Friday-1 AKT on 140110: The Schroedinger equation and path integrals

January-05-14 5:25 PM

Meta tutorial today at 6:10 @ 6180 ! } on board !

Then as in handout.....

What happens to a quantum particle on a pendulum at $T = \frac{\pi}{2}$?

Abstract. This subject is the best one-hour introduction I know for the mathematical techniques that appear in quantum mechanics — in one short lecture we start with a meaningful question, visit Schrödinger's equation, operators and exponentiation of operators, Fourier analysis, path integrals, the least action principle, and Gaussian integration, and at the end we land with a meaningful and interesting answer.

Based a lecture given by the author in the "trivial notions" seminar in Harvard on April 29, 1989. This edition, January 10, 2014.

1. The Question

Let the complex valued function $\psi = \psi(t, x)$ be a solution of the Schrödinger equation

$$\frac{\partial \psi}{\partial t} = -i\left(-\frac{1}{2}\Delta_x + \frac{1}{2}x^2\right)\psi \qquad \text{with} \qquad \psi|_{t=0} = \psi_0.$$

What is $\psi|_{t=T=\frac{\pi}{2}}$?
In fact, the major part of our discussion will work just as well for the general Schrödinger equation,

$$\frac{\partial \psi}{\partial t} = -iH\psi, \qquad H = -\frac{1}{2}\Delta_x + V(x),$$

$$\psi|_{t=0} = \psi_0, \qquad \text{arbitrary } T,$$

where,

- ψ is the "wave function", with $|\psi(t,x)|^2$ representing the probability of finding our particle at time t in position x.
- H is the "energy", or the "Hamiltonian".
- $-\frac{1}{2}\Delta_x$ is the "kinetic energy".
- $V(x)$ is the "potential energy at x".

2. The Solution

The equation $\frac{\partial \psi}{\partial t} = -iH\psi$ with $\psi|_{t=0} = \psi_0$ formally implies

$$\psi(T, x) = \left(e^{-iTH}\psi_0\right)(x) = \left(e^{i\frac{T}{2}\Delta - iTV}\psi_0\right)(x).$$

By Lemma 3.1 with $n = 10^{58} + 17$ and setting $x_n = x$ we find that $\psi(T, x)$ is

$$\left(e^{i\frac{T}{2n}\Delta}e^{-i\frac{T}{n}V}e^{i\frac{T}{2n}\Delta}e^{-i\frac{T}{n}V}\dots e^{i\frac{T}{2n}\Delta}e^{-i\frac{T}{n}V}\psi_0\right)(x_n).$$

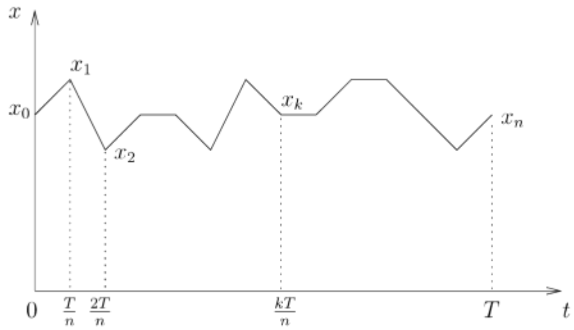
Now using Lemmas 3.2 and 3.3 we find that this is: (c denotes the ever-changing universal fixed numerical constant)

$$c\int dx_{n-1}e^{i\frac{(x_n - x_{n-1})^2}{2T/n}}e^{-i\frac{T}{N}V(x_{n-1})}\dots$$
$$\int dx_1 e^{i\frac{(x_2-x_1)^2}{2T/n}}e^{-i\frac{T}{N}V(x_1)}$$
$$\int dx_0 e^{i\frac{(x_1-x_0)^2}{2T/n}}e^{-i\frac{T}{N}V(x_0)}\psi_0(x_0).$$

Repackaging, we get

$$c\int dx_0\dots dx_{n-1}$$
$$\exp\left(i\frac{T}{2n}\sum_{k=1}^{n}\left(\frac{x_k - x_{k-1}}{T/n}\right)^2 - i\frac{T}{n}\sum_{k=0}^{n-1}V(x_k)\right)$$
$$\psi_0(x_0).$$

Now comes the novelty. keeping in mind the picture



and replacing Riemann sums by integrals, we can write

$$\psi(T,x) = c\int dx_0 \int_{W_{x_0x_n}} \mathcal{D}x$$
$$\exp\left(i\int_0^T dt\left(\frac{1}{2}\dot{x}^2(t) - V(x(t))\right)\right)\psi_0(x_0),$$

where $W_{x_0x_n}$ denotes the space of paths that begin at x_0 and end at x_n,

$$W_{x_0x_n} = \{x : [0,T] \to \mathbb{R} : \ x(0) = x_0, \, x(T) = x_n\},$$

and $\mathcal{D}x$ is the formal "path integral measure".
This is a good time to introduce the "action" $\mathcal{L}$:

$$\mathcal{L}(x) := \int_0^T dt\left(\frac{1}{2}\dot{x}^2(t) - V(x(t))\right).$$

With this notation,

$$\psi(T,x) = c\int dx_0\psi_0(x_0)\int_{W_{x_0x_n}}\mathcal{D}xe^{i\mathcal{L}(x)}.$$

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Let x_c denote the path on which $\mathcal{L}(x)$ attains its minimum value, write $x = x_c + x_q$ with $x_q \in W_{00}$, and get

$$\psi(T,x) = c\int dx_0\psi_0(x_0)\int \quad \mathcal{D}x_q e^{i\mathcal{L}(x_c + x_q)}.$$

Lemma 3.3.

$$\left(e^{i\frac{t}{2}\Delta}\psi_0\right)(x) = c\int dx' e^{i\frac{(x-x')^2}{2t}}\psi_0(x').$$

Proof. In fact, the left hand side of this equality is

Let x_c denote the path on which $\mathcal{L}(x)$ attains its minimum value, write $x = x_c + x_q$ with $x_q \in W_{00}$, and get

$$\psi(T,x) = c\int dx_0\psi_0(x_0)\int_{W_{00}} \mathcal{D}x_q e^{i\mathcal{L}(x_c+x_q)}.$$

In our particular case $\mathcal{L}$ is quadratic in x, and therefore $\mathcal{L}(x_c+x_q) = \mathcal{L}(x_c) + \mathcal{L}(x_q)$ (this uses the fact that x_c is an extremal of $\mathcal{L}$, of course). Plugging this into what we already have, we get

$$\begin{aligned}\psi(T,x) &= c\int dx_0\psi_0(x_0)\int_{W_{00}} \mathcal{D}x_q e^{i\mathcal{L}(x_c)+i\mathcal{L}(x_q)}\\ &= c\int dx_0\psi_0(x_0)e^{i\mathcal{L}(x_c)}\int_{W_{00}} \mathcal{D}x_q e^{i\mathcal{L}(x_q)}.\end{aligned}$$

Now this is excellent news, because the remaining path integral over W_{00} does not depend on x_0 or x_n, and hence it is a constant! Allowing c to change its value from line to line, we get

$$\psi(T,x) = c\int dx_0\psi_0(x_0)e^{i\mathcal{L}(x_c)}.$$

Lemma 3.4 now shows us that $x_c(t) = x_0\cos t + x_n \sin t$. An easy explicit computation gives $\mathcal{L}(x_c) = -x_0x_n$, and we arrive at our final result,

$$\psi(\frac{\pi}{2},x) = c\int dx_0\psi_0(x_0)e^{-ix_0x_n}.$$

Notice that this is precisely the formula for the Fourier transform of ψ_0! That is, the answer to the question in the title of this document is "the particle gets Fourier transformed", whatever that may mean.

3. The Lemmas

Lemma 3.1. *For any two matrices A and B,*

$$e^{A+B} = \lim_{n\to\infty}\left(e^{A/n}e^{B/n}\right)^n.$$

Proof. (sketch) Using Taylor expansions, we see that $e^{\frac{A+B}{n}}$ and $e^{A/n}e^{B/n}$ differ by terms at most proportional to c/n^2. Raising to the nth power, the two sides differ by at most $O(1/n)$, and thus

$$e^{A+B} = \lim_{n\to\infty}\left(e^{\frac{A+B}{n}}\right)^n = \lim_{n\to\infty}\left(e^{A/n}e^{B/n}\right)^n,$$

as required. □

Lemma 3.2.

$$\left(e^{itV}\psi_0\right)(x) = e^{itV(x)}\psi_0(x).$$

□

Lemma 3.3.

$$\left(e^{i\frac{t}{2}\Delta}\psi_0\right)(x) = c\int dx' e^{i\frac{(x-x')^2}{2t}}\psi_0(x').$$

Proof. In fact, the left hand side of this equality is just a solution $\psi(t,x)$ of Schrödinger's equation with $V=0$:

$$\frac{\partial\psi}{\partial t} = \frac{i}{2}\Delta_x\psi, \qquad \psi|_{t=0} = \psi_0.$$

Taking the Fourier transform $\tilde\psi(t,p) = \frac{1}{\sqrt{2\pi}}\int e^{-ipx}\psi(t,x)dx$, we get the equation

$$\frac{\partial\tilde\psi}{\partial t} = -i\frac{p^2}{2}\tilde\psi, \qquad \tilde\psi|_{t=0} = \tilde\psi_0.$$

For a fixed p, this is a simple first order linear differential equation with respect to t, and thus,

$$\tilde\psi(t,p) = e^{-i\frac{tp^2}{2}}\tilde\psi_0(p).$$

Taking the inverse Fourier transform, which takes products to convolutions and Gaussians to other Gaussians, we get what we wanted to prove. □

Lemma 3.4. *With the notation of Section 2 and at the specific case of $V(x) = \frac{1}{2}x^2$ and $T = \frac{\pi}{2}$, we have*

$$x_c(t) = x_0\cos t + x_n\sin t.$$

Proof. If x_c is a critical point of $\mathcal{L}$ on $W_{x_0x_n}$, then for any $x_q \in W_{00}$ there should be no term in $\mathcal{L}(x_c+\epsilon x_q)$ which is linear in ϵ. Now recall that

$$\mathcal{L}(x) = \int_0^T dt\left(\frac{1}{2}\dot x^2(t) - V(x(t))\right),$$

so using $V(x_c+\epsilon x_q) \sim V(x_c) + \epsilon x_q V'(x_c)$ we find that the linear term in ϵ in $\mathcal{L}(x_c+\epsilon x_q)$ is

$$\int_0^T dt\left(\dot x_c\dot x_q - V'(x_c)x_q\right).$$

Integrating by parts and using $x_q(0) = x_q(T) = 0$, this becomes

$$\int_0^T dt\left(-\ddot x_c - V'(x_c)\right)x_q.$$

For this integral to vanish independently of x_q, we must have $-\ddot x_c - V'(x_c) \equiv 0$, or

$\ddot x_c = -V'(x_c)$. (This is the famous $F = ma$ of Newton's, and we have just rediscovered the principle of least action!)

In our particular case this boils down to the equation

$$\ddot x_c = -x_c, \qquad x_c(0) = x_0, \qquad x_c(\pi/2) = x_n,$$

whose unique solution is displayed in the statement of this lemma. □

not done