Note: Where is the Commutation Relation Hiding in the Path Integral Formulation?

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The path integral formulation of quantum mechanics has an advantage over the canonical quantization approach, namely that it provides a more physical intuition to how quantum mechanics arise via summing over paths. Nevertheless, it is mathematically challenging to make sense of path integral. In addition, the [canonical] commutation relation $[\hat{q}, \hat{p}] = i\hbar$ is not apparent in the path integral formulation. Since the commutation relation is central to quantum mechanics, it has to be hidden somewhere within the path integration. This note aims to explain this important issue that nevertheless is not discussed in most textbooks.

> *"There are in this world optimists who feel that any symbol that starts off with an integral sign must necessarily denote something that will have every property that they should like an integral to possess. This is of course quite annoying to us rigorous mathematicians; what is even more annoying is that by doing so they often come up with the right answer."* - E. J. McShane [1]

I. INTRODUCTION: A TOURIST GUIDE TO PATH INTEGRAL

The [Feynman] path integral formulation to quantum mechanics, and subsequently to quantum field theory, can be found in many standard textbooks [2, 3], and so we will not explain it in details. The essential ideas is nicely discussed in [4]: Recall the famous double-slit experiment in quantum mechanics, in which a beam of electrons is fired through two slits. If the electrons are classical particles like tiny balls, then we should expect the screen to have two bright strips corresponding to where the electrons hit, i.e. we would *not* expect interference pattern, which is a characteristic of wave. However, when the experiment is conducted, we observe interference pattern – electrons *do* have wave properties! It is not that the electrons are interfering with each other and thus somehow cause the interference pattern, since by firing the electrons *one at a time*, interference pattern still build up gradually as more and more electrons go through the slits. Quantum mechanically, we often say that the wave function will be the sum of two possible states: one that passes through slit A and one that passes through slit B, and the wave function is in a superposition of states. However there is no reason why we should stop at two slits, we could have three, and then the wave function will be the sum of three possible states. We can also have more than one screen. Therefore we could have say, first screen with 2 slits, second screen with 3 slits etc. and stack them all together. That is, we have to consider all the probabilities of particle passing through the i-th slit of the k-th screen. Now imagine that we increase the number of screens and the number of slits and continue to do so in the limit towards infinity. In the limit with infinitely many slits, *the slits are not there anymore!* Therefore we reached a seemingly absurd [what isn't in quantum mechanics?] conclusion that even in empty space without physical screens, we have to consider the probabilities of the particles taking *all* possible paths from one point to another instead of just the classical path [which is the unique path determined by solving differential equation of the Newtonian equation of motion given some initial condition.] As Zee described it, this is almost Zen.

Although the path integral formulation is made precise by Richard Feynman [5], who also showed that the Schrödinger's equation and the commutation relation can be recovered from path integral formulation, the formulation itself was first invented by Paul Dirac [6], who first formulated the amplitude of a particle to propagate from a point q_i to another point q_f in time $t = t_f - t_i$ by

$$\left\langle q_f \left| e^{-i\hat{H}t} \right| q_i \right\rangle = \int Dq(t) e^{i\int_0^T dt L(q,\dot{q})}, \tag{1}$$

where $\hat{H}$ is the Hamiltonian operator and L is the [classical] Lagrangian. The expression on the left hand side is called the *propagator*

$$K(q_i, q_f; t) = \left\langle q_f \left| e^{-it\hat{H}/\hbar} \right| q_i \right\rangle. \tag{2}$$

II. A MATHEMATICIAN'S LAMENT

Before we review the path integration formulation in more details, we make some remarks about the mathematical problems concerning the path integral. Despite the successfully predicting power of Feynman path integral, it lacks mathematical rigor. Trained as a mathematician, I have difficulty accepting the validity of path

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integral, and for that matter, most of quantum field theory; although as a physicist, I know how to use them and to wave my hands as necessary, deep down I am deeply troubled.

To see why path integral is problematic, note that in Eq.(1), the integration is more appropriately denoted by $\int_\Gamma D\gamma$ where $\gamma : [t_i, t_f] \to \mathbb{R}^d$ is any path connecting the endpoints $\gamma(t_i) = q_i$ and $\gamma(t_f) = q_f$, and Γ is the space of such paths. Here $D\gamma$ should be thought of as a Lebesgue-type measure on the space Γ of paths. Unfortunately, this Lebesgue-type measure *simply does not exist.* This follows from the well-known result in functional analysis that a [nontrivial] translational invariance Lebesgue-type measure cannot be defined on infinite dimensional Hilbert spaces. However, even before Feynman, there already exists similar ideas of path integration, albeit it is formulated to deal with Brownian motion instead of quantum mechanics. This is the *Wiener integral*, formulated by American mathematician Norbert Wiener who made major contributions to stochastic and noise processes as well as cybernetics [In fact, the one-dimensional version of Brownian motion is known as the *Wiener process*, we will return to this later]. Feynman however made no mention of Wiener's works in his paper.

The Wiener measure is not translationally invariance, and one wonders if the Feynman path integral can be understood in a similar way. It turns out that the answer is no: in 1960, Cameron proved that it is not possible to construct "Feynman measure" as a Wiener measure with a complex variance, i.e. as limit of finite dimensional approximations of the expression

$$\frac{e^{\frac{i}{\hbar}\int_0^t \frac{m}{2}\dot{\gamma}(s)^2 ds} D\gamma}{\int e^{\frac{i}{\hbar}\int_0^t \frac{m}{2}\dot{\gamma}(s)^2 ds} D\gamma} \tag{3}$$

as the resulting measure would have infinite total variation, even on bounded sets in path space. This is not the case for the usual Lebesgue measure on $\mathbb{R}^d$, which has finite total variation on *bounded* measurable subsets of $\mathbb{R}^d$. More discussions on the attempts to make mathematical sense of the path integral formulation can be found in the first chapter of [8]. One relatively simple way to make path integral more sensible is to do a "Wick-rotation" by analytic continuation and consider instead a damping factor e^{-S} instead of oscillatory one e^{iS}, where $S = \int_0^t dt\, L(q, \dot{q})$. One then gets precisely a Wiener path integration, which *does* make sense. After calculation has been performed, one can then Wick-rotate back and read off the final answer. Unfortunately, there are subtleties involved in this approach and not all Feynman path integrals allow Wick-rotation.

It must be emphasized that Feynman himself was aware of the lack of rigor in his work, as evidenced from his paper [5] in which he wrote that:

> [...] *one feels like Cavalieri must have felt calculating the volume of a pyramid before the invention of the calculus.*

I often feel that this remark is in a sense too modest. A more appropriate analogy would be that of calculus in its early days, more specifically when it was still plagued by infinitesimals – a very small quantity which is greater than zero yet less than any positive number, if you will. Sometimes we still think in this way, especially in physics (but this is because we already know that if we wish, we could always make it rigorous). The philosopher Berkeley was the first one to challenge the foundation of calculus. He remarked:

> *They are neither finite quantities nor quantities infinitely small, nor yet nothing. May we not call them the ghosts of departed quantities?*

It was due to criticism like this that finally led to rigorous formulation of calculus in terms of ϵ and δ now dreaded by beginning mathematics students [7]. Nevertheless, calculus has yielded many amazing results ever since it was invented by Newton and Leibniz, despite lacking rigorous foundation until Berkeley's objection. This is precisely the state we are currently in for path integration formulation of quantum mechanics.

III. REVIEW OF PATH INTEGRAL FORMULATION

In view of the discussion on the mathematical difficulties in interpreting Feynman path integration, we will make Wick-rotation by setting $\tau = it/\hbar$ and calculate instead the *Euclidean propagator*

$$K(q_i, q_f; \tau) = \left\langle q_f \left| \left(e^{-\frac{\tau \hat{H}}{N}}\right)^N \right| q_i \right\rangle \tag{4}$$

$$= \left\langle q_f \left| e^{-\epsilon \hat{H}} \cdots e^{-\epsilon \hat{H}} \right| q_i \right\rangle; \quad \epsilon = \frac{\tau}{N} \tag{5}$$

$$\tag{6}$$

We can now insert $N-1$ copies of the completeness relation

$$\int_{\mathbb{R}} dq_i \, |q_i\rangle \langle q_i| = 1 \tag{7}$$

into the propagator and obtain

$$K(q_i,q_f;t) = \int_{\mathbb{R}} dq_{N-1}\cdots\int_{\mathbb{R}} dq_1 \left\langle q_f \left| e^{-\epsilon\hat{H}} \right| q_{N-1}\right\rangle \left\langle q_{N-1} \left| e^{-\epsilon\hat{H}} \right| q_{N-2}\right\rangle \cdots \left\langle q_1 \left| e^{-\epsilon\hat{H}} \right| q_i\right\rangle . \quad (8)$$

Now each factor

$$\left\langle q_{i+1} \left| e^{-\epsilon\hat{H}} \right| q_i\right\rangle = \int_{\mathbb{R}} dp \left\langle q_{i+1} \left| e^{-\epsilon\hat{H}} \right| p\right\rangle \langle p|q_i\rangle \quad (9)$$

$$= e^{-\epsilon V(q_i)} \int_{\mathbb{R}} dp\; e^{-\frac{\epsilon p^2}{2m}} \left[\frac{e^{\frac{ip(q_{i+1}-q_i)}{\hbar}}}{2\pi\hbar}\right] \quad (10)$$

$$= \frac{e^{-\epsilon V(q_i)}}{2\pi\hbar}\left[\sqrt{\frac{2\pi m}{\epsilon}} e^{-\frac{(q_{i+1}-q_i)^2}{(2\epsilon/m)\hbar^2}}\right] \quad (11)$$

$$= \frac{1}{2\pi\hbar}\sqrt{\frac{2\pi m}{\epsilon}} e^{-\frac{m}{2\epsilon\hbar^2}(q_{i+1}-q_i)^2} e^{-\epsilon V(q_i)} \quad (12)$$

$$\equiv N(\epsilon) e^{\epsilon\mathcal{L}}, \quad (13)$$

where

$$N(\epsilon) \equiv \frac{1}{\hbar}\sqrt{\frac{m}{2\pi\epsilon}}, \quad (14)$$

and

$$\mathcal{L} = -\frac{m}{2\hbar^2}\left(\frac{q_{i+1}-q_i}{\epsilon}\right)^2 - \frac{1}{2}\left[V(x_{i+1}) + V(x_i)\right], \quad (15)$$

where we have used the *mid-point prescription* to the potential term discretization. In the second equality above we have used the fact that

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}, \quad (16)$$

while in the third line we have evaluated the Gaussian-type integral via the standard formula

$$\int_{\mathbb{R}} (e^{-\frac{1}{2}ax^2 + iJx})\; dx = \sqrt{\frac{2\pi}{a}} e^{-\frac{J^2}{2a}}. \quad (17)$$

Hence, with $q_0 = q_i$ and $q_N = q_f$, we have

$$K(q_i,q_f,\tau) = \int_{\mathbb{R}} \prod_{n=1}^{N-1} dq_n \prod_{n=0}^{N-1} \left\langle q_{n+1} \left| e^{-\epsilon\hat{H}} \right| q_n\right\rangle \quad (18)$$

$$= \int_{\mathbb{R}} \prod_{n=1}^{N-1} dq_n \prod_{n=0}^{N-1} N(\epsilon) e^{\epsilon\mathcal{L}(q_{n+1},q_n)} \quad (19)$$

$$= \int_{\mathbb{R}} \prod_{n=1}^{N-1} dq_n \left(\frac{m}{2\pi\epsilon\hbar^2}\right)^{\frac{N}{2}} e^{\epsilon\sum_{n=0}^{N-1}\mathcal{L}(x_{n+1},x_n)}. \quad (20)$$

Thus,

$$K(q_i,q_f;\tau) \equiv \int Dq e^{-S} \quad (21)$$

where

$$\int Dq \equiv \int_{\mathbb{R}} \prod_{n=1}^{N-1} dq_n \left(\frac{m}{2\pi\epsilon\hbar^2}\right)^{\frac{N}{2}}, \quad (22)$$

and

$$S = \epsilon\sum_{n=0}^{N-1}\frac{m}{2\hbar^2}\left(\frac{q_{n+1}-q_n}{\epsilon}\right)^2 - \epsilon\sum_{n=0}^{N-1} V(q_n). \quad (23)$$

Taking formal limit $\epsilon \to 0$,

$$S \to \int_0^\tau \frac{m}{2\hbar^2}\left(\frac{dq}{d\tau}\right)^2 + V(q). \quad (24)$$

Upon Wick-rotate back to Minkowski time we finally obtain

$$K = \int Dq\; e^{iS/\hbar};\;\; S = \int_0^t \left[\frac{m}{2}\left(\frac{dq}{dt}\right)^2 - V(q)\right] dt \quad (25)$$

IV. WHERE IS THE COMMUTATION RELATION HIDING?

We now begin to track down the commutation relation. This section is based on the useful Appendix A of [9] as well as on the original paper of Feynman [5]. For simplicity we first set $\hbar = 1$.

Without loss of generality we can take $t_i = 0$ and $t_f = T$. Then in the equation

$$\langle q_f, T|q_i, 0\rangle = \int dq \,\langle q_f, T|q, t\rangle \langle q, t|q_i, 0\rangle . \quad (26)$$

One may write each of the amplitudes as a path integral and thus finds

$$\int [dq]_{q_i,0}^{q_f,T} e^{i\int_0^T dt L} = \int dq \int [dq]_{q_i,t}^{q_f,T} e^{i\int_t^T dt\ L} \int [dq]_{q_i,0}^{q_f,t} e^{i\int_0^t dt\ L}, \quad T \geq t \geq 0. \tag{27}$$

That is, the path integral on $[0, T]$ breaks up into separate path integrals on $[0, t]$ and $[t, T]$ and an ordinary integral over $q(t)$.

Consider now a path integral with the additional insertion of a factor of $q(t)$, where $0 < t < T$. Then we have

$$\int [dq]_{q_i,0}^{q_f,T} e^{iS} q(t) = \int dq \langle q_f, T|q, t\rangle\, q\, \langle q, t|q_i, 0\rangle \tag{28}$$

$$= \int dq \langle q_f, T\,|\hat{q}(t)|\, q, t\rangle \langle q, t|q_i, 0\rangle \tag{29}$$

$$= \langle q_f, T\,|\hat{q}(t)|\, q_i, 0\rangle\,. \tag{30}$$

Therefore we see that: *$q(t)$ in the functional integral translates into $\hat{q}(t)$ in the matrix element.* Similarly we can show that for a product of two insertions $q(t)q(t')$ [which, being variables of integration, is equal to $q(t')q(t)$], where $t, t' \in [0, T]$, we have

$$\int [dq]_{q_i,0}^{q_f,T} e^{iS} q(t)q(t') = \langle q_f, T\,|T[\hat{q}(t)\hat{q}(t')]|\, q_i, 0\rangle\,, \tag{31}$$

where T denotes the time-ordered product

$$T[\hat{A}(t)\hat{B}(t')] = \theta(t-t')\hat{A}(t)\hat{B}(t') + \theta(t'-t)\hat{B}(t)\hat{A}(t), \tag{32}$$

where θ denotes the Heaviside Step Function. That is, *The order of terms in a matrix operator product corresponds to an order in time of the corresponding factors in the path integral.*

Indeed, due to the way the path integral is constructed out of successive infinitesimal time slices, two or more insertions in the path integral will always correspond to the time-ordered product of operators in the matrix element. Now, the equation of motion is obtained via taking the functional derivative

$$\frac{\delta S}{\delta q(t)} = 0. \tag{33}$$

Indeed, we have, via integration by part,

$$\int [dq]_{q_i,0}^{q_f,T} e^{iS} \frac{\delta S}{\delta q(t)} F = -i \int [dq]_{q_i,0}^{q_f,T} \left[\frac{\delta}{\delta q(t)} e^{iS}\right] F \tag{34}$$

$$= i \int [dq]_{q_i,0}^{q_f,T} e^{iS} \frac{\delta F}{\delta q(t)}. \tag{35}$$

Thus, for initial state ψ_t and final state ψ_f, we have, upon restoring $\hbar$,

$$\left\langle \psi_f \left| \frac{\delta F}{\delta q_k} \right| \psi_t \right\rangle = -\frac{i}{\hbar} \left\langle \psi_f \left| F \frac{\delta S}{\delta q_k} \right| \psi_i \right\rangle. \tag{36}$$

Therefore, we see that two different functionals may give the same result for the transition element between any two states. We say that they are equivalent and symbolize the relation by

$$-\frac{\hbar}{i}\frac{\delta F}{\delta q_k} \overset{S}{\longleftrightarrow} F\frac{\delta S}{\delta q^k}. \tag{37}$$

Here the symbol $\overset{S}{\longleftrightarrow}$ emphasizes the fact that functionals equivalent under one action may not be equivalent under another. Now, discretizing, we have $S = \sum S(q_{i+1}, q_i)$ so that

$$-\frac{\hbar}{i}\frac{\delta F}{\delta q^k} \overset{S}{\longleftrightarrow} F\left[\frac{\delta S(q_{k+1}, q_k)}{\delta q^k} + \frac{\delta S(q_k, q_{k-1})}{\delta q^k}\right]. \tag{38}$$

This equation is correct to zero and first order in ϵ. *In this equation hides the Newtonian equations of motion, as well as the commutation relation.*

We recall from the previous section that in the one-dimensional quantum mechanical problem,

$$S(q_{k+1}, q_k) = \frac{m\epsilon}{2}\left[\frac{q_{k+1} - q_k}{\epsilon}\right]^2 - \epsilon V(q_{k+1}), \tag{39}$$

so we obtain

$$\frac{\delta S(q_{k+1}, q_k)}{\delta q_k} = -\frac{m(q_{k+1} - q_k)}{\epsilon}, \tag{40}$$

and

$$\frac{\delta S(q_k, q_{k-1})}{\delta q_k} = \frac{m(q_k - q_{k-1})}{\epsilon} - \epsilon V'(q_k) \tag{41}$$

where V' is the derivative of the potential, i.e. [minus of] force. Therefore,

$$-\frac{\hbar}{i}\frac{\delta F}{\delta q^k} \overset{S}{\longleftrightarrow} F\left[-m\left(\frac{q_{k+1} - q_k}{\epsilon} - \frac{q_k - q_{k-1}}{\epsilon}\right) - \epsilon V'(q_k)\right]. \tag{42}$$

If F does not depend on q_k, this gives Newton's equations of motion. Since the LHS is now zero, we get, upon dividing both sides by ϵ,

$$0 \overset{S}{\longleftrightarrow} -\frac{m}{\epsilon}\left(\frac{q_{k+1} - q_k}{\epsilon} - \frac{q_k - q_{k-1}}{\epsilon}\right) - V'(q_k), \tag{43}$$

i.e.

$$V'(q_k) \overset{S}{\longleftrightarrow} -\frac{m}{\epsilon}\left[\frac{q_{k+1} - q_k}{\epsilon} - \frac{q_k - q_{k-1}}{\epsilon}\right]. \tag{44}$$

In other words, the transition element of mass times acceleration between any two states is indeed equal to the transition element of force $-V'(q_k)$ between the same states.

Now, if F *does* depend upon q_k, say $F = q_k$, then we get

$$-\frac{\hbar}{i} \overset{S}{\longleftrightarrow} q_k \left[-m \left(\frac{q_{k+1} - q_k}{\epsilon} - \frac{q_k - q_{k-1}}{\epsilon} \right) - \epsilon V'(q_k) \right]. \quad (45)$$

Neglecting terms of order ϵ, one has

$$m \left(\frac{q_{k+1} - q_k}{\epsilon} \right) q_k - m \left(\frac{q_k - q_{k-1}}{\epsilon} \right) q_k \overset{S}{\longleftrightarrow} \frac{\hbar}{i}. \quad (46)$$

Taking extra care of the time ordering when going back to operator formulation, this is precisely the commutation relation

$$\hat{p}\hat{q} - \hat{q}\hat{p} = \frac{\hbar}{i}. \quad (47)$$

V. A WIENER PROCESS APPROACH TOWARDS NON-COMMUTATIVITY

We now briefly explain another method to extract the commutation relation out of the path integral, which is largely based on [10]. Instead of the Feynman's path integral, let us considered its Wick-rotated version, interpreted as a Wiener integral. Consider the Wiener process, which is just a one-dimensional random walk, with the [Euclidean] action

$$S = -\int \left(\frac{dq}{dt} \right)^2 dt. \quad (48)$$

The path $q(t)$ is fluctuating, with derivative defined as the limit of discrete difference:

$$\frac{\Delta q}{\Delta t} = \frac{q(t+\epsilon) - q(t)}{\epsilon}. \quad (49)$$

The product $q\dot{q}$ is actually ambiguous: it depends on the discretization, so that it can be interpreted as either

$$q(t) \frac{q(t+\epsilon) - q(t)}{\epsilon}, \quad (50)$$

or as

$$q(t+\epsilon) \frac{q(t+\epsilon) - q(t)}{\epsilon}. \quad (51)$$

The first corresponds to $\hat{q}(t)\hat{p}(t)$ while the second one represents $\hat{p}(t)\hat{q}(t)$ since the operator order is the time ordering as we have previously discussed. From the perspective of Stochastic calculus, the velocity is a *forward difference* in the Ito sense, and therefore is always slightly ahead in time.

The difference of the two yields

$$\frac{(q(t+\epsilon) - q(t))^2}{\epsilon}. \quad (52)$$

In ordinary calculus, the difference will go to zero in the limit $\epsilon \to 0$. However, this is not the case for Stochastic calculus. In particular, the distance a random walk moves is proportional to $\sqrt{t}$.

[Remark: One way to see this is as follows: The random variable dq in a sense, represents an accumulation of random influences over the interval dt. By the Central Limit Theorem, dq has a normal distribution. The variance of a random variable (which is the accumulation of independent effects over an interval of time) is proportional to the length of the interval, i.e. dt. The standard deviation of dq is thus proportional to the square root of dt].

Consequently,

$$q(t+\epsilon) - q(t) \sim \sqrt{\epsilon}. \quad (53)$$

This in turn implies that, we have from Eq.(52),

$$\frac{(q(t+\epsilon) - q(t))^2}{\epsilon} \sim \frac{\sqrt{\epsilon}^2}{\epsilon} = 1, \quad (54)$$

instead of zero. We thus obtained

$$[\hat{q}, \hat{p}] = 1, \quad (55)$$

the Euclidean version of the commutation relation. This is actually in essence, the consequence of the celebrated *Ito's Lemma*.

Upon Wick-rotating back to Lorentzian signature, we obtain ($\hbar = 1$)

$$[\hat{q}, \hat{p}] = i \quad (56)$$

in quantum mechanics.

We remark that the equalities obtained in Eq.(55) and Eq.(56) are actually only *weak equality*: they are valid only in the sense the of sense of distributions. For a Brownian motion, the result is actually saying that the position is correlated with the [infinite] value of the velocity [since the paths are actually continuous but non-differentiable, which is clear from Eq.(53), since the ratio that defines the derivative will diverge in the limit $\epsilon \to 0$], so that the future position is actually finitely correlated with the average velocity given the past position. The past value is of course completely uncorrelated with the current [forward] velocity.

VI. CONCLUSION

We conclude by merely emphasizing that discretization is crucial in the path integral formulation, for it is via careful analysis on the discretization that one can recover the commutation relation $[\hat{q}, \hat{p}] = i\hbar$ of quantum mechanics.

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