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FORMALIZING FEYNMAN'S DERIVATION OF SCHRODINGER EQUATION

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ABSTRACT

Feynman's derivation of Schrodinger Equation (SE) shows how Dirac's expression is equivalent, even if seemingly approximate, with SE.[1] This equivalence may be made exact even when extended to E^3. In this article we prove this equivalence for simple case when the Lagrangian is simply the difference between kinetic and potential energy.

Key Word: Schrodinger Equation, Feynman, Derivation, Integral Equation, Lagrangian, Dirac

INTRODUCTION

Feynman's formulation of path integral makes use of equivalence between Dirac's integral equation and Schrodinger's partial differential equation. However Dirac didn't recover SE from his equation, it was Feynman who did[1][2]. Feynman recovered SE by setting $A\exp(iS/\hbar)$ as quantum mechanical wave propagator. He at first set the propagator to equal $\exp(iS/\hbar)$ then expanding out everything in power series, making the lowest order approximation, he found out that he needed to adjust a proportionality constant to make its left and right hand side equal. This derivation made heavy uses of approximation, thus it may seem to be an approximate equality. This equality however, is actually an exact equality. In this article we'll provide an exact mathematical derivation of 3 dimensional SE, and one dimensional case follows easily. In deriving SE, only basic assumptions are made, and in doing so we have avoid as much as possible approximation steps. All approximate equalities in the last step then are turned exact by a limiting procedure. The derivation itself follows roughly Feynman's lead, minus the physical intuition features to appeal mathematical rigor.

Quantum Mechanical Wave Function Propagator

Huygens' principle proposed by Christiaan Huygens in 1678 stated that every point reached by luminous disturbance may become source for secondary waves, which is commonly called wavelets, the form of these secondary waves determines the form of the primary wave at later time. Mathematically it takes the form of

$$\psi_p(\boldsymbol{r}_p, t_p) = \int \psi_s(\boldsymbol{r}_s, t_s)dC$$

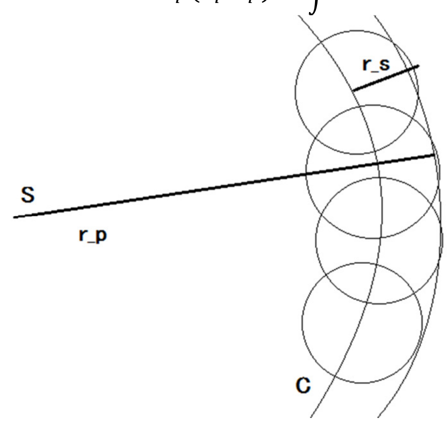

Figure 1

Where r_p and r_s is as indicated in above figure and the integration is to be taken over the surface C. Thus, ψ_p only contains information about disturbance along surface C. To get complete information about the shape of wave function we integrate over the whole space. The idea of propagator of wave function is that there exists a function $G(r_p, r_s, t_p, t_s)$ called the kernel or propagator of wave function such that

$$\psi_p(\boldsymbol{r}_p, t_p) = \int G(\boldsymbol{r}_p, \boldsymbol{r}_s, t_p, t_s)\psi_p(\boldsymbol{r}_s, t_s)d^3r_s$$

Or

$$G(\boldsymbol{r}_p, \boldsymbol{r}_s, t_p, t_s)\psi_p(\boldsymbol{r}_s, t_s) = \psi_s(\boldsymbol{r}_s, t_s)$$

The propagator as $t_s \to t_p$, exhibits a certain property of Dirac delta function. To show this we simply evaluate the limit when $t_s \to t_p$

$$\psi_p(\boldsymbol{r}_p, t_p) = \int G(\boldsymbol{r}_p, \boldsymbol{r}_s, t_p, t_s)\psi_p(\boldsymbol{r}_s, t_p)d^3r_s$$

Which by definition we know that for arbitrary $a < k < b$ we have

$$X(k) = \int_a^b G \times X(l)dl$$
$$G = \delta(l - k)$$

Later in the derivation we'll find that our quantum mechanical wave propagator reduces to Dirac delta.

The propagator of quantum mechanical wave function is found to be proportional to $exp(iS/\hbar)$ by Feynman[1][2] after reading a paper by Dirac.

Approximating Propagator and Finding Proportionality Constant

From Feynman's own derivation[1][2][3] we know that the propagator of quantum mechanical wave function is proportional to $exp(iS/\hbar)$ as is found by Feynman. In the simplest case the Lagrangian is simply the difference between kinetic and potential energy.

$$L = \frac{1}{2}m\boldsymbol{v}(t) \cdot \boldsymbol{v}(t) - U(\boldsymbol{r}(t))$$

Thus for small time interval $\epsilon = t_2 - t_1$

$$S = \int_{t_1}^{t_2} Ldt \approx L_{ave}\epsilon = (K_{ave} - U_{ave})\epsilon$$
$$K_{ave} = \frac{1}{2}m\frac{(\boldsymbol{y} - \boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x})}{\epsilon^2}$$
$$U_{ave} = U(\frac{1}{2}(\boldsymbol{x} + \boldsymbol{y}))$$

With $\boldsymbol{y}$ and $\boldsymbol{x}$ defined as

$$\boldsymbol{y} = \int_0^{t_2} \boldsymbol{v}\, dt = \boldsymbol{r}(t_2)$$
$$\boldsymbol{x} = \int_0^{t_1} \boldsymbol{v}\, dt = \boldsymbol{r}(t_1)$$

or

$$S \approx \frac{m}{2\epsilon}(\boldsymbol{y} - \boldsymbol{x}) \cdot (\boldsymbol{x} - \boldsymbol{y}) - \epsilon U(\frac{1}{2}(\boldsymbol{x} + \boldsymbol{y}))$$

We note that as ϵ tends to 0, the approximate equalities will become exact equalities. To show this, we know that Lagrangian is a function that depends on time t.

$$L(t) = K(\boldsymbol{v}(t)) - U(\boldsymbol{r}(t))$$

By mean value theorem, we know that there exists t_m such that for $t_1 < t_m < t_2$ we have

$$\frac{\int_{t_1}^{t_2} L(t)dt}{t_2 - t_1} = L(t_m)$$

Invoking another mean value theorem, K_{ave} then can be expressed as

$$K_{ave} = \frac{1}{2}m\frac{(\boldsymbol{y} - \boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x})}{\epsilon^2} = \frac{1}{2}m\boldsymbol{v}_v \cdot \boldsymbol{v}_v$$

Where component of $\boldsymbol{v}_v$ are defined such that for each components y_i and x_i of $\boldsymbol{y}$ and $\boldsymbol{x}$ there exists some $t_{v,i}$ with $t_1 < t_{v,i} < t_2$, s.t.

$$\frac{y_i - x_i}{t_2 - t_1} = \frac{\int_{t_1}^{t_2} v_i(t)\, dt}{t_2 - t_1} = v_i(t_{v,i})$$

Or to be explicit $v_i(t_{v,i})$'s are components of $\boldsymbol{v}_v$.

We can express $\frac{1}{2}(\boldsymbol{x} + \boldsymbol{y}) = \boldsymbol{z}$, assuming component z_i of $\boldsymbol{z}$ lies in between components y_i and x_i of $\boldsymbol{y}$ and $\boldsymbol{x}$ as well as the continuity of $\boldsymbol{r}(t)$ within $t_1 \leq t \leq t_2$, then by intermediate value theorem for each components z_i of $\boldsymbol{z}$ we have for some $t_{x,i}$ with $t_1 < t_{x,i} < t_2$,

$$z_i = r_i(t_{x,i})$$

Then substituting back we have

$$S = \int_{t_1}^{t_2} Ldt = L(t_m)\epsilon$$
$$= \left\{\frac{1}{2}m\boldsymbol{v}(t_m) \cdot \boldsymbol{v}(t_m) - U(\boldsymbol{r}(t_m))\right\}\epsilon$$
$$L_{ave}\epsilon = \left\{\frac{1}{2}m\boldsymbol{v}_v \cdot \boldsymbol{v}_v - U(\boldsymbol{z})\right\}\epsilon$$

Now taking the limit as $t_2 \to t_1$, and by squeeze theorem we have for each $t_{v,i}$'s and $t_{x,i}$'s

$$t_1 = t_{v,i} = t_m = t_{x,i} = t_2$$

Thus, $L_{ave}\epsilon \to S$ as $\epsilon = t_2 - t_1 \to 0$.

The approximation also applies to velocity dependent potential, though our derivation involves only position-only dependent potential.

Plugging $L_{ave}\epsilon$ as approximation for the action we have

$$G(\boldsymbol{x}, \boldsymbol{y}) = A\, exp\left(\frac{iS}{\hbar}\right) \approx exp\left(\frac{im}{2\hbar\epsilon}(\boldsymbol{y} - \boldsymbol{x})^2\right) \exp\left(-\frac{i}{\hbar}\epsilon U\left(\frac{1}{2}(\boldsymbol{x} + \boldsymbol{y})\right)\right)$$

Wherein A is undetermined constant to be fitted into the equation. Plugging back into the integral equation, while setting $t_1 = t$, yields

$$\Psi(\boldsymbol{x}, t + \epsilon) \approx \int A\, exp\left(\frac{im}{2\hbar\epsilon}(\boldsymbol{y} - \boldsymbol{x})^2\right) \exp\left(-\frac{i}{\hbar}\epsilon U\left(\frac{1}{2}(\boldsymbol{x} + \boldsymbol{y})\right)\right) \times \Psi(\boldsymbol{y}, t)d^3y$$

As ϵ tends to 0 we want the above approximate equality to turn into an exact equality. The second exponential will fall off to 1. Then by suitably choosing proportionality constant A we have

$$\Psi(\boldsymbol{x}, t + \epsilon) \approx \int A\, exp\left(\frac{im}{2\hbar\epsilon}\sum(y_j - x_j)^2\right) \times \Psi(\boldsymbol{y}, t)d^3y$$

From Gaussian integral we know of $\int_{-\infty}^{\infty} \exp(-\gamma x^2)\, dx = \sqrt{\frac{\pi}{\gamma}}$. Thus, the proportionality constant, to make the right and left hand side equals as $\epsilon \to 0$, is required to be

$$A = \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{3}{2}}$$

But we also know of a Dirac delta representation $\delta(x) = \lim_{\alpha\to 0}\frac{1}{\sqrt{2\pi i\alpha}}\exp(\frac{ix^2}{2\alpha})$. That is the proportionality constant turns our propagator into a representation of Dirac delta as $\epsilon \to 0$. Thus, the propagator function indeed reduce to Dirac delta as $\epsilon = t_2 - t_1 \to 0$. Hence, as $\epsilon \to 0$, we have

$$\Psi(\boldsymbol{x},t) = \int \prod_{j=1}^{3}\{\delta(y_j - x_j)\} \times \Psi(\boldsymbol{y},t)d^3y$$

Computationally it means that we only need to integrate over a small neighborhood of $\boldsymbol{x}$ to know how the wave function behaves in short time ϵ.

Expansion and Helpful Identities

From here on, we'll derive Schrodinger Equation following roughly Feynman's[3] leads.
Starting with

$$\Psi(\boldsymbol{x},t+\epsilon) \approx \int A \prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}(y_j - x_j)^2\right)\right\}\exp\left(-\frac{i}{\hbar}\epsilon U\left(\frac{1}{2}(\boldsymbol{x}+\boldsymbol{y})\right)\right) \times \Psi(\boldsymbol{y},t)d^3y$$

Use substitution $\boldsymbol{\zeta} = \boldsymbol{y} - \boldsymbol{x}$, to get

$$\Psi(\boldsymbol{x},t+\epsilon) \approx \int A \prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)\right\}\exp\left(-\frac{i}{\hbar}\epsilon U\left(\boldsymbol{x}+\frac{\boldsymbol{\zeta}}{2}\right)\right) \times \Psi(\boldsymbol{x}+\boldsymbol{\zeta},t)d^3\zeta$$

Expanding everything out[4], except $exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)$ factor, like what Feynman did gives

$$\beta \coloneqq -\frac{i}{\hbar}\epsilon U\left(\boldsymbol{x}+\frac{\boldsymbol{\zeta}}{2}\right)$$

$$exp(\beta) = 1 + \beta + \frac{\beta^2}{2!} + \frac{\beta^3}{3!} + \cdots$$

$$U\left(\boldsymbol{x}+\frac{\boldsymbol{\zeta}}{2}\right) = \left\{1 + \left(\sum_{j=1}^{3}\frac{\zeta_j}{2}\frac{\partial}{\partial x_j}\right) + \frac{1}{2!}\left(\sum_{j=1}^{3}\frac{\zeta_j}{2}\frac{\partial}{\partial x_j}\right)^2 + \cdots + \frac{1}{n!}\left(\sum_{j=1}^{3}\frac{\zeta_j}{2}\frac{\partial}{\partial x_j}\right)^n + \cdots\right\}U(\boldsymbol{x})$$

$$\Psi(\boldsymbol{x}+\boldsymbol{\zeta},t) = \left\{1 + \left(\sum_{j=1}^{3}\zeta_j\frac{\partial}{\partial x_j}\right) + \frac{1}{2!}\left(\sum_{j=1}^{3}\zeta_j\frac{\partial}{\partial x_j}\right)^2 + \cdots + \frac{1}{n!}\left(\sum_{j=1}^{3}\zeta_j\frac{\partial}{\partial x_j}\right)^n + \cdots\right\}\Psi(\boldsymbol{x},t)$$

We know of Gaussian integral

$$\int_{-\infty}^{\infty}\exp(-\gamma x^2)\,dx = \sqrt{\frac{\pi}{\gamma}}$$

Using Feynman's favorite, differentiating under the integral sign gives

$$\int_{-\infty}^{\infty}x^2\exp(-\gamma x^2)\,dx = \frac{1}{2\gamma}\sqrt{\frac{\pi}{\gamma}}$$

Differentiating γ n times we have

$$\int_{-\infty}^{\infty}(-x^2)^n\exp(-\gamma x^2)\,dx = \frac{\partial^n}{\partial\gamma^n}\sqrt{\frac{\pi}{\gamma}}$$

$$\frac{\partial^n}{\partial\gamma^n}\sqrt{\frac{\pi}{\gamma}} = \left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)\left(-\frac{5}{2}\right)\dots\left(-\frac{2n-1}{2}\right)\sqrt{\pi}\gamma^{-\frac{2n+1}{2}}$$

$$= \left(-\frac{1}{2}\right)^n(2n-1)!!\sqrt{\pi}\,\gamma^{-\frac{2n+1}{2}}$$

$$\int_{-\infty}^{\infty}(x^2)^n\exp(-\gamma x^2)\,dx = \frac{1}{2^n}(2n-1)!!\sqrt{\pi}\,\gamma^{-\frac{2n+1}{2}}$$

For $n > 0$, where we have defined $l!! = 1 \times 3 \times 5 \times \dots \times l$ as double factorial.

Other identities which will be of uses are

$$\int_{-\infty}^{\infty}(odd\ function)dx = 0$$

$$(odd\ function) \times (even\ function) = (odd\ function)$$

We have a formula for trinomial expansion

$$(A+B+C)^n = \sum_{i,j,k}\frac{n!}{i!\,j!\,k!}A^iB^jC^k$$

While $i + j + k = n$
With above identities it's possible to evaluate every terms of

$$\Psi(\boldsymbol{x},t+\epsilon) \approx \int A \prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)\right\} \times \left(1 + \beta + \frac{\beta^2}{2!} + \frac{\beta^3}{3!} + \cdots\right) \times \Psi(\boldsymbol{x}+\boldsymbol{\zeta},t)d^3\zeta$$

Derivation

To ease our calculation we'll state it beforehand that we'll divide both sides of the integral equation by ϵ, and take the limit $\epsilon \to 0$, making any nonlinear terms of ϵ in the $exp(\beta)$ factor dies off. So, we have

$$\Psi(\boldsymbol{x},t+\epsilon) \approx \int A \prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)\right\} \times \{\Psi(\boldsymbol{x}+\boldsymbol{\zeta},t) + \beta\Psi(\boldsymbol{x}+\boldsymbol{\zeta},t)\}d^3\zeta$$

To get more picture on what's happening inside each terms we will write out expanded form of the equation. First, we redefine some terms to avoid notational mess.

$$N_n = \frac{1}{n!}\left(\sum_{j=1}^{3}\zeta_j\frac{\partial}{\partial x_j}\right)^n\Psi(\boldsymbol{x},t)$$

$$P_p = \frac{1}{p!}\left(\sum_{j=1}^{3}\zeta_j\frac{\partial}{\partial x_j}\right)^p\Psi(\boldsymbol{x},t)$$

$$O_o = \frac{1}{o!}\left(\sum_{j=1}^{3}\frac{\zeta_j}{2}\frac{\partial}{\partial x_j}\right)^o U(\boldsymbol{x})$$

With above notations we have

$$\Psi(\boldsymbol{x}+\boldsymbol{\zeta},t) = \sum_{n=0}^{\infty} N_n = \sum_{p=0}^{\infty} P_p$$

$$\beta = -\frac{i}{\hbar}\epsilon U\left(\boldsymbol{x}+\frac{\boldsymbol{\zeta}}{2}\right) = -\frac{i}{\hbar}\epsilon\sum_{o=0}^{\infty} O_o$$

Hence the integral equation may be expressed as

$$\Psi(\boldsymbol{x},t+\epsilon) \approx \int A\prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)\right\}\times\left(\sum_{n=0}^{\infty}N_n\right)d^3\zeta$$
$$-\frac{i}{\hbar}\epsilon\int A\prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)\right\}$$
$$\times\left(\sum_{o=0}^{\infty}O_o\right)\left(\sum_{p=0}^{\infty}P_p\right)d^3\zeta$$

Notice how each terms with odd n in the first integral term all have odd power with respect to one or more of three variables. Because only odd+even equals odd, implying one (or more) of the variables have odd power(s) whenever n is odd. Thus making the integrand odd function with respect to that variable(s), hence making them vanishes when evaluated. Similarly, each terms of the 2nd integral may be expressed as terms of $(\sum\zeta_j)^o(\sum\zeta_j)^p$, for each terms having odd $o+p$, all of the expanded terms have odd power with respect to one or more variables. Thus, we only need to evaluate terms having even n and even $o+p$ and drop the odd terms. Also any terms in the sum having odd power with respect to one or more variables will automatically vanishes when evaluated, reducing further the number of terms needed to be evaluated.

Yet for further ease of the calculation, we state it again that in the last step of the derivation we'll divide both side of the integral equation by ϵ and take the limit $\epsilon\to 0$. We know that only terms having at most $\epsilon^{5/2}$ will survive, since A contributes $\epsilon^{-3/2}$ and again ϵ^{-1} from the final step. From Gaussian integral we know that only terms having $\left(\int_{-\infty}^{\infty}\exp(-\gamma\zeta^2)\,d\zeta\right)^3$ or $\left(\int_{-\infty}^{\infty}\exp(-\gamma\zeta^2)\,d\zeta\right)^2\times\int_{-\infty}^{\infty}\zeta^2\exp(-\gamma\zeta^2)\,d\zeta$ will survives, since they contributes $\gamma^{-3/2}$ and $\gamma^{-5/2}$ or $\epsilon^{3/2}$ and $\epsilon^{5/2}$ respectively.

Now having enough information about quite a few of simplifications that may be made, let's start calculating the first few terms that we know won't vanish.

Lowest order of first integral term (n=0)

$$\int A\prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)\right\}\Psi(\boldsymbol{x},t)d^3\zeta = \Psi(\boldsymbol{x},t)$$

1st order of the first integral vanishes (n=1)

2nd order of first integral term (n=2)

$$\frac{1}{2}\int A\prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)\right\}\sum_{j=1}^{3}\zeta_j^2\frac{\partial^2}{\partial x_j^2}\Psi(\boldsymbol{x},t)d^3\zeta$$
$$=\frac{i\hbar\epsilon}{2m}\sum_{j=1}^{3}\frac{\partial^2\Psi(\boldsymbol{x},t)}{\partial x_j^2} = \frac{i\hbar\epsilon}{2m}\nabla^2\Psi(\boldsymbol{x},t)$$

The mixed derivative terms of n=2 are odd function with respect to 2 variables thus vanishes (though only 1 needed to make them vanishes).

Lowest order of the second integral (o=p=0)

$$-\frac{i\epsilon}{\hbar}U(\boldsymbol{x})\int A\prod_{j=1}^{3}\left\{exp\left(\frac{im}{2\hbar\epsilon}\zeta_j^2\right)\right\}\Psi(\boldsymbol{x},t)d^3\zeta$$
$$= -\frac{i\epsilon}{\hbar}U(\boldsymbol{x})\Psi(\boldsymbol{x},t)$$

Higher order terms of the two integrals have nonlinear factor of ϵ when evaluated, thus vanishes in the final step, hence gathering terms we obtain

$$\Psi(\boldsymbol{x},t+\epsilon)\approx\Psi(\boldsymbol{x},t)-\frac{i\epsilon}{\hbar}U(\boldsymbol{x})\Psi(\boldsymbol{x},t)+\frac{i\hbar\epsilon}{2m}\nabla^2\Psi$$

Multiplying by $i\hbar$ for both sides and rearranging we have

$$i\hbar\frac{\Psi(\boldsymbol{x},t+\epsilon)-\Psi(\boldsymbol{x},t)}{\epsilon}\approx U(\boldsymbol{x})\Psi(\boldsymbol{x},t)-\frac{\hbar^2}{2m}\nabla^2\Psi$$

Taking as $\epsilon\to 0$ it is exactly the (time-dependent) Schrodinger Equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(\frac{-\hbar^2}{2m}\nabla^2+U\right)\Psi$$

All of previous approximate equalities turned into exact equalities since we have made it such that each of above equalities turn exact upon only one condition, that is limiting $\epsilon\to 0$. Hence stating that propagator function of quantum mechanical wave function is equal to $A\exp(iS/\hbar)$, with suitably chosen constant A, makes it equivalent with Schrodinger's Equation, with the former being integral equation and the later differential equation.

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