\hbar i\Delta t})^{N/2}$$
$$\times \exp[\frac{i}{\hbar}\Delta t \sum_{i=1}^{N}\{\frac{m}{2}(\frac{x_i - x_{i-1}}{\Delta t})^2 - V(x_{i-1})\}]$$

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). Mathematically, we had better to use

$$\frac{i}{\hbar}\int_{t'}^{t} dt L(x,\dot{x}) = \frac{i}{\hbar}\int_{t'}^{t} dt_1 L(x(t_1), \dot{x}(t_1))$$



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

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

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

Thus we have

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

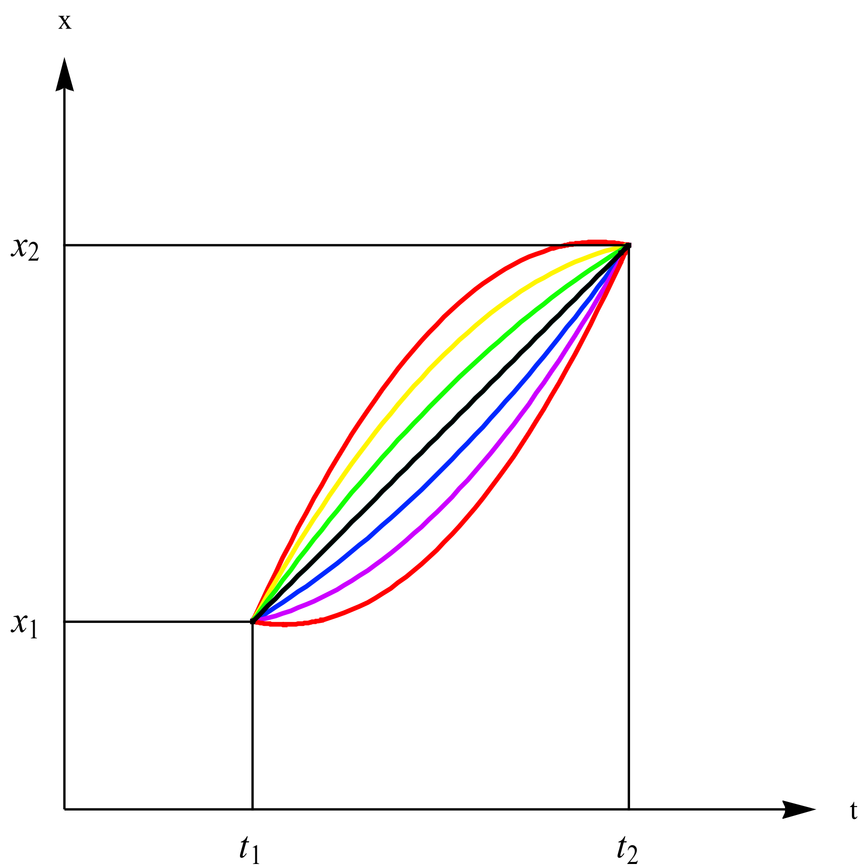
where

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

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

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

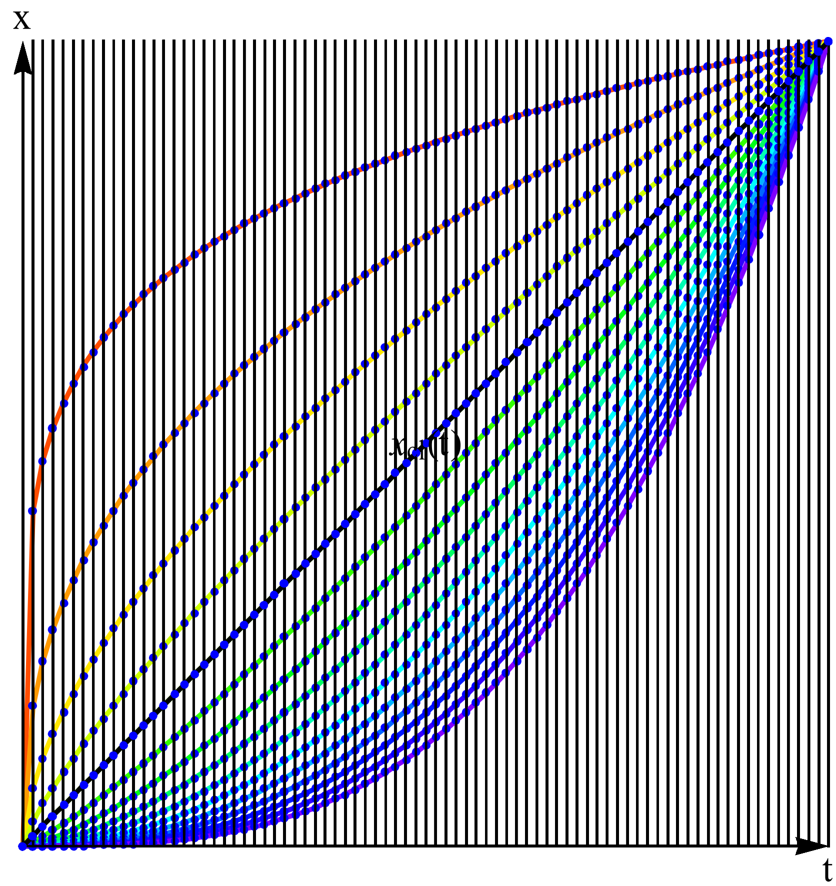


This expression is known as Feynman's path integral (configuration space path integral). $S[x(t)]$ is the value of the action evaluated for a particular path taken by the particle. If one wants to know the quantum mechanical amplitude for a point particle at x', at time t' to reach a position x, at time t, one integrates 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 knows what the initial and final positions are. The trajectory can deviate from the classical trajectory if the difference in the action is roughly within $\hbar$.

((REFERENCE))

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

((**Note**))

We can use the Baker-Campbell-Hausdorff theorem for the derivation of the Feynman path integral. We have a Hamiltonian

$$\hat{H} = \hat{T} + \hat{V}$$

where $\hat{T}$ is the kinetic energy and $\hat{V}(\hat{x})$ is the potential energy. We consider

$$\begin{aligned}\exp(-\frac{i}{\hbar}\hat{H}\Delta t) &= \exp[-\frac{i}{\hbar}(\hat{T}+\hat{V})\Delta t] \\ &= \exp(\hat{P}+\hat{Q})\end{aligned}$$

where

$$\hat{P} = -\frac{i}{\hbar}\hat{T}\Delta t, \qquad \hat{Q} = -\frac{i}{\hbar}\hat{V}\Delta t$$

We use the Baker-Campbell-Hausdorff theorem

$$\exp(\hat{P})\exp(\hat{Q}) = \exp\{\hat{P}+\hat{Q}+\frac{1}{2}[\hat{P},\hat{Q}]+\frac{1}{12}[\hat{P},[\hat{P},\hat{Q}]]-\frac{1}{12}[\hat{Q},[\hat{P},\hat{Q}]]+...\}$$

with

$$[\hat{P},\hat{Q}] = (-\frac{i}{\hbar})^2(\Delta t)^2[\hat{T},\hat{V}]$$

$$[\hat{P},[\hat{P},\hat{Q}]] = (-\frac{i}{\hbar})^3(\Delta t)^3[\hat{T},[\hat{T},\hat{V}]]$$

$$[\hat{Q},[\hat{P},\hat{Q}]] = (-\frac{i}{\hbar})^3(\Delta t)^3[\hat{V},[\hat{T},\hat{V}]]$$

In the limit of $\Delta t \to 0$, we get

$$\begin{aligned}\exp(-\frac{i}{\hbar}\hat{H}\Delta t) &= \exp(\hat{P}+\hat{Q}) \\ &= \exp(\hat{P})\exp(\hat{Q}) \\ &= \exp(-\frac{i}{\hbar}\hat{T}\Delta t)\exp(-\frac{i}{\hbar}\hat{V}\Delta t)\end{aligned}$$

Using this, we get the matrix element

$$\begin{aligned}\left\langle x_j \right| \exp(-\frac{i}{\hbar}\hat{H}\Delta t)\left| x_{j+1} \right\rangle &= \left\langle x_j \right| \exp(-\frac{i}{\hbar}\hat{T}\Delta t)\exp(-\frac{i}{\hbar}\hat{V}\Delta t)\left| x_{j+1} \right\rangle \\ &= \left\langle x_j \right| \exp(-\frac{i\Delta t}{2m\hbar}\hat{p}^2)\left| x_{j+1} \right\rangle \exp(-\frac{i}{\hbar}V(x_{j+1})\Delta t)\end{aligned}$$

or

$$\left\langle x_j \right| \exp(-\frac{i}{\hbar}\hat{H}\Delta t)\left| x_{j+1} \right\rangle = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2} \exp\{\frac{i}{\hbar}[\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{(\Delta t)^2} - V(x_{j+1})]\Delta t)]$$

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,

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

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

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

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

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

....

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

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;
ϵ=Δt

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
h1 = ((x1 - x')^2 + (x2 - x1)^2) // Expand;
```

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

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

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

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

$$\texttt{f2 =} \int_{-\infty}^{\infty} \texttt{g1}\, dx2\ \texttt{// Simplify}\left[\#,\ \texttt{Im}\left[\frac{m}{\epsilon\,\hbar}\right] > 0\right]\ \&$$

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

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

$$\texttt{f3 =} \int_{-\infty}^{\infty} \texttt{g2}\, dx3\ \texttt{// Simplify}\left[\#,\ \texttt{Im}\left[\frac{m}{\epsilon\,\hbar}\right] > 0\right]\ \&$$

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

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

$$\texttt{f4 =} \int_{-\infty}^{\infty} \texttt{g3}\, dx4\ \texttt{// Simplify}\left[\#,\ \texttt{Im}\left[\frac{m}{\epsilon\,\hbar}\right] > 0\right]\ \&$$

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

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). Then 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 extremum 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 time *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,

$$dx_i = dy_i,$$

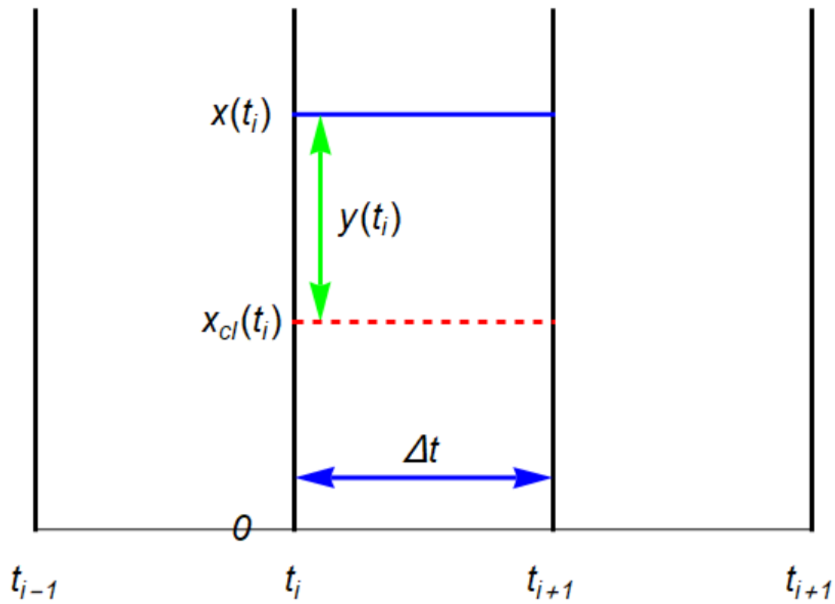


Fig. $x(t_i) = x_{cl}(t_i) + y(t_i)$. $x_{cl}(t_i)$ is constant for $t_i \le t \le t_i + \Delta t = t_{i+1}$, which is independent of the path, while $x(t_i)$ and $y(t_i)$ are also constant for $t_i \le t \le t_i + \Delta t = t_{i+1}$, but depends on the path chosen. So that we have $\mathrm{d}\,x(t_i) = dy(t_i)$ which depends on the choice of path.

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

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

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

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

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

REFERENCES

S.Rajasekar and R. Velusamy, Quantum Mechanics II, Advanced Topics (CRC Press, 2015).

((**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

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

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

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

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

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

$$f = x_1{}^2 + (x_2 - x_1)^2 + (x_3 - x_2)^2 + ... + (x_{N-1} - x_{N-2})^2 + x_{N-1}{}^2$$
$$= 2(x_1{}^2 + x_2{}^2 + ... + x_{N-1}{}^2) - 2(x_1x_2 + x_2x_3 + ... + x_{N-2}x_{N-1})$$

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. Calculation of the average $\langle\psi|\hat{A}|\psi\rangle$

In order to understand the above discussion, for the sake of clarity, we discuss the fundamental mathematics in detail.

6.1 The average $\langle\psi|\hat{A}|\psi\rangle$ under the original basis $\{|b_i\rangle\}$

We consider the two bases {$|b_i\rangle$, $|a_i\rangle$}, where the new basis {$|a_i\rangle$} is related to the original basis {}$|b_i\rangle$ through a unitary operator $\hat{U}$,

$$|a_j\rangle = \hat{U}|b_j\rangle, \qquad |b_j\rangle = \hat{U}^+|a_j\rangle, \qquad \langle b_j| = \langle a_j|\hat{U},$$

with $\hat{U}^+\hat{U} = \hat{1}$. $|a_i\rangle$ is the eigenket of the Hermitian operator $\hat{A}$ with the eigenvalue a_i.

$$\hat{A}|a_i\rangle = a_i|a_i\rangle.$$

Note that

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

or

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

In other word, the matrix element of $\hat{U}$ is independent of the kind of basis (this is very important property). We also note that

$$\langle a_i|\hat{A}|a_j\rangle = \langle b_i|\hat{U}^+\hat{A}\hat{U}|b_j\rangle = a_i\delta_{ij} \qquad \text{(diagonal matrix)}$$

Here we define the Column matrices for the state $|\psi\rangle$ of the system,

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ . \\ . \\ . \\ \beta_n \end{pmatrix} \qquad \boldsymbol{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ . \\ . \\ . \\ \alpha_n \end{pmatrix} \qquad \text{(matrix form)}$$

with

$$\beta_i = \langle b_i | \psi \rangle, \qquad \alpha_i = \langle a_i | \psi \rangle.$$

We now consider the average over the state $|\psi\rangle$ under the original basis $\{|b_i\rangle\}$.

$$\begin{aligned}
\langle A \rangle &= \langle \psi | \hat{A} | \psi \rangle \\
&= \sum_{i,j} \langle \psi | b_i \rangle \langle b_i | \hat{A} | b_j \rangle \langle b_i | \psi \rangle \\
&= \sum_{i,j} \langle b_i | \psi \rangle^* \langle b_i | \hat{A} | b_j \rangle \langle b_i | \psi \rangle \\
&= \sum_{i,j} \beta_i^* A_{ij} \beta_i \\
&= \begin{pmatrix} \beta_1^* & \beta_2^* & . & . & . & \beta_n^* \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & . & . & . & A_{1n} \\ A_{21} & A_{22} & . & . & . & A_n \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ A_{n1} & A_{n2} & . & . & . & A_{nn} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ . \\ . \\ . \\ \beta_n \end{pmatrix} \\
&= \boldsymbol{\beta}^+ \mathbf{A} \boldsymbol{\beta}
\end{aligned}$$

(matrix form), using the closure relation. The relation between $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$ is obtained as follow.

$$\begin{aligned}
\alpha_i &= \langle a_i | \psi \rangle \\
&= \sum_j \langle a_i | b_j \rangle \langle b_j | \psi \rangle \\
&= \sum_j \langle a_i | b_j \rangle \beta_j \\
&= \sum_j \langle b_i | \hat{U}^+ | b_j \rangle \beta_j
\end{aligned}$$

or

$$\boldsymbol{\alpha} = \mathbf{U}^+ \boldsymbol{\beta} \qquad \text{(matrix form)}$$

since $\langle a_i | = \langle b_i | \hat{U}^+$.

6.2 The average $\langle \psi | \hat{A} | \psi \rangle$ under the new basis $\{| a_i \rangle\}$

Next, we now consider the average under the new basis $\{| a_i \rangle\}$.

$$\begin{aligned}
\langle A \rangle &= \langle \psi | \hat{A} | \psi \rangle \\
&= \sum_{i,j} \langle \psi | a_i \rangle \langle a_i | \hat{A} | a_j \rangle \langle a_j | \psi \rangle \\
&= \sum_{i,j} \langle a_i | \psi \rangle^* \langle a_i | \hat{A} | a_j \rangle \langle a_j | \psi \rangle \\
&= \sum_{i,j} \alpha_i^* a_i \delta_{ij} \alpha_i \\
&= \begin{pmatrix} \alpha_1^* & \alpha_2^* & . & . & . & \alpha_n^* \end{pmatrix} \begin{pmatrix} a_1 & 0 & . & . & . & 0 \\ 0 & a_2 & . & . & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & 0 & . & . & . & a_n \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ . \\ . \\ . \\ \alpha_n \end{pmatrix} \\
&= \sum_{i,j} a_i |\alpha_i|^2
\end{aligned}$$

6.3 The calculation of the average using Mathematica

(i) Find eigenvalue and eigenkets of matrix ***A*** by using Mathematica

Eigensystem[**A**]

which leads to the eigenvalues a_i and eigenkets, $\left|a_i\right\rangle$. The eigenkets ahould be normalized using the program **Normalize**. When the system is degenerate (the same eigenvalues but different states), further we need to use the program Orthogonize for all eigenkets obtained by doing the process of Eigensystem[**A**]

(ii) Determine the unitary matrix ***U***

Unitary matrix ***U*** is defined as

$$\mathbf{U} = \begin{pmatrix} \langle b_1|a_1\rangle & \langle b_1|a_2\rangle & . & . & . & \langle b_1|a_n\rangle \\ \langle b_2|a_1\rangle & \langle b_2|a_2\rangle & . & . & . & \langle b_2|a_n\rangle \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ \langle b_n|a_1\rangle & \langle b_n|a_2\rangle & . & . & . & \langle b_n|a_n\rangle \end{pmatrix}$$
$$= \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & . & . & . & \mathbf{u}_n \end{pmatrix}$$

where

$$\mathbf{u}_i = \begin{pmatrix} \langle b_1|a_i\rangle \\ \langle b_2|a_i\rangle \\ \langle b_3|a_i\rangle \\ . \\ . \\ \langle b_n|a_i\rangle \end{pmatrix} \qquad \text{(matrix form of eigenkets)}$$

Thus, we have

$$\boldsymbol{\alpha} = \mathbf{U}^{+}\boldsymbol{\beta}, \qquad \boldsymbol{\beta} = \mathbf{U}\boldsymbol{\alpha} \qquad \text{(matrix form)}$$

where

$$\mathbf{U} = \left(\mathbf{u}_1 \ \mathbf{u}_2 ......\mathbf{u}_n \ \right)$$

and

$$\mathbf{U}^{+} = \begin{pmatrix} \mathbf{u}_1^{\ *} \\ \mathbf{u}_2^{\ *} \\ . \\ . \\ . \\ \mathbf{u}_n^{\ *} \end{pmatrix}$$

Note that

$$\boldsymbol{\beta}^{+}\mathbf{A}\boldsymbol{\beta} = (\boldsymbol{\alpha}^{+}\hat{\mathbf{U}}^{+}\mathbf{A}\mathbf{U}\boldsymbol{\alpha}) = (\boldsymbol{\alpha}^{+}\tilde{\mathbf{A}}\boldsymbol{\alpha})$$

where

$$\hat{\mathbf{U}}^{+}\mathbf{A}\mathbf{U} = \begin{pmatrix} a_1 & 0 & . & . & . & 0 \\ 0 & a_2 & . & . & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & 0 & . & . & . & a_n \end{pmatrix} \qquad \text{(diagonal matrix)}$$

6.4 Example-1 (3x3 matrix)

Here we discuss a typical example, ***A*** is 3x3 matrix.

$$
\begin{aligned}
f &= 2(\beta_1^2 + \beta_2^2 + \beta_3^2 - \beta_1\beta_2 - \beta_2\beta_3 - \beta_3\beta_1) \\
&= \boldsymbol{\beta}^+ \mathbf{A} \boldsymbol{\beta} \\
&= \begin{pmatrix} \beta_1^* & \beta_2^* & \beta_3^* \end{pmatrix} \mathbf{A} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} \\
&= \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 \end{pmatrix} \mathbf{A} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}
\end{aligned}
$$

Where β_1, β_2, and β_3 are real,

$$
\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}, \qquad \boldsymbol{\beta}^+ = \begin{pmatrix} \beta_1^* & \beta_2^* & \beta_3^* \end{pmatrix} = \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 \end{pmatrix} = \boldsymbol{\beta}^T ,
$$

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

Eigenvalue problem of matrix $\boldsymbol{A}$ (we solve the problem using **Mathematica. The system is degenerate**)

$$
\mathbf{A}\phi_1 = a_1\phi_1 , \qquad \mathbf{A}\phi_2 = a_2\phi_2 , \qquad \mathbf{A}\phi_3 = a_3\phi_3 .
$$

where the eigenvalues and eigenkets are as follows,

$$
a_1 = 3, \qquad \phi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},
$$

$$a_2 = 3, \qquad \phi_2 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix},$$

$$a_3 = 0, \qquad \phi_3 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

under the basis $\{|b_i\rangle\}$. The unitary matrix can be obtained as

$$\mathbf{U} = \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix}, \qquad \mathbf{U}^+ = \begin{pmatrix} \phi_1^+ \\ \phi_2^+ \\ \phi_3^+ \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix}$$

$$\mathbf{U}^+\mathbf{U} = 1, \qquad \mathbf{U}^+\mathbf{A}\mathbf{U} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} = \mathbf{U}\boldsymbol{\alpha} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix}\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}\alpha_1 + \frac{1}{\sqrt{6}}\alpha_2 + \frac{1}{\sqrt{3}}\alpha_3 \\ -\frac{2}{\sqrt{6}}\alpha_2 + \frac{1}{\sqrt{3}}\alpha_3 \\ -\frac{1}{\sqrt{2}}\alpha_1 + \frac{1}{\sqrt{6}}\alpha_2 + \frac{1}{\sqrt{3}}\alpha_3 \end{pmatrix}$$

Thus, we have

$$
\begin{aligned}
f &= \boldsymbol{\beta}^{+}\mathbf{A}\boldsymbol{\beta} \\
&= \boldsymbol{\alpha}^{+}(\mathbf{U}^{+}\mathbf{A}\mathbf{U})\boldsymbol{\alpha} \\
&= \begin{pmatrix} \alpha_1^* & \alpha_2^* & \alpha_3^* \end{pmatrix} \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} \\
&= a_1 |\alpha_1|^2 + a_2 |\alpha_2|^2 + a_3 |\alpha_3|^2 \\
&= 3\alpha_1^{\ 2} + 3\alpha_2^{\ 2} + 0\alpha_3^{\ 2}
\end{aligned}
$$

6.5 Example-2 4x4 matrix

We also discuu the second example; ***A*** is 4x4 matrix.

$$
\begin{aligned}
f &= \beta_1^{\ 2} + 2\beta_2^{\ 2} + 2\beta_3^{\ 2} + \beta_4^{\ 2} - 2\beta_1\beta_2 - 2\beta_2\beta_3 - 2\beta_3\beta_1 \\
&= \boldsymbol{\beta}^{+}\mathbf{A}\boldsymbol{\beta} \\
&= \begin{pmatrix} \beta_1^* & \beta_2^* & \beta_3^* & \beta_4^* \end{pmatrix} \mathbf{A} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix} \\
&= \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 & \beta_4 \end{pmatrix} \mathbf{A} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix}
\end{aligned}
$$

Where β_1, β_2, β_3 and β_4 are real,

$$
\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix} \qquad \boldsymbol{\beta}^{+} = \begin{pmatrix} \beta_1^* & \beta_2^* & \beta_3^* & \beta_4^* \end{pmatrix} = \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 & \beta_4 \end{pmatrix} = \boldsymbol{\beta}^{T}
$$

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

Eigenvalue problem of matrix **A** (using **Mathematica**)

$$\mathbf{A}\phi_1 = a_1\phi_1, \qquad \mathbf{A}\phi_2 = a_2\phi_2,$$

$$\mathbf{A}\phi_3 = a_3\phi_3, \qquad \mathbf{A}\phi_4 = a_4\phi_4$$

The eigenvalues and eigenkets are obtained as follows,

$$a_1 = 2 + \sqrt{2}, \qquad \phi_1 = \begin{pmatrix} \frac{1}{2\sqrt{2+\sqrt{2}}} \\ -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} \\ \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} \\ -\frac{1}{2\sqrt{2+\sqrt{2}}} \end{pmatrix},$$

$$a_2 = 2, \qquad \phi_2 = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \end{pmatrix},$$

$$a_3 = 2-\sqrt{2}, \qquad \phi_3 = \begin{pmatrix} \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} \\ \frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} \\ -\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} \\ -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} \end{pmatrix}.$$

$$a_4 = 0, \qquad \phi_4 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}.$$

The unitary matrix:

$$\begin{aligned} \mathbf{U} &= \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 & \phi_4 \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2\sqrt{2+\sqrt{2}}} & \frac{1}{2} & \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & -\frac{1}{2} & \frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & -\frac{1}{2} & -\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ -\frac{1}{2\sqrt{2+\sqrt{2}}} & \frac{1}{2} & -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & \frac{1}{2} \end{pmatrix}, \end{aligned}$$

$$\mathbf{U}^{+} = \begin{pmatrix} \phi_1^{+} \\ \phi_2^{+} \\ \phi_3^{+} \\ \phi_4^{+} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2\sqrt{2+\sqrt{2}}} & -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & -\frac{1}{2\sqrt{2+\sqrt{2}}} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & \frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} & -\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} & -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

$$\mathbf{U}^{+}\mathbf{U} = 1, \qquad \mathbf{U}^{+}\mathbf{A}\mathbf{U} = \begin{pmatrix} 2+\sqrt{2} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2-\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix} = \mathbf{U}\boldsymbol{\alpha} = \begin{pmatrix} \frac{1}{2\sqrt{2+\sqrt{2}}} & \frac{1}{2} & \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & -\frac{1}{2} & \frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & -\frac{1}{2} & -\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ -\frac{1}{2\sqrt{2+\sqrt{2}}} & \frac{1}{2} & -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix},$$

or

$$\begin{pmatrix}\beta_1\\ \beta_2\\ \beta_3\\ \beta_4\end{pmatrix}=\begin{pmatrix}\frac{1}{2\sqrt{2+\sqrt{2}}}\alpha_1+\frac{1}{2}\alpha_2+\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}}\alpha_3+\frac{1}{2}\alpha_4\\ -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}}\alpha_1-\frac{1}{2}\alpha_2+\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}}\alpha_3+\frac{1}{2}\alpha_4\\ \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}}\alpha_1-\frac{1}{2}\alpha_2-\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}}\alpha_3+\frac{1}{2}\alpha_4\\ -\frac{1}{2\sqrt{2+\sqrt{2}}}\alpha_1+\frac{1}{2}\alpha_2-\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}}\alpha_3+\frac{1}{2}\alpha_4\end{pmatrix}.$$

Thus, we have

$$\begin{aligned}f &= \boldsymbol{\beta}^{+}\mathbf{A}\boldsymbol{\beta}\\ &= \boldsymbol{\alpha}^{+}(\mathbf{U}^{+}\mathbf{A}\mathbf{U})\boldsymbol{\alpha}\\ &= \begin{pmatrix}\alpha_1^{*} & \alpha_2^{*} & \alpha_3^{*} & \alpha_4^{*}\end{pmatrix}\begin{pmatrix}2+\sqrt{2} & 0 & 0 & 0\\ 0 & 2 & 0 & 0\\ 0 & 0 & 2-\sqrt{2} & 0\\ 0 & 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\\ \alpha_4\end{pmatrix}\\ &= a_1|\alpha_1|^2+a_2|\alpha_2|^2+a_3|\alpha_3|^2+a_4|\alpha_4|^2\\ &= (2+\sqrt{2})\alpha_1^{\,2}+2\alpha_2^{\,2}+(2-\sqrt{2})\alpha_3^{\,2}+0\alpha_4^{\,2}\end{aligned}$$

7. Equivalence with Schrödinger 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

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

or

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

in the $|x\rangle$ representation.

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

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

or

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

where

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

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

8. 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

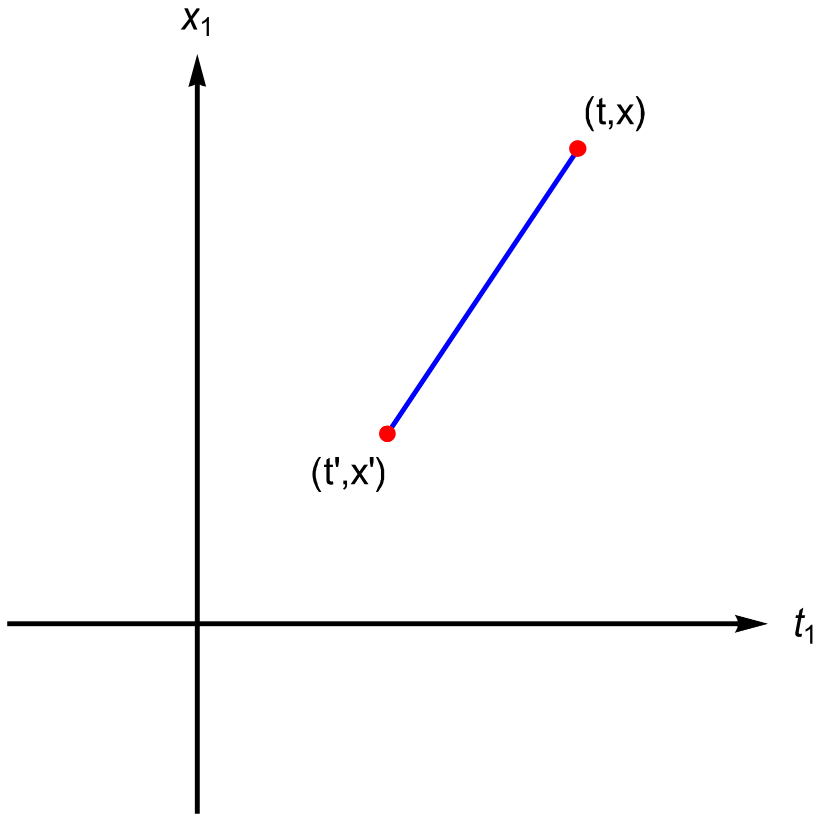
$$\dot{x} = a ,$$

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

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

((**Mathematics**))

Feynman path integral for free particle

```
Clear["Global`"];
x[t_] := +A1 t + B1;
s1 = x[ti] - xi == 0;
s2 = x[tf] - xf == 0;
```

```
s3 = Solve[{s1, s2}, {A1, B1}]
```

$$\left\{\left\{A1 \to -\frac{-xf + xi}{tf - ti},\ B1 \to -\frac{ti\ xf - tf\ xi}{tf - ti}\right\}\right\}$$

```
x1 = x[t1] /. s3[[1]] // FullSimplify
```

$$\frac{t1\ xf - ti\ xf - t1\ xi + tf\ xi}{tf - ti}$$

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

$$\frac{xf - xi}{tf - ti}$$

Lagrangian

```
L1 = (1/2 m (D[x1, t1])^2) // FullSimplify
```

$$\frac{m\,(xf - xi)^2}{2\,(tf - ti)^2}$$

Action S

```
s1 = Integrate[L1, {t1, ti, tf}] //
  FullSimplify
```

$$\frac{m\,(xf - xi)^2}{2\,(tf - ti)}$$

```
s2 =
 s1 //. {tf → (T + ti), xf → xi + X, xi → 0} //
  FullSimplify
```

$$\frac{m\,X^2}{2\,T}$$

((**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 $\dfrac{S}{\hbar}$ (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
```

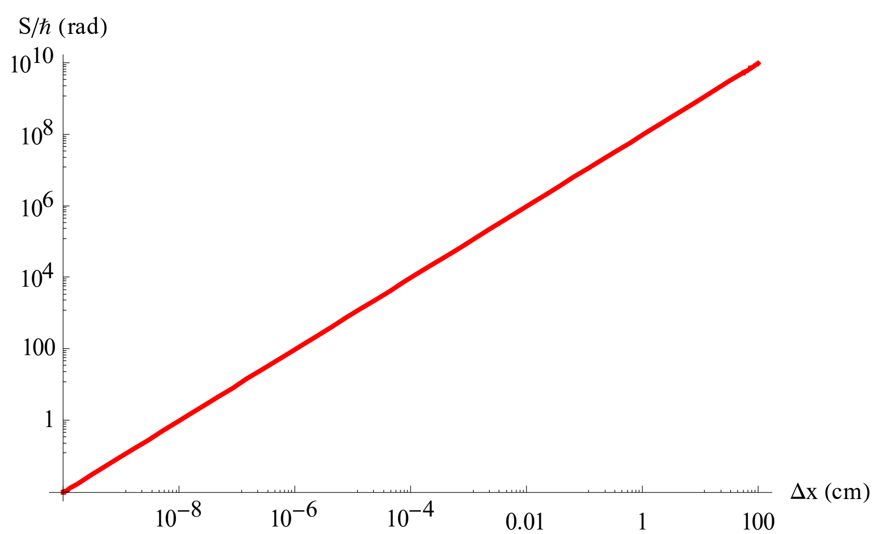
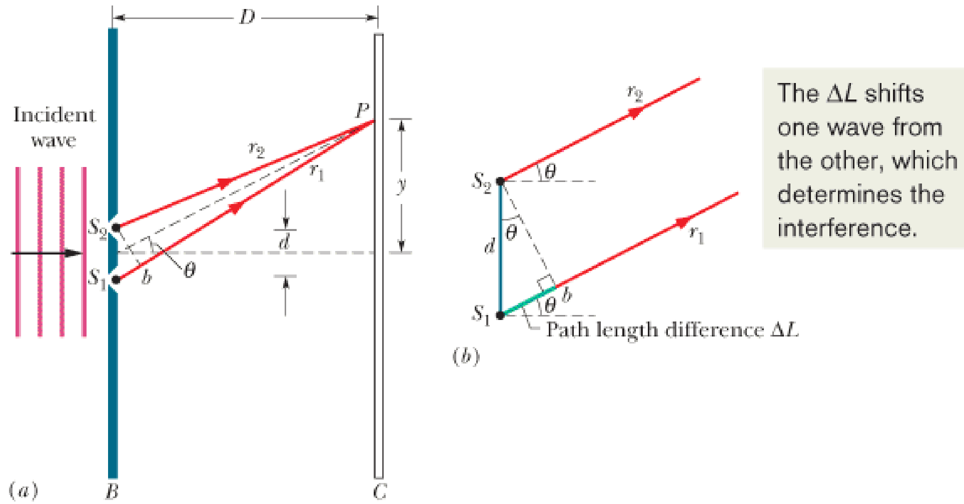


Fig. $\dfrac{S}{\hbar}$ (radian) as a function of Δx (cm), where $v = c/137$. m is the mass of electron.

9. 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 $\dfrac{\Delta S}{\hbar}$ 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

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

10. What is the Lagrangian for photon?

((**Landau-Lifshitz**))

For a particle, we have the Hamilton equations

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{r}}, \qquad \boldsymbol{v} = \dot{\boldsymbol{r}} = \frac{\partial H}{\partial \boldsymbol{p}}$$

In view of the analogy, we can immediately write the corresponding equation for rays:

$$\dot{\boldsymbol{k}} = -\frac{\partial \omega}{\partial \boldsymbol{r}}, \qquad \boldsymbol{v} = \dot{\boldsymbol{r}} = \frac{\partial \omega}{\partial \boldsymbol{k}}$$

In vacuum, $\omega = ck$, so that $\dot{\boldsymbol{k}} = 0$, $\boldsymbol{v} = c\boldsymbol{n}$ ($\boldsymbol{n}$ is a unit vector along the direction of propagation); in other words, in vacuum the rays are straight lines, along which the light travels with velocity *c*.

Pursuing the analogy, we can establish for geometrical optics a principle analogous to the principle of least action in mechanics. However, it cannot be written in Hamiltonian form as $\delta \int L dt = 0$, since it turns out to be impossible to introduce, for rays, a function analogous to the Lagrangian of a particle. Since the Lagrangian of a particle is related to the Hamiltonian H by the equation

$$L = \boldsymbol{p} \cdot \frac{\partial H}{\partial \boldsymbol{p}} - H,$$

replacing the Hamiltonian H by the angular frequency ω and the momentum by the wave vector $\boldsymbol{k}$, we should have to write for the Lagrangian in optics, $\boldsymbol{k} \cdot \frac{\partial \omega}{\partial \boldsymbol{k}} - \omega$. But this expression is equal to zero, since $\omega = ck$.But this expression is also clear directly from the consideration that the propagation of rays is analogous to the motion of particles with zero mass.

As is well, in the case where the energy is constant, the principle of least action for particles can also be written in the form of the so-called principle of Maupertuis:

$$\delta S = \delta \int \boldsymbol{p} \cdot d\boldsymbol{l} = 0$$

where the integration extends over the trajectory of the particle between two of its points. In this expression the momentum is assumed to be a function of the energy and the coordinates. The analogous principle for rays is called Fermat's principle. In this case, we can write by analogy:

$$\delta \psi = \int \boldsymbol{k} \cdot d\boldsymbol{l} = 0$$

In vacuum, $\boldsymbol{k} = \frac{\omega}{c} \boldsymbol{n}$, and we obtain ($d\boldsymbol{l} \cdot \boldsymbol{n} = dl$:

$$\delta \int dl = 0$$

which corresponds to rectilinear propagation of the rays.

((**REFERENCE**))

L.D. Landau and E.M. Lifshitz, The Classical Theory of Fields (Pergamon, 1996).

((**Note**))

From a view-point of the phaser diagram for the interference, photons are one of the best examples. I will use this example for the explanation of photon propagator. It seems to me that theorists hesitate to use the word of photon. Why is that? It is hard to find the expression of the action S for photon, even if the path integral is expressed by $\exp(\frac{i}{\hbar}px)$; plane-wave form. The Lagrangian form of photon is not simple compared to that of particle (such as electron).

11. Single slit experiment

In order to understand the path integral method, let us go back to the Young's double slit experiment. We obtain an interference pattern, independent of whether we use a light source, or particle (electron) source. This can, of course, be explained by saying that there is a probability amplitude associated with each path. Note that a path integral approach offers a road to quantum mechanics for systems that are not readily accessible via Hamiltonian mechanics (Merzbacher, 1998). In his book, Feynman discussed the principle of least action for particles (Feynman, 1964).

Is it possible to say intuitively that

$$L = T = cp,$$

where T is the kinetic energy of photon, c is the velocity of light, and p is the momentum.? The momentum p is expressed by

$$p = \hbar k = \frac{2\pi\hbar}{\lambda},$$

where λ is the wave length of photon. Then the action S can be evaluated as

$$S = \int L dt = \int cp dt = cp\Delta t = p\Delta x$$

where p is assumed to be constant and $\Delta x = c\Delta t$. Then we have

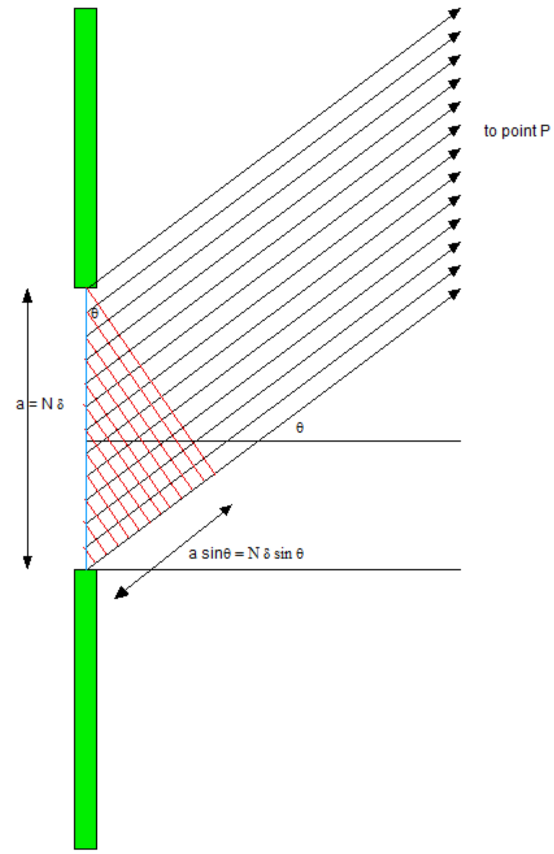
$$\exp(\frac{i}{\hbar}S) = \exp(\frac{i}{\hbar}px) = \exp(ikx)$$

The phase of change in wave function for photon is

$$\Delta\phi = k\Delta x$$

where k is the wave number.

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

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

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

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

((**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

$$k(r_2 - r_1) = \varphi = k\delta \sin\theta = k(\frac{a}{N}\sin\theta)$$

$$k(r_3 - r_2) = \varphi$$

$$k(r_4 - r_3) = \varphi$$

$$-----------------------$$

$$k(r_N - r_{N-1}) = \varphi$$

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

$$k(r_2 - r_1) = \varphi$$

$$k(r_3 - r_1) = 2\varphi$$

$$k(r_4 - r_1) = 3\varphi$$

$$-----------------------$$

$$(r_N - r_1) = (N-1)\varphi$$

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 $N\rightarrow\infty$, where

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

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

$$I_m = I_0N^2 = \frac{c\varepsilon_0}{2}[NE_0(r)]^2 = \frac{c\varepsilon_0}{2}E_0{}^2$$

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

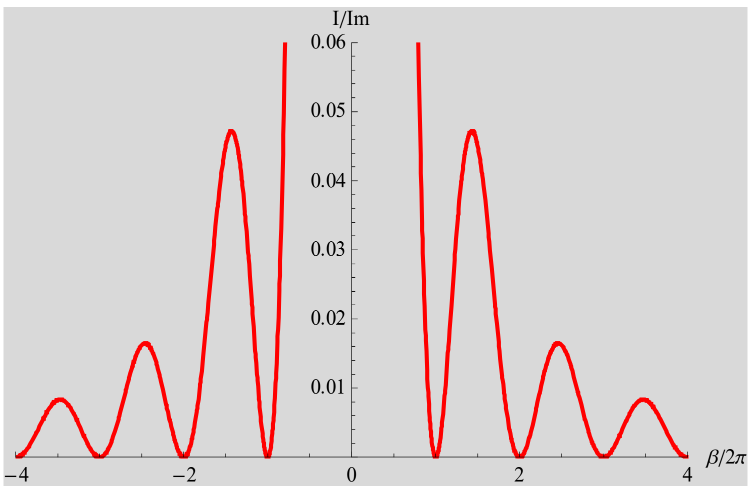
$$\varphi = k\delta\sin\theta$$

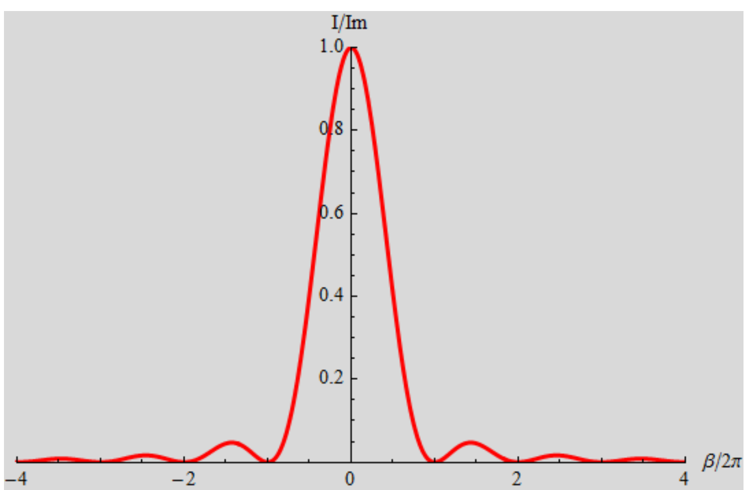
where $a = N\delta$. We make a plot of the relative intensity I/I_m as a function of β.

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

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 occurs in directions in direction θ_m such that

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

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

12. Phasor diagram

(i) The system with two paths

The phasor diagram can be used for the calculation of the double slilts (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).

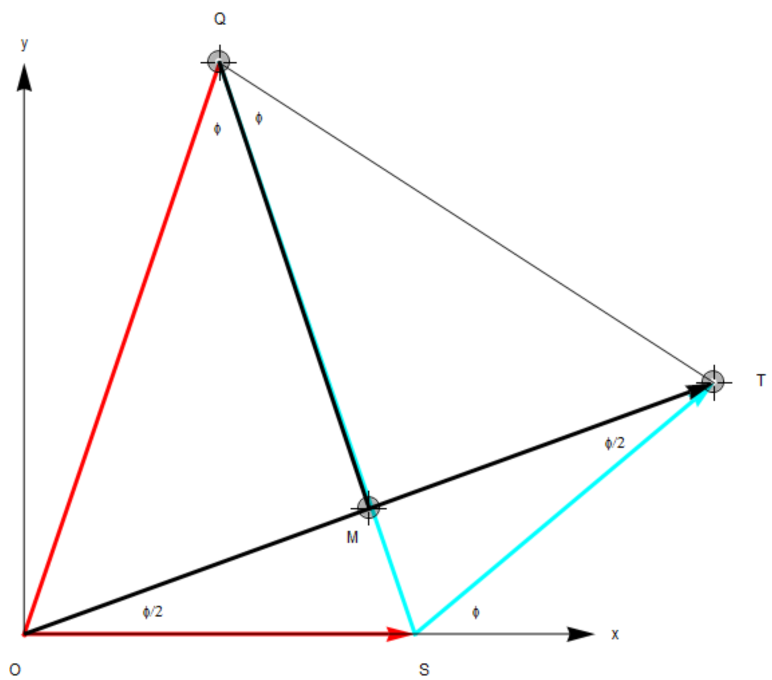


Fig. Phasor diagram for the double slit.

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 $(\overline{OT})^2$,

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

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.

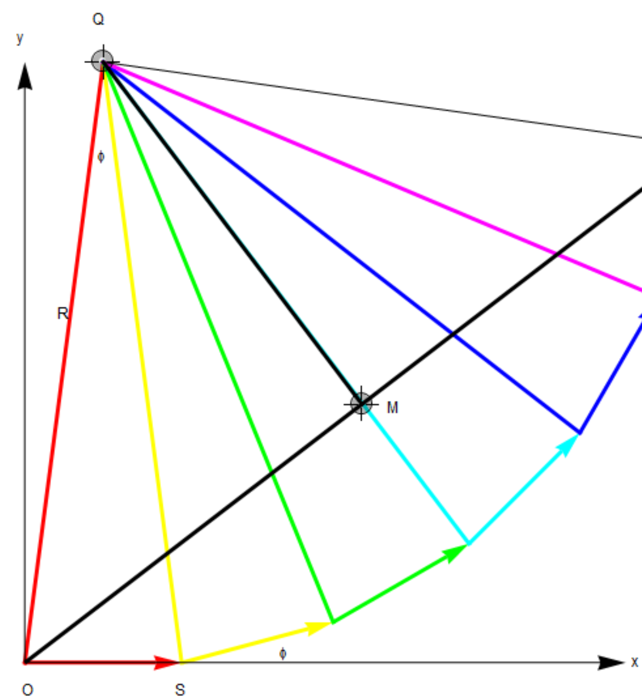


Fig. The resultant amplitude of N = 6 equally spaced sources with net successive phase difference φ. $\beta = N\,\varphi = 6\,\varphi$.

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

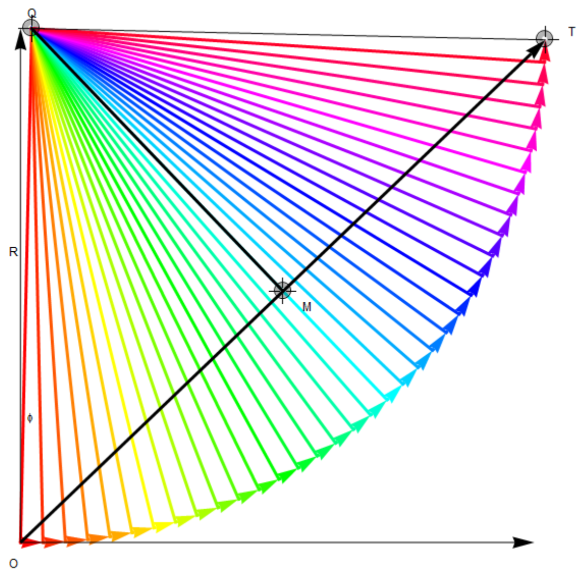
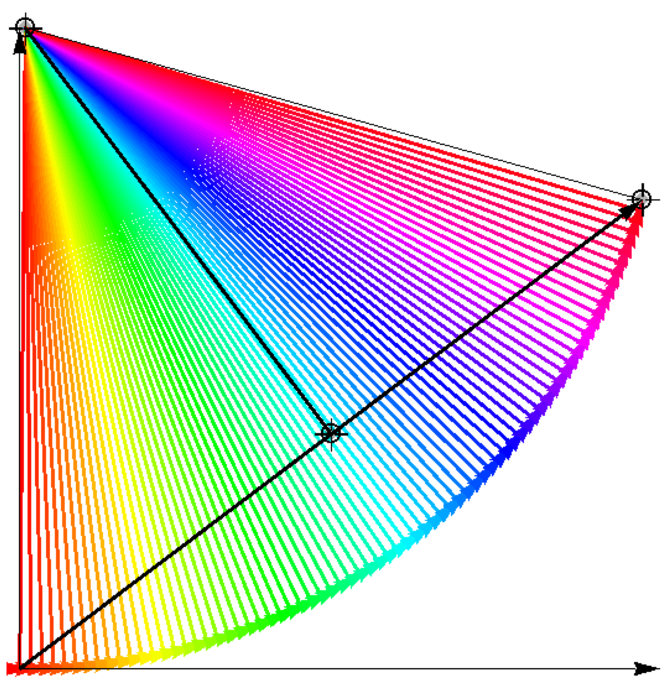


Fig. The resultant amplitude of N = 36 equally spaced sources with net successive phase difference φ.

(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.

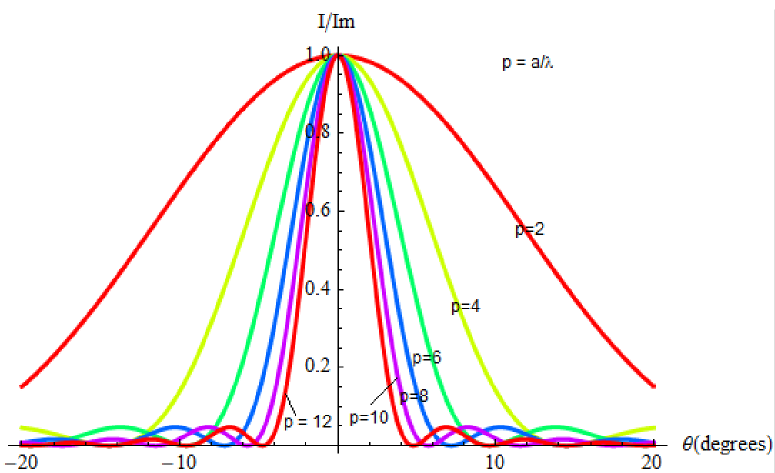


Fig. The relative intensity in single-slit diffraction for various values of the ratio $p = a/\lambda$. The wider the slit is the narrower is the central diffraction maximum.

13. Gravity: Feynman path integral

((**Calculation from the classical limit**))

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

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

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

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

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

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

((**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
```

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

14. Simple harmonics: Feynman path integral

((Classical limit))

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

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

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

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

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

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

The Hamilton's principle function is

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

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

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 $t-t'\to 0$, 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 $t-t'\to 0$, *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

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

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

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

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

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
```

$\frac{1}{2}$ m ω0 $\left(-2\ x\ x0 + \left(x^2 + x0^2\right)\ \mathrm{Cos}[(t - t0)\ \omega0]\right)$ 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

$$\psi(\xi,t)=\int_{-\infty}^{\infty}K(\xi,t;\xi',0)\psi(\xi',0)d\xi'$$

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

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

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

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

or

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

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

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]};
```

$$\texttt{KSH}[\xi\_,\ t\_,\ \xi 1\_] := \sqrt{\frac{1}{2\pi\, i\, \texttt{Sin}[\omega 0\ t]}}\ \texttt{Exp}\left[\frac{i}{2\ \texttt{Sin}[\omega 0\ t]}\left(\left(\xi^2 + \xi 1^2\right)\texttt{Cos}[\omega 0\ t] - 2\,\xi\,\xi 1\right)\right];$$

$$\varphi 0[\xi\_] := \pi^{-1/4}\ \texttt{Exp}\left[-\frac{(\xi - \xi 0)^2}{2}\right];$$

$$\texttt{f1} = \int_{-\infty}^{\infty} \texttt{KSH}[\xi,\ t,\ \xi 1]\ \varphi 0[\xi 1]\, d\xi 1\ \texttt{// FullSimplify[\#, \{Im[Cot[t }\omega 0\texttt{]] > -1, }\omega 0\, t > 0\texttt{\}] \&}$$

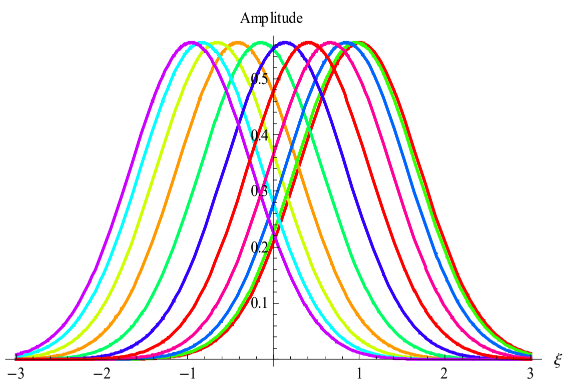
$$\frac{e^{-\frac{\left(\xi^2+\xi 0^2\right)\mathrm{Cot}[t\,\omega 0]+i\,\xi\,(\xi+2\,i\,\xi 0\,\mathrm{Csc}[t\,\omega 0])}{2\,(i+\mathrm{Cot}[t\,\omega 0])}}\sqrt{-i\,\mathrm{Csc}[t\,\omega 0]}}{\pi^{1/4}\sqrt{1 - i\,\mathrm{Cot}[t\,\omega 0]}}$$

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

$$\frac{e^{-(\xi - \xi 0\,\mathrm{Cos}[t\,\omega 0])^2}}{\sqrt{\pi}}$$

```
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"}]
```



15. 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

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

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

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 dimensions.

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

We now consider the wave function:

$$\langle x|\psi(t=0)\rangle = \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}} \exp(ik_0 x - \frac{x^2}{4\sigma_x{}^2}).$$

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

$$\begin{aligned}
\langle k|\psi(t=0)\rangle &= \int dx \langle k|x\rangle\langle x|\psi(t=0)\rangle \\
&= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}} \frac{1}{\sqrt{2\pi}} \int dx \exp(-ikx)\exp(ik_0 x - \frac{x^2}{4\sigma_x{}^2}) \\
&= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}} \frac{1}{\sqrt{2\pi}} 2\sigma_x\sqrt{\pi} \exp[-\sigma_x{}^2(k-k_0)^2] \\
&= \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\sigma_x} \exp[-\sigma_x{}^2(k-k_0)^2]
\end{aligned}$$

or

$$\begin{aligned}
|\langle k|\psi(t=0)\rangle|^2 &= \sqrt{\frac{2}{\pi}}\sigma_x \exp[-2\sigma_x{}^2(k-k_0)^2] \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\left(\frac{1}{2\sigma_x}\right)} \exp[-\frac{(k-k_0)^2}{2\left(\frac{1}{2\sigma_x}\right)^2}]. \\
&= \frac{1}{\sqrt{2\pi}\sigma_k} \exp[-\frac{(k-k_0)^2}{2\sigma_k{}^2}]
\end{aligned}$$

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

Then we get the wave function at time t,

$$
\begin{aligned}
\langle x|\psi(t)\rangle &= \int dx' K(x,t;x',0)\langle x'|\psi(0)\rangle \\
&= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}} \sqrt{\frac{m}{2\pi i\hbar t}} \int dx' \exp[ik_0 x' - \frac{x'^2}{4\sigma_x^{\ 2}} + \frac{im(x-x')^2}{2\hbar t}] \\
&= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}} \sqrt{\frac{m}{2\pi i\hbar t}} 2\sqrt{\pi} \frac{1}{\sqrt{\frac{1}{\sigma_x^{\ 2}} - \frac{2im}{t\hbar}}} \exp[-\frac{mx(x-4ik_0\sigma_x^{\ 2}) + 2ik_0^{\ 2} t\hbar\sigma_x^{\ 2}}{4m\sigma_x^{\ 2} + 2it\hbar}] \\
&= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}} \frac{1}{\sqrt{1 + \frac{it\hbar}{2m\sigma_x^{\ 2}}}} \exp[-\frac{x(x-4ik_0\sigma_x^{\ 2}) + 2ik_0^{\ 2}\frac{t\hbar}{m}\sigma_x^{\ 2}}{4\sigma_x^{\ 2}(1 + \frac{it\hbar}{2m\sigma_x^{\ 2}})}] \\
&= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}} \frac{1}{\sqrt{1 + \frac{it\hbar}{2m\sigma_x^{\ 2}}}} \exp[-\frac{\{x(x-4ik_0\sigma_x^{\ 2}) + 2ik_0^{\ 2}\frac{t\hbar}{m}\sigma_x^{\ 2}\}(1 - \frac{it\hbar}{2m\sigma_x^{\ 2}})}{4\sigma_x^{\ 2}(1 + \frac{it\hbar}{2m\sigma_x^{\ 2}})(1 - \frac{it\hbar}{2m\sigma_x^{\ 2}})}] \\
&= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x}} \frac{1}{\sqrt{1 + \frac{it\hbar}{2m\sigma_x^{\ 2}}}} \exp[-\frac{(x - \frac{\hbar k_0 t}{m})^2}{4\sigma_x^{\ 2}(1 + \frac{t^2\hbar^2}{4m^2\sigma_x^{\ 4}})} - i\frac{m(8k_0 mx\sigma_x^{\ 4} + t(x^2 - 4k_0^{\ 2}\sigma_x^{\ 4})\hbar)}{8m^2\sigma_x^{\ 4}(1 + \frac{t^2\hbar^2}{4m^2\sigma_x^{\ 4}})}]
\end{aligned}
$$

Since

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

the probability is obtained as

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

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:

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

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

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

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

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

where

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

Therefore

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

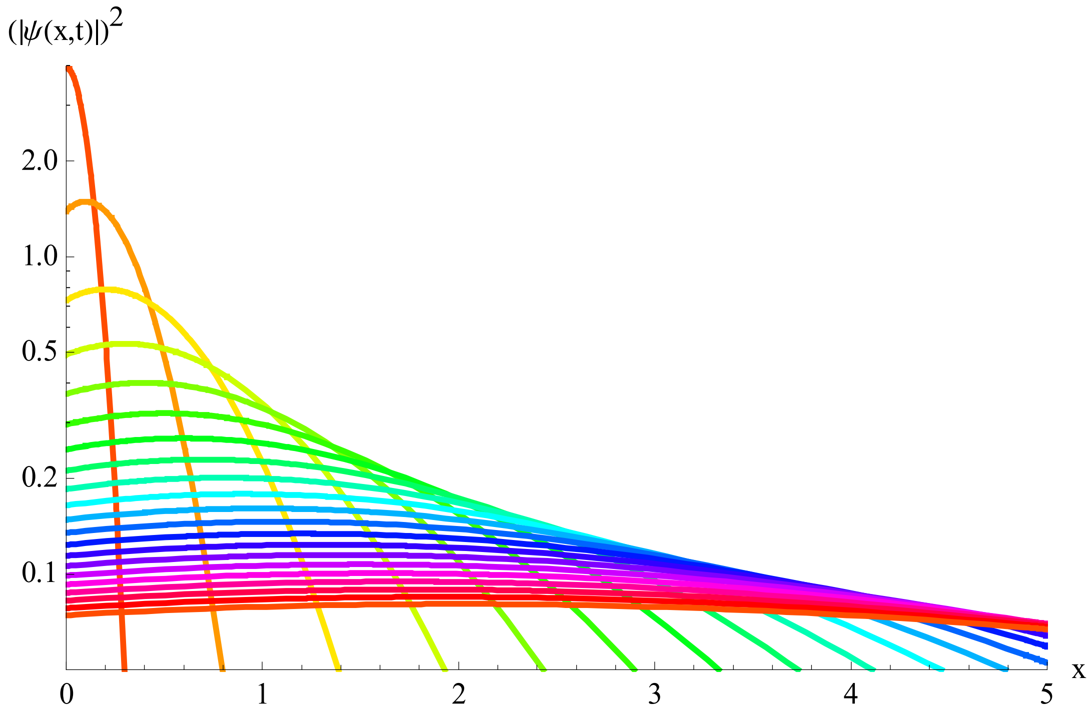


Fig. Plot of $|\langle x|\psi(t)\rangle|^2$ as a function of x where the time t is changed as a parameter.

In summary, we have

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

and

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

16. 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

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

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.

17. Mathematica

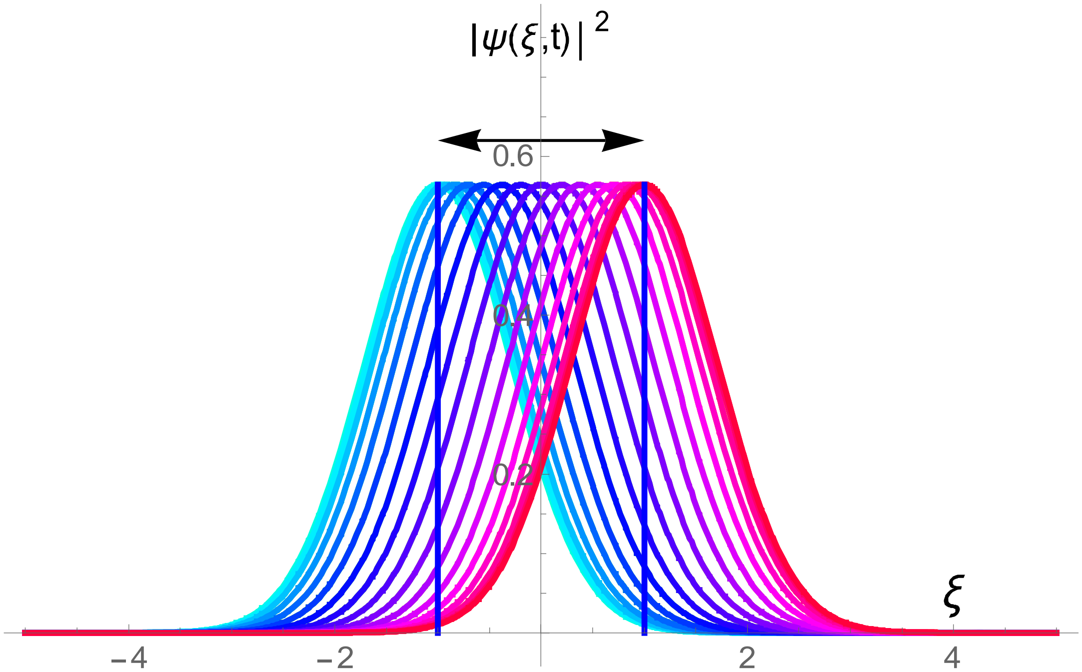
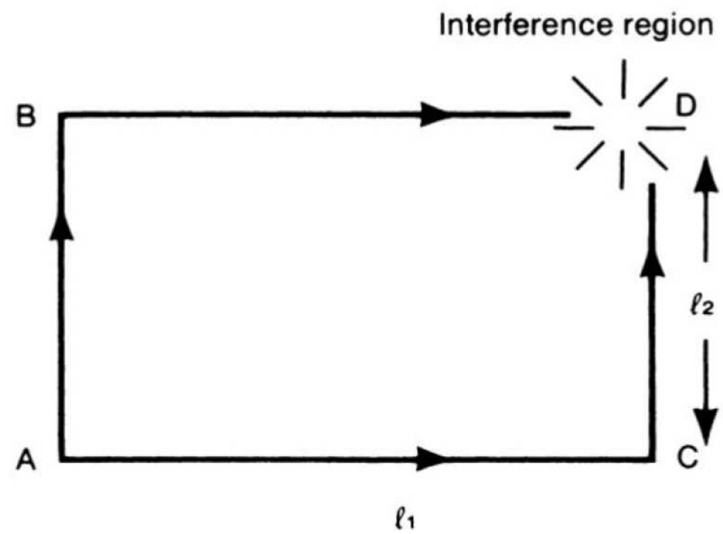


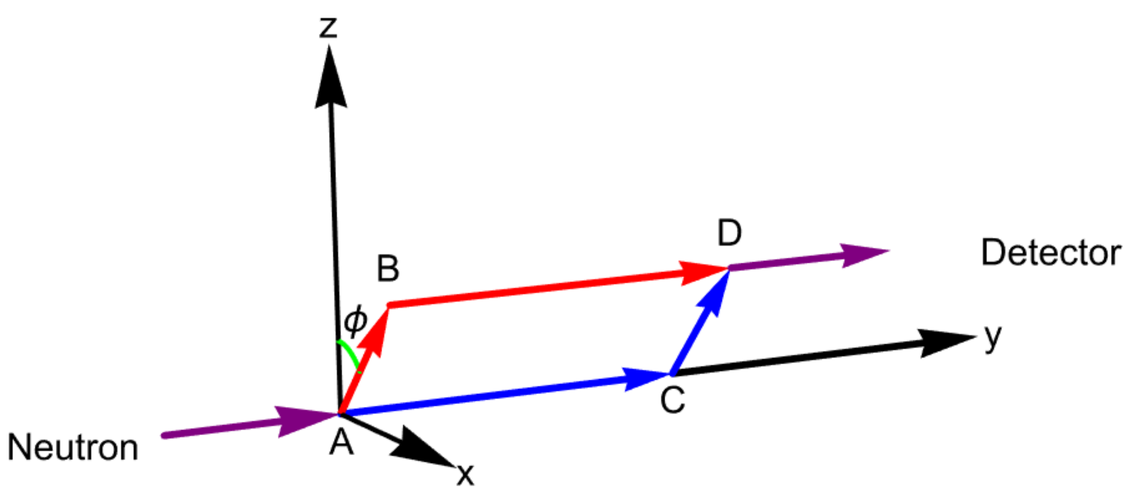
Fig. The time dependence of $\left|\psi(\xi,t)\right|^2 = \dfrac{1}{\pi^{1/2}}\exp[-(\xi-\xi_0\cos\omega_0 t)^2]$, where ξ_0=1. $T = 2\pi/\omega_0$. The peak shifts from ξ = 0 at t = 0 to ξ = 0 at t = T/4, ξ = ξ_0 at t = T/2, ξ = - ξ_0 at t = 3T/4, and ξ = 0 at t = T.

18. Neutron interferometry

A neutron beam is split into two beams by an interferometer. The relative phase of the two beams is varied by rotating the interferometer around the AC of the incident beam. (R. Colella, A.W. Overhauser, and S.A. Werner [Phys. Rev. Lett. 34, 1472 (1975)].

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 $l_2 \sin\phi$.





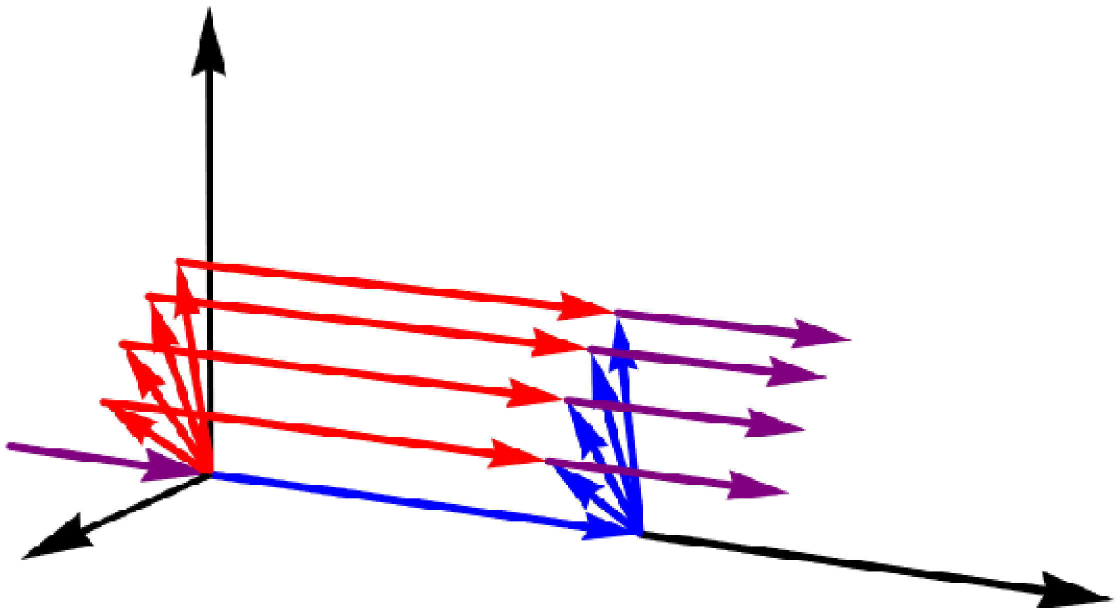


Fig. Experimental cobfiguration for neutron interefernce due to gravity. There are two paths; path A-B-D and path A-C-D. ϕ is the rotation angle from the z axis in the z-x plane.

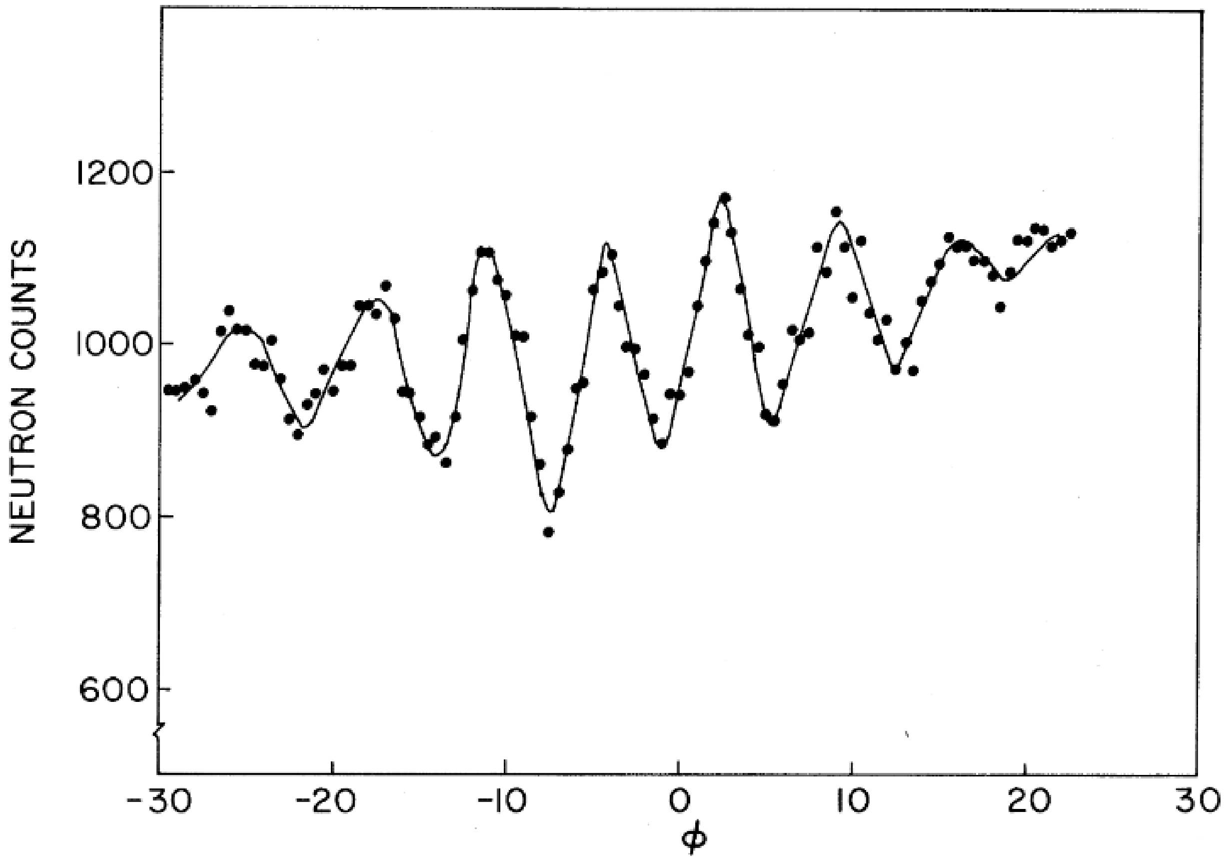


Fig. Dependence of gravity-induced phase on angle of rotation ϕ. From R. Colella, A. W. Overhauser, and S. A. Werner, Phys.. Rev. Lett. **34** (1975) 1472.

((**Note**))
The action is obtained as

$$S_{cl}(x,t,x',t') = -\frac{m[g^2(t-t')^4 - 12(x-x')^2 + 12g(t-t')^2(x+x')]}{24(t-t')}$$

where x is the height Along the path BD, $t-t' = T = \frac{l_1}{v}$, and $x = x' = x_0 = l_1 \sin\phi$. Along the path AC, $t-t' = T = \frac{l_1}{v}$, and $x = x' = x_0 = 0$

$$\begin{aligned} S_{cl}(x_0,T) &= -\frac{m(g^2T^4 + 12gT^2 2x_0)}{24T} \\ &= -\frac{m(g^2T^3 + 24Tgx_0)}{24} \end{aligned}$$

From the previous discussion we have the propagator for the gravity

$$K(x,t;x_0,t_0) = A\exp(\frac{i}{\hbar}S_{cl})$$
$$= \exp(-\frac{i}{24\hbar}mg^2T^3 - \frac{ix_0mgT}{\hbar})$$
$$= A_1\exp(-\frac{ix_0mgT}{\hbar})$$

For the path ABD and path ACD, we have

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

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

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

or

$$\Delta\theta = -\frac{1}{2\hbar}\frac{m^2gl_1l_2}{\frac{2\pi\hbar}{\lambda}}\sin\phi = -\frac{m^2gl_1l_2\lambda}{4\pi\hbar^2}\sin\phi = -\varepsilon\sin\phi.$$

or

$$\Delta\theta = -\frac{1}{2\hbar}\frac{m^2gl_1l_2}{mv}\sin\phi = -\frac{mgl_1l_2\lambda}{2\hbar v}\sin\phi = -\varepsilon\sin\phi,$$

where p is the momentum

$$p = mv.$$

The time T is related to l_1 as

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

The intensity for the interference is

$$
\begin{aligned}
|\psi|^2 &= \left|1 + e^{i\Delta\theta}\right|^2 \\
&= 4\cos^2(\frac{1}{2}\Delta\theta) \quad . \\
&= 4\cos^2(\frac{\varepsilon \sin\phi}{2})
\end{aligned}
$$

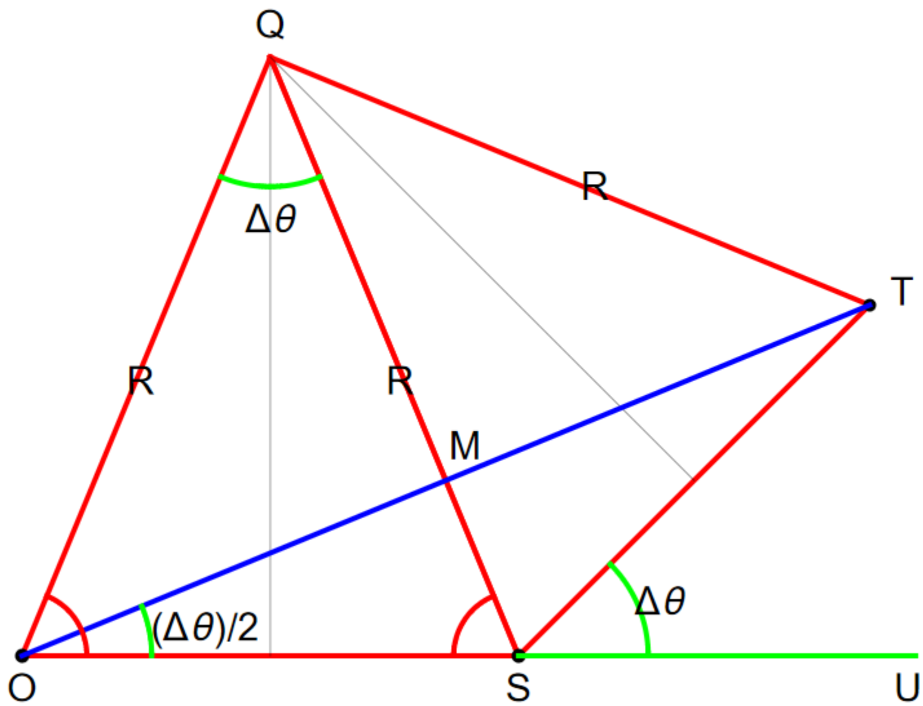


Fig. The phasor diagram. The intensity corresponds to the length $\overline{OT}$, where $\overline{OS} = \overline{ST} = 1$.

Note that

$$
\varepsilon = -\frac{mgl_1 l_2}{2\hbar v},
$$

where m is the mass of neutron. We consider the thermal neutron at the temperature $T = 300$ K. The energy of neutron is given by $E = \frac{1}{2}mv^2 = \frac{3}{2}k_B T$. The thermal energy is

$$
E = 38.778 \text{ meV}.
$$

The average velocity v is evaluated as

$$v = \sqrt{\frac{3k_B T}{m}} = 2.72374\times 10^3 \text{ m/s.}$$

The wavelength is

$$\lambda = \frac{2\pi\hbar}{mv} = 1.452 \text{ Å.}$$

So that, we have

$$\frac{mg}{2\hbar v} = 2.85931 \text{ (1/cm}^2\text{)}$$

The intensity I is evaluated as

$$I = 4\sin^2\left(\frac{mgl_1 l_2}{4\hbar v}\cos\phi\right) = 4\sin^2(1.4297 l_1 l_2 \cos\phi)$$

We assume that the area $l_1 l_2 = 6\ cm^2$. We make a plot of the intensity I as a function of the rotation angle ϕ (radian).

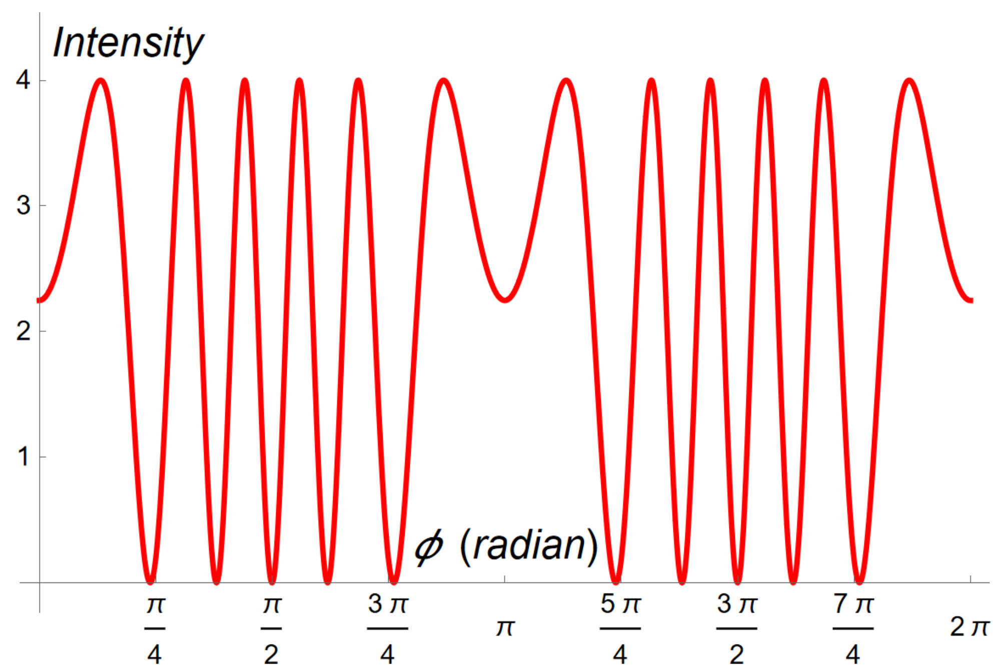


Fig. Plot of the intensity (neutron interference due to gravity) as a function of rotation angle ϕ (rad).

((**Mathematica**)) **We use the cgs units for the calculation**.

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

rule1 = {kB → 1.3806504 × 10^-16, g → 980.7,
    ℏ → 1.054571628 × 10^-27, mn → 1.674927211 × 10^-24,
    meV → 1.602176487 × 10^-15};

v1 = Sqrt[(3 kB T)/mn] /. T → 300 /. rule1; v1 // ScientificForm
```

2.72374×10^{5}

```
(3 kB T)/(2 meV) /. T → 300 /. rule1
```

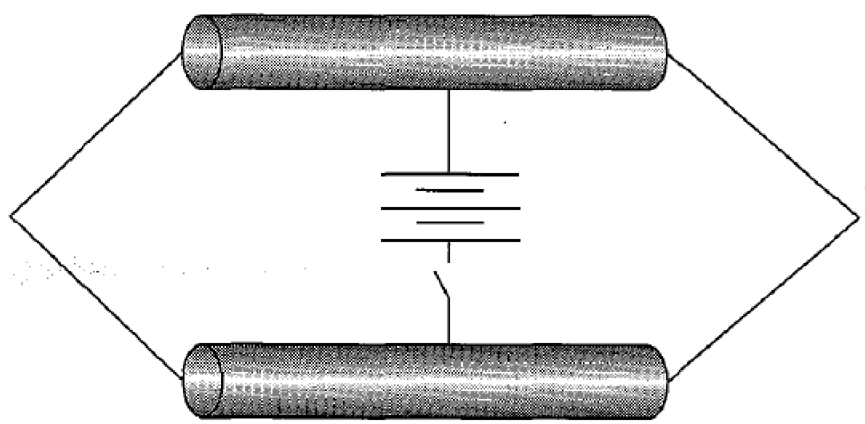
38.778

```
(mn g)/(2 ℏ v1) //. rule1
```

2.85931

```
F1[a1_] := 4 Sin[1.4296 a1 Cos[ϕ]]^2;
Q1 = Plot[F1[6], {ϕ, 0, 2 π},
   PlotStyle → {Hue[0], Thick},
   Ticks → {Range[0, 2 π, π / 4], Range[0, 5, 1]}];
Q2 =
  Graphics[
   {Text[Style["ϕ (°)", Black, 15, Italic], {π, 0.3}],
    Text[Style["Intensity", Black, 15, Italic],
     {0.6, 4.3}]}];
Show[Q1, Q2, PlotRange → All]
```

19. 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

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

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

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

We assume that

$$\phi = \frac{q(V_1 - V_2)}{\hbar}\Delta t .$$

Then we have

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

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

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

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 $\boldsymbol{A}$ and scalar potential ϕ are related to the magnetic field $\boldsymbol{B}$ and electric field $\boldsymbol{E}$ 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 χ is an arbitrary function. The new wave function is related to the old wave function through

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

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

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

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

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

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

20. 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 $q = -e$ ($e>0$), $\boldsymbol{A}$ 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 ***B***.

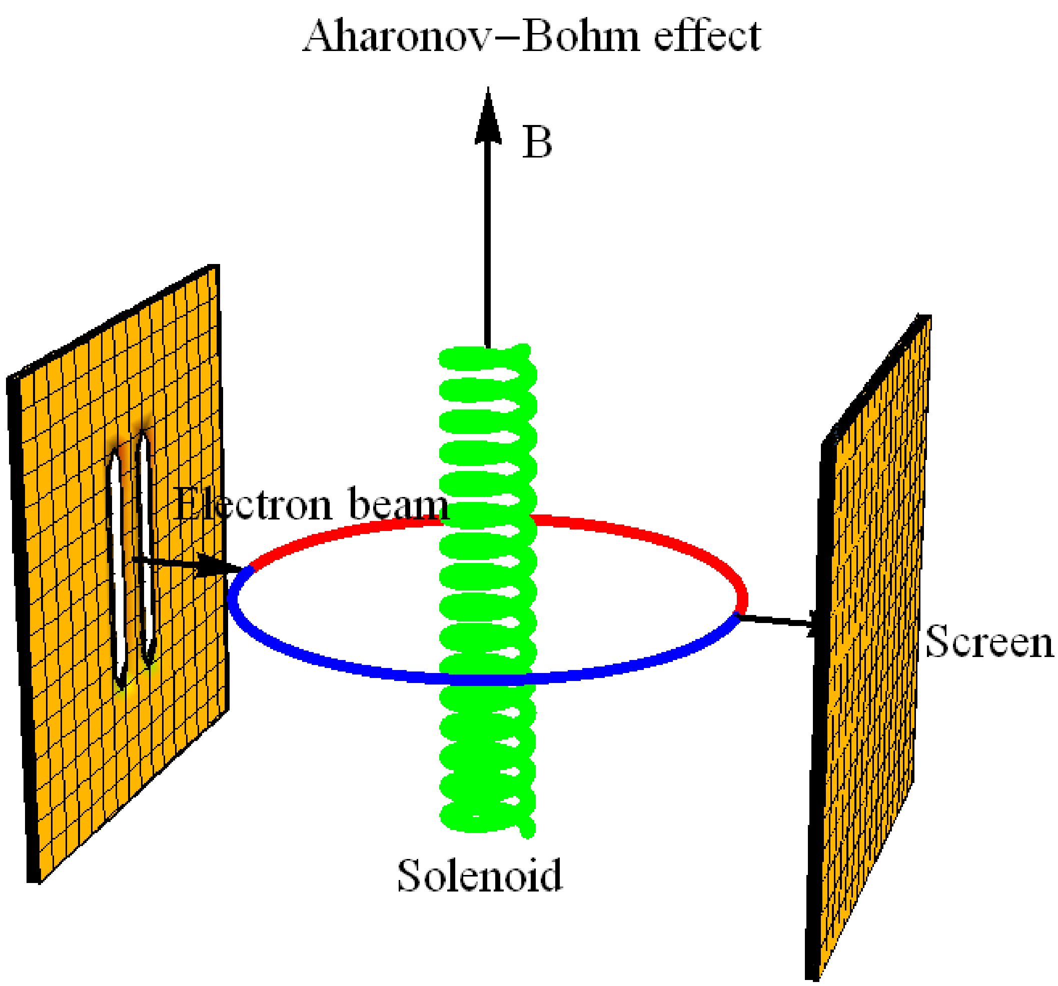


Fig. Schematic diagram of the Aharonov-Bohm experiment. Electron beams are split into two paths that go to either a collection of lines of magnetic flux (achieved by means of a long solenoid). The beams are brought together at a screen, and the resulting quantum interference pattern depends upon the 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)

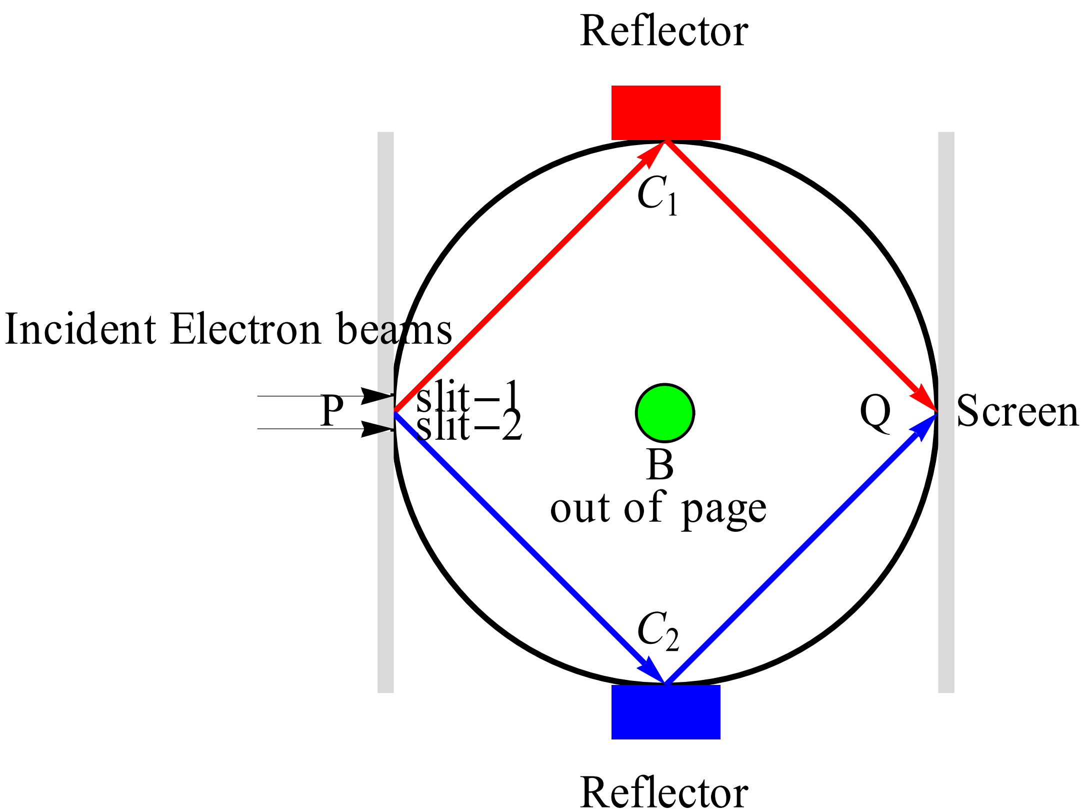


Fig. Schematic diagram of the Aharonov-Bohm experiment. Incident electron beams go into the two narrow slits (one beam denoted by blue arrow, and the other beam denoted by red arrow). The diffraction pattern is observed on the screen. The reflector plays a role of mirror for the optical experiment. The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

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

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

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

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

$$\frac{2\pi c\hbar}{e} = 4.1356675\times10^{-7} \text{ Gauss cm}^2.$$

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

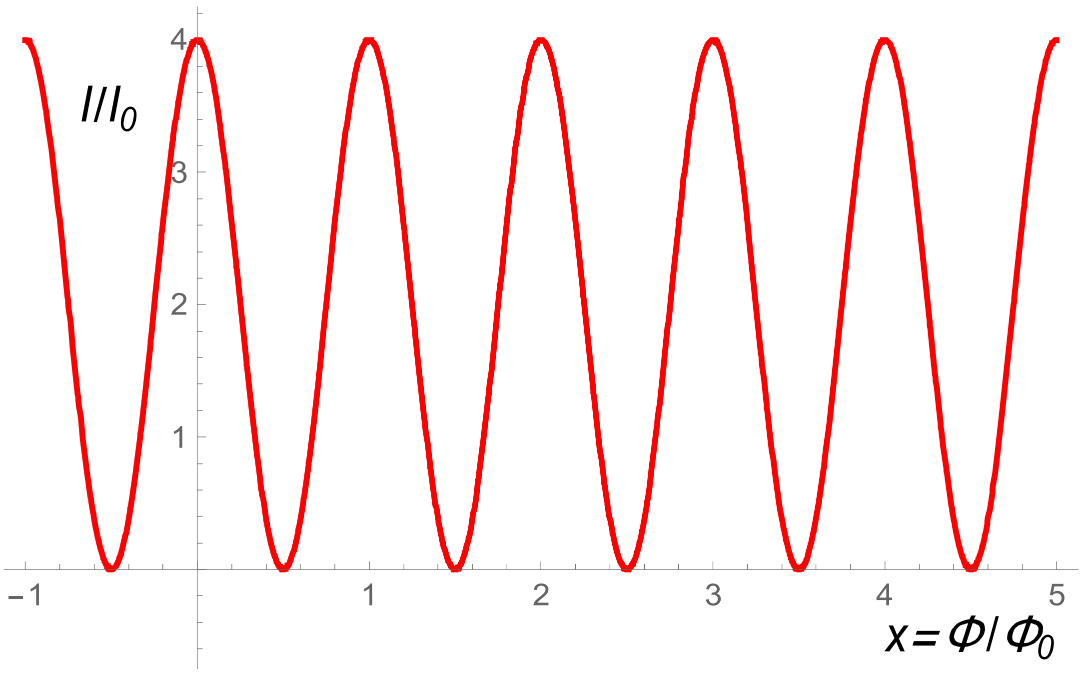
$$\Phi_0 = \frac{2\pi c\hbar}{2e} = 2.067833758(46) \times 10^{-7} \text{ Gauss cm}^2. \quad \text{(NIST)}$$

We note that

$$\Delta\theta = \frac{e}{c\hbar}\Phi = \frac{\Phi}{\Phi_0}\frac{e\Phi_0}{c\hbar} = \pi\frac{\Phi}{\Phi_0}$$

The intensity is

$$\begin{aligned} I &= I_0(1+e^{i\Delta\theta})(1+e^{-i\Delta\theta}) \\ &= 2I_0[1+\cos(\Delta\theta)] \\ &= 4\cos^2\left(\frac{\Delta\theta}{2}\right) \\ &= 4\cos^2\left(\pi\frac{\Phi}{\Phi_0}\right) \end{aligned}$$



Suppose that the area for the region of magnetic field is $A = 1$ mm^2 =10^{-2} cm^2.

$$\frac{\Phi}{\Phi_0} = \frac{10^{-2}B}{2.06783\times 10^{-7}} = \frac{10^5 B}{2.06783}$$

If $B = 0.3G$, $\quad\Phi/\Phi_0 = 1.45\times 10^4$.

If $B = 1$ mG, $\quad\Phi/\Phi_0 = 48$.

If $B = 0.01$ mG, $\quad\Phi/\Phi_0 = 0.48$.

((Note))

Equivalence between Aharonov Bohm effect and Feynman path integral

Lagrangian:

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

Canonical momentum:

$$\mathbf{P} = \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}.$$

Vector potential and scalar potential:

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

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

The gauge transformation is defined by

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

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

where χ is an arbitrary function. The new wave function of free particle ($\boldsymbol{A}$'=0) $\psi'(\boldsymbol{r})$ is related to the original wave function $\psi(\boldsymbol{r})$ through

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

For the Aharonov-Bohm effect, we assume that

$$\mathbf{A}' = 0 = \mathbf{A} + \nabla\chi, \qquad\qquad \chi = -\int \boldsymbol{A}\cdot d\boldsymbol{r}.$$

So that the original wavefunction $\psi(\boldsymbol{r})$ is

$$\begin{aligned}\psi(\boldsymbol{r}) &= \exp(-\frac{iq}{\hbar c}\chi)\psi'(\boldsymbol{r}) \\ &= \exp(-\frac{iq}{\hbar c}\chi)\psi'(\boldsymbol{r}) \\ &= \psi'(\boldsymbol{r})\exp(\frac{iq}{\hbar c}\int \boldsymbol{A}\cdot d\boldsymbol{r})\end{aligned}$$

with

$$\chi = -\int \mathbf{A}\cdot d\mathbf{r},$$

$$\psi'(\boldsymbol{r}) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) = \exp(i\int \boldsymbol{k}\cdot d\boldsymbol{r}). \qquad \text{(free-particle wave function)}$$

Thus, we have the original wavefunction as

$$\begin{aligned}
\psi(r) &= \exp(i\int \mathbf{k}\cdot d\mathbf{r})\exp(\frac{iq}{\hbar c}\int \mathbf{A}\cdot d\mathbf{r}) \\
&= \exp(\frac{i}{\hbar}\int \hbar\mathbf{k}\cdot d\mathbf{r} + \frac{iq}{\hbar c}\int \mathbf{A}\cdot d\mathbf{r}) \\
&= \exp[\frac{i}{\hbar}(\int \hbar\mathbf{k}\cdot d\mathbf{r} + \frac{q}{c}\int \mathbf{A}\cdot d\mathbf{r})] \\
&= \exp[\frac{i}{\hbar}\int (\mathbf{p}+\frac{q}{c}\mathbf{A})\cdot d\mathbf{r} \\
&= \exp[\frac{i}{\hbar}S]
\end{aligned}$$

The integral is over a certain path in the 3D real space. It is found that that S is the action and given by

$$S = \int \mathbf{P}\cdot d\mathbf{r} = \int (\mathbf{p}+\frac{q}{c}\mathbf{A})\cdot d\mathbf{r}, \qquad \text{(Feynman path integral)}$$

where

$$\mathbf{P} = \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}.$$

In conclusion, we show that the Aharonov-Bohm (AB) effect can be explained by the Feynman path integral. In other words, the AB effect is equivalent to the Feynman path integral.

21. Example-1: Feynman path integral

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

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

The Gaussian position-space wave packet evolves in time as

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

where

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

(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 $\frac{1}{2\pi}\frac{1}{\sqrt{\sigma^4+\frac{\hbar^2t^2}{m^2}}}$.

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

22. 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

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

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

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

or

$$\begin{aligned}
\langle x|\psi(t)\rangle &= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m\pi}{2\pi i\hbar t(\frac{1}{2} - \frac{im\sigma^2}{2\hbar t})}}\exp[\frac{imx^2}{2\hbar t} + \frac{\left(ik_0 - \frac{imx}{\hbar t}\right)^2}{4(\frac{1}{2\sigma^2} - \frac{im}{2\hbar t})}] \\
&= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{i\hbar t - \frac{im}{2\hbar t}(2i\hbar t\sigma^2)}}\exp[\frac{imx^2}{2\hbar t} - \frac{\left(\frac{mx}{\hbar t} - k_0\right)^2}{2(\frac{\hbar t - im\sigma^2}{\sigma^2\hbar t})}] \\
&= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m} + \sigma^2}}\exp[\frac{imx^2}{2\hbar t} + \frac{\left(\frac{mx}{\hbar t} - k_0\right)^2}{2im(\frac{\sigma^2 + \frac{i\hbar t}{m}}{\sigma^2\hbar t})}] \\
&= \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{\frac{i\hbar t}{m} + \sigma^2}}\exp[\frac{imx^2}{2\hbar t} + \frac{\sigma^2\hbar t}{2im}\frac{\left(\frac{mx}{\hbar t} - k_0\right)^2}{\sigma^2 + \frac{i\hbar t}{m}}]
\end{aligned}$$

or

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

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

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

where

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

Then we have

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

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

(i) The height of $\left|\langle x|\psi(t)\rangle\right|^2$ 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 $v_g=\frac{\hbar k_0}{m}$.

23. 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_{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

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

24. Comment by Roger Penrose on Feynman path integral

Roger Penrose: Road to the Reality. A Complete Guide to the Law of the Universe (Jonathan Cape London, 2004).

Here is a very interesting comment by Roger Penrose (Nobel laureate, 2020) on the Feynman Path integral. The content is the same, but some sentences are appropriately revised.

The Lagrangian is in many respects more appropriate than a Hamiltonian when we are concerned with a relativistic theory. The standard Schrödinger/Hamiltonian quantization procedures lie uncomfortably with the spacetime symmetry of relativity. However, unlike the Hamiltonian, which is associated with a choice of time coordinate, the Lagrangian can be taken to be a completely relativistically invariant entity.

The basic idea, like so many of the ideas underlying the formalism of quantum theory, is one that goes back to Dirac, although the person who carried it through as a basis for relativistic quantum theory was Feynman. Accordingly, it is commonly referred to as the formulation in terms of Feynman path integrals or Feynman sum over histories.

The basic idea is a different perspective on the fundamental quantum mechanical principle of complex linear superposition. Here, we think of that principle as applied, not just to specific quantum states, but to entire spacetime histories. We tend to think of these histories as 'possible alternative classical trajectories' (in configuration space). The idea is that in the quantum world, instead of there being just one classical 'reality', represented by one such trajectory (one history). There is a great complex superposition of all these 'alternative realities' (superposed alternative histories). Accordingly, each history is to be assigned a complex weighting factor, which we refer to as an amplitude if the total is normalized to modulus unity, so the squared modulus of an amplitude gives us a probability. We are usually interested in amplitudes for getting from a point *a* to a point *b* in configuration space.

The magic role of the Lagrangian is that it tells us what amplitude is to be assigned to each such history. If we know the Lagrangian *L*, then we can obtain the action *S*, for that history (the action being just the integral of *L* for that classical history). The complex amplitude to be assigned to that particular history is then given by the deceptively simple formula

$$\text{Complex amplitude} \propto \exp(\frac{i}{\hbar}S) = \exp[\frac{i}{\hbar}\int L dt].$$

For each history, there will be some action *S*, where *S* is the integral of the Lagrangian along the path. All the histories are supposed to 'coexist' in quantum superposition, and each history is assigned a complex amplitude $\exp(iS/\hbar)$. How are we to make contact with Lagrange's requirement, perhaps just in some approximate sense, that there should be a particular history singled out for which the action is indeed stationary?

The idea is that those histories within our superposition that are far away from a 'stationary-action' history will basically have their contributions cancel out with the contributions from neighboring histories. This is because the changes in *S* that come about when the history is varied will produce phase angles $\exp(iS/\hbar)$ that vary all around the clock, and so will cancel out on the average. Only if the history is very close to one for which the action is large and stationary (so the argument runs), will its contribution begin to be reinforced by those of its neighbors, rather than cancelled by them. because in this case there will be a large bunching of phase angles in the same direction.

This is indeed a very beautiful idea. In accordance with the 'path-integral' philosophy, not only should we obtain the classical history as the major contributor to the total amplitude—and therefore to the total probability—but also the smaller quantum corrections to this classical behavior, arising from the histories that are not quite classical and give contributions that do not quite cancel out, which may often be experimentally observable.

25. Action in the Feynman path integral

The Feynman approach was inspired by Dirac's paper (1933) on the role of the Lagrangian and the least-action principle in quantum mechanics. This eventually led Feynman to represent the propagator of the Schrödinger equation by the complex-valued path integral which now bears his name. At the end of the 1940s Feynman (1950, 1951) worked out, on the basis of the path integrals, a new formulation of quantum electrodynamics and developed the well-known diagram technique for perturbation theory

We start with the Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L_{cl}}{\partial \mathbf{v}}\right)=\frac{\partial L_{cl}}{\partial \mathbf{r}},$$

or

$$\frac{d}{dt}\mathbf{P}=\frac{\partial L_{cl}}{\partial \mathbf{r}},$$

The conjugate momentum ***P*** can be derived as

$$\mathbf{P}=\int\frac{\partial L_{cl}}{\partial \mathbf{r}}dt=\frac{\partial}{\partial \mathbf{r}}\int L_{cl}dt,$$

or

$$\int\mathbf{P}\cdot d\mathbf{r}=\int L_{cl}dt.$$

Here we use a type of techniques which is used in the Feynman-Hellmann theorem;

$$\langle\psi(\lambda)|\frac{\partial\hat{H}}{\partial\lambda}|\psi(\lambda)\rangle=\frac{\partial}{\partial\lambda}\langle\psi(\lambda)|\hat{H}|\psi(\lambda)\rangle.$$

Thus, the action S_{cl} can be expressed by

$$S_{cl}=\int L_{cl}dt=\int\mathbf{P}\cdot d\mathbf{r}.$$

in the Feynman path integral. The change in phase of the wave function is

$$\Delta\theta = \frac{1}{\hbar} S_{cl} = \frac{1}{\hbar}\int \mathbf{P}\cdot d\mathbf{r}.$$

This simple form of the phase is essential point derived from the Feynman path integral.

26. Wave function for a charged particle in the presence of magnetic field

From the theory of the Feynman path integral, it is found that the change in phase of the wave function is closely related to the action of classical Lagrangian, even for the phenomena of quantum mechanics. The change in phase in the presence of a vector potential ***A***, is given by

$$\Delta\theta = \frac{1}{\hbar}\int \mathbf{P}\cdot d\mathbf{r},$$

where ***P*** is the canonical momentum and ***p*** is the kinetic momentum, L_{cl} is the Lagrangian and is defined by

$$L_{cl} = \frac{1}{2} m\mathbf{v}^2 + \frac{q}{c}\mathbf{A}\cdot\mathbf{v},$$

where *e* is the charge of particle and *m* is the mass. The canonical momentum ***P*** is defined by

$$\mathbf{P} = \frac{\partial L_{cl}}{\partial \mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}.$$

From the classical Lagrange theory. The equation of motion is governed by the Lagrange equation,

$$\frac{d}{dt}\mathbf{P} = \frac{d}{dt}\left(\frac{\partial L_{cl}}{\partial \mathbf{v}}\right) = \frac{\partial L_{cl}}{\partial \mathbf{r}}.$$

The time derivative of the kinetic momentum ***p*** is equal to an external force ***F*** such as Lorentz force,

$$\frac{d\mathbf{p}}{dt} = \mathbf{F}, \qquad \text{(Newton's second law)}$$

which will be shown later. In quantum mechanics, it is known that the canonical momentum ***P*** (but not ***p***) is expressed by the differential operator

$$\mathbf{P} = \frac{\hbar}{i}\nabla .$$

We will discuss the application of the Feynman path integral in the next section 2S.

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

((**Mathematica**))

$$\int_{-\infty}^{\infty} \mathrm{Exp}\left[\frac{-a}{2}x^2\right] dx$$

$$\mathrm{ConditionalExpression}\left[\frac{\sqrt{2\pi}}{\sqrt{a}}, \mathrm{Re}[a]>0\right]$$

$$\int_{-\infty}^{\infty} \mathrm{Exp}\left[\frac{-a}{2}x^2+b\,x\right] dx$$

$$\mathrm{ConditionalExpression}\left[\frac{e^{\frac{b^2}{2a}}\sqrt{2\pi}}{\sqrt{a}}, \mathrm{Re}[a]>0\right]$$

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 $\dot{x}=\frac{dx}{dt}$. 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.

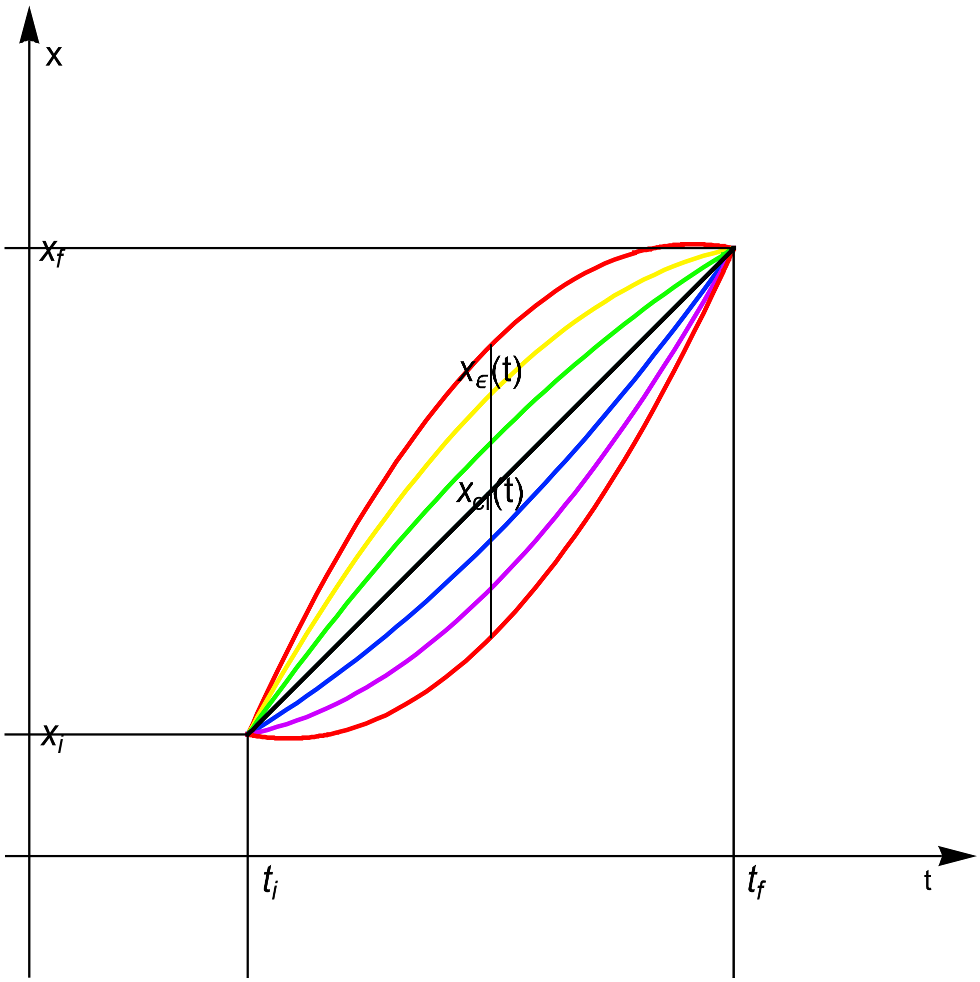

Fig.

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

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

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 $\varepsilon = 0$.

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

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

$$\begin{aligned}
\frac{\partial S[x_\varepsilon]}{\partial \varepsilon} &= \int_{t_i}^{t_f} \{\frac{\partial L}{\partial x}\eta(t) + \frac{\partial L}{\partial \dot{x}}\dot{\eta}(t)\}dt \\
&= \int_{t_i}^{t_f} \frac{\partial L}{\partial x}\eta(t)dt + \frac{\partial L}{\partial \dot{x}}\eta(t)\}|_{t_i}^{t_f} - \int_{t_i}^{t_f} \frac{d}{dt}(\frac{\partial L}{\partial \dot{x}})\eta(t)dt \\
&= \int_{t_i}^{t_f} [\frac{\partial L}{\partial x} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{x}})]\eta(t)dt
\end{aligned} \tag{1}$$

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,

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

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

APPENDIX-III: Lagrangian of charged particle in the electromagnetic field

(III-1) Lagrangian of free particle
((L.D. Landau and E.M. Lifshitz))

In the course of an infinitesimal time interval dt the moving clocks go a distance d***r***. Let us ask what time interval (proper time $d\tau$) is indicated for this period by the moving clocks. In a system of coordinates linked to the moving clocks, the latter are at rest, $d\mathbf{r}' = 0$. Because of the invariance of intervals

$$c^2 (d\tau)^2 - (d\mathbf{r}')^2 = c^2 (d\tau)^2 = c^2 (dt)^2 - (d\mathbf{r})^2$$

or

$$\begin{aligned} d\tau &= (dt)^2 - \frac{1}{c^2}(d\mathbf{r})^2 \\ &= dt\sqrt{1 - \frac{1}{c^2}(\frac{d\mathbf{r}}{dt})^2} \\ &= dt\sqrt{1 - \frac{v^2}{c^2}} \end{aligned}$$

where $\mathbf{v} = \dfrac{d\mathbf{r}}{dt}$ is the velocity. Integrating this expression, we can obtain the time interval indicated by the moving clocks when the elapsed time according to a clock at rest is $\Delta\tau$. The action S is given by

$$S = \int L dt = -mc^2 \int d\tau = -mc^2 \int dt \sqrt{1 - \frac{v^2}{c^2}},$$

yielding to the expression of the Lagrangian for the free particle as

$$L = -mc^2 \sqrt{1 - \frac{v^2}{c^2}}.$$

where m is the mass of the particle. Note that the units of L is erg.

(III-2) Four-potential of the electromagnetic field.

The four-dimensional vector for the scalar potential and vector potential,

$$A^\mu = (\phi, \mathbf{A}), \qquad \text{(Gaussian)}$$

$$A^\mu = (\frac{\phi}{c}, \mathbf{A}). \qquad \text{(SI units)}$$

Hereafter, we use the Gaussian units for the four-dimension potential. We note that

$$x^\mu = (ct, \mathbf{r}), \qquad x_\mu = (ct, -\mathbf{r}),$$

and

$$x^\mu x_\mu = c^2 t^2 - r^2.$$

Generalized potential U is obtained as

$$\begin{aligned} U dt &= \frac{q}{c} A_\mu dx^\mu \\ &= \frac{q}{c}(c\phi dt - \mathbf{A} \cdot d\mathbf{r}) \\ &= q(\phi dt - \frac{1}{c}\mathbf{A} \cdot \frac{d\mathbf{r}}{dt} dt) \\ &= q(\phi - \frac{1}{c}\mathbf{A} \cdot \mathbf{v}) dt \end{aligned}$$

or

$$U = q(\phi - \frac{1}{c}\mathbf{A}\cdot\mathbf{v}).$$

where q is a charge of particle. The Lagrangian for a charged particle in an electromagnetic field has the form

$$\begin{aligned} L &= K - U \\ &= -mc^2\sqrt{1-\frac{v^2}{c^2}} - q(\phi - \frac{1}{c}\mathbf{A}\cdot\mathbf{v}) \end{aligned}$$

The action S is expressed by

$$S = \int_{t'}^{t} L dt_1 = \int_{t'}^{t} (-mc^2\sqrt{1-\frac{v^2}{c^2}} + \frac{q}{c}\mathbf{A}\cdot\mathbf{v} - q\phi) dt_1$$

The generalized momentum is

$$\mathbf{P} = \frac{\partial L}{\partial \mathbf{v}} = \frac{mv}{\sqrt{1-\frac{v^2}{c^2}}} + \frac{q}{c}\mathbf{A} = \mathbf{p} + \frac{q}{c}\mathbf{A},$$

with

$$\mathbf{p} = \frac{m\mathbf{v}}{\sqrt{1-\frac{v^2}{c^2}}}.$$

We also note that

$$S_{cl} = \int \mathbf{P}\cdot d\mathbf{r}. \qquad \text{(Feynman path integral)}$$

The Hamiltonian H is obtained as follows.

$$
\begin{aligned}
H &= \mathbf{P}\cdot\mathbf{v} - L \\
&= (\mathbf{p} + \frac{q}{c}\mathbf{A})\cdot\mathbf{v} + mc^2\sqrt{1-\frac{v^2}{c^2}} + q(\phi - \frac{1}{c}\mathbf{A}\cdot\mathbf{v}) \\
&= \frac{m\mathbf{v}^2}{\sqrt{1-\frac{v^2}{c^2}}} + mc^2\sqrt{1-\frac{v^2}{c^2}} + q\phi \\
&= \frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}} + q\phi
\end{aligned}
$$

or

$$
\begin{aligned}
(\frac{H-q\phi}{c})^2 &= \frac{m^2c^2}{1-\frac{v^2}{c^2}} \\
&= \frac{m^2c^2(1-\frac{v^2}{c^2}) + m^2v^2}{1-\frac{v^2}{c^2}} \\
&= m^2c^2 + c^2\mathbf{p}^2 \\
&= m^2c^2 + (\mathbf{P} - \frac{q}{c}\mathbf{A})^2
\end{aligned}
$$

or else

$$
H = \sqrt{m^2c^4 + c^2(\mathbf{P} - \frac{q}{c}\mathbf{A})^2} + q\phi
$$

For low velocities, i.e., for classical mechanics, the Lagrangian goes over into

$$
L = \frac{1}{2}mv^2 + \frac{q}{c}\mathbf{A}\cdot\mathbf{v} - q\phi
$$

and the Hamiltonian is

$$
\begin{aligned}
H &= \mathbf{P}\cdot\mathbf{v} - L \\
&= \frac{m\mathbf{v}^2}{\sqrt{1-\frac{v^2}{c^2}}} + mc^2\sqrt{1-\frac{v^2}{c^2}} + q\phi \\
&= \frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}} + q\phi
\end{aligned}
$$

In this approximation,

$$\mathbf{p} = m\mathbf{v} = \mathbf{P} - \frac{q}{c}\mathbf{A}$$

The final form of the Hamiltonian is given by

$$\tilde{H} = H - mc^2 = \frac{1}{2m}\mathbf{p}^2 + q\phi = \frac{1}{2m}(\mathbf{P} - \frac{q}{c}\mathbf{A})^2 + q\phi$$

(III-3) Derivation of Lorentz force from Lagrangian

The Lorentz force, which is a force on a particle with a charge q due to an electric field $\boldsymbol{E}$ and magnetic field $\boldsymbol{B}$,

$$\mathbf{F} = q(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B})$$

where $\boldsymbol{v}$ is the velocity of particle

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}, \qquad \text{(electric field)}$$

$$\mathbf{B} = \nabla\times\mathbf{A}. \qquad \text{(magnetic field)}$$

The gauge transformation is defined by

$$A' = A + \nabla\chi, \qquad \phi' = \phi - \frac{1}{c}\frac{\partial\chi}{\partial t}$$

where χ is an arbitrary function. Suppose that the Lagrangian L is expressed as

$$
\begin{aligned}
L &= -mc^2\sqrt{1-\frac{v^2}{c^2}} - q(\phi - \frac{1}{c}\mathbf{A}\cdot\mathbf{v}) \\
&\cong \frac{1}{2}m\mathbf{v}^2 - q(\phi - \frac{1}{c}\mathbf{A}\cdot\mathbf{v}) \\
&= T - U
\end{aligned}
$$

is the velocity-dependent potential energy. Note that

$$
\mathbf{P} = \frac{\partial L}{\partial \mathbf{v}} = \frac{m\mathbf{v}}{\sqrt{1-\frac{\mathbf{v}^2}{c^2}}} + \frac{q}{c}\mathbf{A} = \mathbf{p} + \frac{q}{c}\mathbf{A}
$$

Lagrange equation is

$$
\frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{v}}\right) = \frac{\partial L}{\partial \mathbf{r}} = \nabla L ,
$$

with

$$
\nabla L = \nabla(-q\phi + \frac{q}{c}\mathbf{v}\cdot\mathbf{A}) ,
$$

where $\frac{d}{dt}$ is a total derivative. We note that

$$
\begin{aligned}
\nabla(\mathbf{v}\cdot\mathbf{A}) = {} & (\mathbf{v}\cdot\nabla)\mathbf{A} + (\mathbf{A}\cdot\nabla)\mathbf{v} \\
& + \mathbf{v}\times(\nabla\times\mathbf{A}) + \mathbf{A}\times(\nabla\times\mathbf{v})
\end{aligned}
$$

Since ***v*** and ***r*** are independent variables in the Lagrangian, we have

$$
(\mathbf{A}\cdot\nabla)\mathbf{v} = 0 , \qquad \mathbf{A}\times(\nabla\times\mathbf{v}) = 0
$$

leading to

$$
\nabla(\mathbf{v}\cdot\mathbf{A}) = (\mathbf{v}\cdot\nabla)\mathbf{A} + \mathbf{v}\times(\nabla\times\mathbf{A})
$$

We note that

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{v}}\right) = \frac{d}{dt}(\mathbf{p} + \frac{q}{c}\mathbf{A})$$
$$= \frac{d\mathbf{p}}{dt} + \frac{q}{c}\frac{d\mathbf{A}}{dt}$$
$$= \frac{d\mathbf{p}}{dt} + \frac{q}{c}[\frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{A}]$$

with

$$\frac{dA_i}{dt} = \frac{\partial A_i}{\partial t} + \dot{x}\frac{\partial A_i}{\partial x} + \dot{y}\frac{\partial A_i}{\partial y} + \dot{z}\frac{\partial A_i}{\partial z}$$
$$= \frac{\partial A_i}{\partial t} + (\mathbf{v}\cdot\nabla)A_i$$

or

$$\frac{d\mathbf{A}}{dt} = \frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{A}]$$

So that, we have

$$\nabla L = -q\nabla\phi + \frac{q}{c}\nabla(\mathbf{v}\cdot\mathbf{A})$$

We get the final form of the Lagrange equation as

$$\frac{d\mathbf{p}}{dt} + \frac{q}{c}[\frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{A}] = -q\nabla\phi + \frac{q}{c}\nabla(\mathbf{v}\cdot\mathbf{A})$$

or

$$\frac{d\mathbf{p}}{dt} = q(-\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}) + \frac{q}{c}[\nabla(\mathbf{v}\cdot\mathbf{A}) - (\mathbf{v}\cdot\nabla)\mathbf{A}]$$
$$= q(-\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}) + \frac{q}{c}\mathbf{v}\times(\nabla\times\mathbf{A})$$
$$= q(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B})$$

which is equivalent to the Lorentz force, with

$$\nabla(\mathbf{v}\cdot\mathbf{A})-(\mathbf{v}\cdot\nabla)\mathbf{A}=\mathbf{v}\times(\nabla\times\mathbf{A})=\mathbf{v}\times\mathbf{B}$$

(III-4) Gauge transformation

The original Lagrangian L_0 is changed into a new Lagrangian L_0' during the Gauge transformation,

$$\begin{aligned}
L_0' &= -q(\phi' - \frac{1}{c}\mathbf{A}'\cdot\mathbf{v}) \\
&= -q(\phi - \frac{1}{c}\frac{\partial\chi}{\partial t}) + \frac{q}{c}(\mathbf{A}+\nabla\chi\cdot\mathbf{v}) \\
&= L_0 + \frac{q}{c}(\frac{\partial\chi}{\partial t}+\nabla\chi\cdot\mathbf{v}) \\
&= L_0 + \frac{q}{c}\frac{d\chi(\mathbf{r},t)}{dt}
\end{aligned}$$

But as we know, adding to the Lagrangian a total time derivative of a function of ***r*** and *t* does not change the equations of motion. The function $\frac{d\chi}{dt}$ always satisfies the Lagrange equation. Note that

$$\frac{d}{dt}[\frac{\partial}{\partial\dot{\mathbf{r}}}\frac{d\chi}{dt}]=\frac{d}{dt}[\frac{\partial\chi}{\partial\mathbf{r}}]=\frac{\partial}{\partial\mathbf{r}}\frac{d\chi}{dt}$$

since

$$\begin{aligned}
\frac{d\chi}{dt} &= \frac{\partial\chi}{\partial t}+\dot{x}\frac{\partial\chi}{\partial x}+\dot{y}\frac{\partial\chi}{\partial y}+\dot{z}\frac{\partial\chi}{\partial z} \\
&= \frac{\partial\chi}{\partial t}+(\mathbf{v}\cdot\nabla)\chi
\end{aligned}$$

$$\frac{d}{dt}[\frac{\partial}{\partial\dot{x}}\frac{d\chi}{dt}]=\frac{d}{dt}[\frac{\partial\chi}{\partial x}]=\frac{\partial}{\partial x}\frac{d\chi}{dt},$$

$$\frac{d}{dt}[\frac{\partial}{\partial\dot{y}}\frac{d\chi}{dt}]=\frac{d}{dt}[\frac{\partial\chi}{\partial y}]=\frac{\partial}{\partial y}\frac{d\chi}{dt},$$

$$\frac{d}{dt}[\frac{\partial}{\partial\dot{z}}\frac{d\chi}{dt}]=\frac{d}{dt}[\frac{\partial\chi}{\partial z}]=\frac{\partial}{\partial z}\frac{d\chi}{dt}.$$

In other words,

$$\frac{d}{dt}(\frac{\partial}{\partial \dot{\mathbf{r}}}L') = \frac{\partial}{\partial \mathbf{r}}L'$$

is equal to

$$\frac{d}{dt}(\frac{\partial}{\partial \dot{\mathbf{r}}}L_0) = \frac{\partial}{\partial \mathbf{r}}L_0$$

independent of the form $\frac{d\chi}{dt}$.

((**Comment**))
Yasushi Takahashi (Note on Mathematical Physics, Kodansha, 1992) in Japanese.

"It may be reasonable to use the expression of the Lagrangian (classical system) given by

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

The reason is why the Lagrange equation for this form of Lagrangian yields the equation of motion of the charged particles with charge q with the Lorentz force $\boldsymbol{F}$,

$$\frac{d\mathbf{p}}{dt} = \mathbf{F} = q(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}).$$

(III-5) Feynman path integral

$$S_{cl} = \int \mathbf{P}\cdot d\mathbf{r} = \int (\mathbf{p} + \frac{q}{c}\mathbf{A})\cdot d\mathbf{r}$$

For the closed path

$$\begin{aligned}\oint \mathbf{A}\cdot d\mathbf{r} &= \int (\nabla\times\mathbf{A})\cdot d\mathbf{a} \\ &= \int \mathbf{B}\cdot d\mathbf{a} \\ &= \Phi_B\end{aligned}$$

((**Stokes' theorem**))

$$\frac{1}{\hbar}\oint \frac{q}{c}\mathbf{A}\cdot d\mathbf{r} = \frac{q}{c\hbar}\Phi_B$$

Magnetic quantum flux (fluxoid)

$$\Phi_0 = \frac{hc}{2e} = \frac{2\pi\hbar c}{2e} = \frac{\pi\hbar c}{e}.$$

$$\Phi_0 = 2.0678\times 10^{-7} \text{ Gauss cm}^2 \qquad \text{(cgs units)}$$

or

$$\Phi_0 = 2.0678\times 10^{-15} \text{ T m}^2 \qquad \text{(SI units)}$$

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