

Notes on a Histories Formulation of Quantum Mechanics

Rafael D. Sorkin, Perimeter Institute, September 2011

These notes introduce the formalism of the path-integral or “sum-over-histories”. Although the basic ideas are more general, we limit ourselves here to the nonrelativistic case of eternal point particles.

Histories and Events

We will consider the motion of a nonrelativistic point particle (or particles) and refer to its world line (or the collection of their world lines) as its *history*, denoting an arbitrary history by γ . Classical physics takes the point of view that each possible reality corresponds to a *single* such history γ . An *event* (like the event “it is raining outside”) then corresponds to a set A of histories such that the event happens if and only if γ belongs to A , i.e. if and only if $\gamma \in A$.^{*}

The dynamical laws and the predictions that result from them then tell us something about what the actual γ will do. But the laws never pin γ down fully. Even in a deterministic theory like classical Hamiltonian mechanics, they fail to specify the initial conditions; and in a stochastic theory like the theory of Brownian motion, the laws never furnish more than probabilities.

Now let us turn to the quantum world. From the histories standpoint, histories and events are still the basic concepts, but their relationship with reality is less straightforward than it was classically. The problem of sorting out this relationship, one might say, is precisely what the problem of quantum foundations is all about. The concept of “anahomomorphic coevent” gives rise to a particular proposal about how this is to be done,

^{*} As in the case of rain, the events of interest will usually consist of all histories that possess some property, and we will often use the same symbol to denote this subset of history-space and the property that selects it. For another example of an event, think of all the worldlines that pass through a given spacetime region.

according to which reality, rather than being a single history, is a kind of polynomial in histories. In the simplest case, it is simply a set of histories. However, the purpose of these notes is not to describe anhomomorphic coevents. Rather, we will stick to the path-integral formalism itself, aiming to show how quantum mechanics looks when presented in this way, and where familiar mathematical constructions like state-vectors, operators and the Schrödinger equation come from.

The quantum measure

The mathematics of path-integrals is much closer to the mathematics of stochastic processes than it is to that of Hamiltonian mechanics. For a classical stochastic process, the dynamics is specified by a *probability measure* μ on the space Ω of all histories. This measure assigns to every suitable subset $A \subseteq \Omega$ a positive real number $\mu(A) \in [0, 1]$ which is interpreted as the probability that event A actually happens. (Recall that the technical term *event* denotes a subset $A \subseteq \Omega$.) In the quantal generalization of this framework, the dynamics is specified by a *generalized measure* μ which assigns to the event $A \subseteq \Omega$ a positive real number, $\mu(A) \geq 0$.

In certain circumstances, one knows from experience that $\mu(A)$ can still be interpreted as the probability that event A happens. This is the meaning of the “Born rule” when A represents a “pointer reading” or macroscopic measurement outcome. But in general such a probability interpretation is not possible, since μ does not respect the additivity condition $\mu(A \sqcup B) = \mu(A) + \mu(B)$. Instead μ has to be used in a less direct manner to make predictions, and the required rules are still not very clear. It seems fair at a minimum to assert that events A with $\mu(A) = 0$ (or very tiny) are “precluded” in the sense that “for all practical purposes”, the event will not occur.

The basic formula that defines $\mu(A)$ in nonrelativistic quantum mechanics is the following.

$$\mu(A) = \int_{\gamma \in A^T} d\nu(\gamma) \int_{\bar{\gamma} \in A^T} d\nu(\bar{\gamma}) e^{iS(\gamma) - iS(\bar{\gamma})} \delta(\gamma(T), \bar{\gamma}(T)). \quad (1)$$

Here, A^T denotes the set of all histories that can be derived from elements of A by *truncation* at time T , $\gamma(t)$ denotes the location (in configuration space Q) of γ at time t , and

the “truncation time” $t = T$ can be chosen freely, as long as it is late enough for it to be decided by then whether or not $\gamma \in A$. In equation (1) there is also implicit some specification of initial conditions for γ . Except in a cosmological context, these will normally be given by an initial wave function — in effect a complex endpoint-contribution to $S(\gamma)$ — possibly in combination with the condition that γ belong to some specified subset of Ω . Notice that the integration variables γ and $\bar{\gamma}$ in (1) are completely independent dummy variables.

In equation (1), $S(\gamma)$ is called the *action-functional*, and it takes the form $S(\gamma) = \int dt L(t)$, where (for a single, nonrelativistic particle referred to some chosen reference frame)

$$L(t) = \frac{m\dot{\gamma}(t)^2}{2} - V(\gamma(t), t), \quad (2)$$

m being the particle’s mass and $V(q, t)$ the potential. Also, $e^{iS(\gamma)}$ is called the “amplitude” of γ and $d\nu(\gamma)$ is called the *integration-measure* or *measure-factor*. [This must not be confused with the quantum measure μ itself. Indeed, the analogy with the Wiener process suggests that in a rigorous formulation, neither $d\nu(\gamma)$ nor e^{iS} will be defined separately, and only their product will have meaning.]

We note without proof that μ obeys the sum rule,

$$\mu(A \sqcup B \sqcup C) - \mu(A \sqcup B) - \mu(B \sqcup C) - \mu(A \sqcup C) + \mu(A) + \mu(B) + \mu(C) = 0$$

where \sqcup is disjoint union. This sum rule implies that $\mu(A)$ can always be written as a double integral $\int_{\gamma \in A} d\nu(\gamma) \int_{\bar{\gamma} \in A} d\nu(\bar{\gamma})$ as in (1). It does not imply that the integrand takes the specific form appearing in (1), however.

In fact, even in nonrelativistic quantum mechanics, the form (1) requires generalization when non-bosonic identical particles are involved, and in certain other situations.*

* In the case of indistinguishable particles, one can sometimes circumvent the generalization by attaching artificial labels to the particles, thereby rendering them formally distinguishable. The effect of the statistical phase-factors is then absorbed into a symmetry-condition on the multi-particle wave function, this being the approach followed, implicitly, in most textbooks.

In such cases, an additional phase-factor $\chi(\gamma, \bar{\gamma})$ must be inserted into (1) which can depend on the topological class to which the *combined* path $\gamma \cup \bar{\gamma}$ belongs. The amplitude thus becomes a function of γ and $\bar{\gamma}$ jointly, rather than a product of separate amplitudes for γ and $\bar{\gamma}$. A similar viewpoint is helpful in connection with Galilean invariance and with motion in a magnetic field.

Wave functions and states

It is a feature of (1) that $\mu(A)$ can be expressed as

$$\mu(A) = \int |\psi_A(q, T)|^2 dq$$

where

$$\psi_A(q, T) = \int_{\gamma \in A^T} d\nu(\gamma) e^{iS(\gamma)} \delta(q, \gamma(T)) . \quad (3)$$

In this way, ψ summarizes everything about the subset A that is needed to compute $\mu(A)$. It also summarizes everything about A that is needed to compute the relative measure of some *future* subset B . In other words, if B is some condition on the portion of γ lying to the future of some time T_0 , and if the condition A lies to the past of T_0 , then we can compute $\mu(A \cap B)$ knowing nothing about A other than the ψ_A to which it gives rise at time T_0 . We have in fact,

$$\begin{aligned} \mu(B \cap A) = & \\ & \int_{\gamma \in B_{T_0}^{T_1}} d\nu(\gamma) \int_{\bar{\gamma} \in B_{T_0}^{T_1}} d\nu(\bar{\gamma}) e^{iS(\gamma) - iS(\bar{\gamma})} \delta(\gamma(T_1), \bar{\gamma}(T_1)) \psi_A(\gamma(T_0), T_0) \psi_A(\bar{\gamma}(T_0), T_0)^* , \quad (4) \end{aligned}$$

where T_1 is some truncation time to the future of the “support” [see equation (7)] of B and $B_{T_0}^{T_1} := \{\gamma: [T_0, T_1] \rightarrow Q \mid \gamma \text{ satisfies } B\}$. In this way, $\psi_A(\cdot, T_0)$ serves as an *initial condition* for predictions to the future of T_0 . Thus, ψ provides both a *summary of the past* and an *initial condition for the future*. It is inherent in the form of (1) that such summaries are possible, but there is no reason for this possibility to persist in more general forms of quantum mechanics. If it did not persist, then a wave function like $\psi(q, t)$ would no longer be useful.

For each time t (or more generally for each spacelike hypersurface), the possible wave functions $\psi(\cdot, t)$ form a Hilbert space that we will call \mathcal{H}_t , the inner product being given by

$$\langle \psi_2 | \psi_1 \rangle = \int dq \psi_2(q, t)^* \psi_1(q, t) . \quad (5)$$

Notice that there is a separate Hilbert space for each time (or hypersurface) t .

Functionals, propagators and operators

Let \mathcal{O} be a function that attaches a complex number $\mathcal{O}(\gamma)$ to each history γ . We will follow tradition in calling \mathcal{O} a *functional* in reference to the fact that its argument γ , a trajectory, can also be represented as a function. By writing

$$\text{supp } \mathcal{O} \subseteq (t_0, t_1) \quad \text{or} \quad t_0 < \text{supp } \mathcal{O} < t_1 \quad (6)$$

we mean that $\mathcal{O}(\gamma)$ depends only on the portion of γ between times t_0 and t_1 . We similarly write

$$\text{supp } A \subseteq (t_0, t_1) \quad (7)$$

to mean that the property defining the event A refers only to the portion of γ between times t_0 and t_1 . This is a special case of (6) if we take $\mathcal{O} = \chi_A$ to be the *characteristic function* of $A \subseteq \Omega$, i.e. the function defined by $\chi_A(\gamma) = 1$ if $\gamma \in A$, $\chi_A(\gamma) = 0$ if $\gamma \notin A$.

For given times $t_1 \leq t_2$ and a functional \mathcal{O} with support between t_1 and t_2 , we can define an operator $\mathcal{U}_{\mathcal{O}}(t_2, t_1): \mathcal{H}_{t_1} \rightarrow \mathcal{H}_{t_2}$ by the condition

$$\psi_2 = \mathcal{U}_{\mathcal{O}}(t_2, t_1)\psi_1 \iff \psi_2(q_2, t_2) = \int_{\gamma \in \Omega_{t_1}^{t_2}} d\nu(\gamma) \mathcal{O}(\gamma) e^{iS(\gamma)} \delta(q_2, \gamma(t_2)) \psi_1(\gamma(t_1)) \quad (8)$$

Here $\Omega_{t_1}^{t_2}$ is the set of all partial (or “truncated”) paths running between times t_1 and t_2 . When $\mathcal{O}(\gamma) \equiv 1$ we write $\mathcal{U}_{\mathcal{O}}$ as just plain \mathcal{U} and call it the “propagator”. When $\mathcal{O} = \chi_A$ for some event A , we write $\mathcal{U}_{\mathcal{O}}$ as \mathcal{U}_A and call it the “conditional propagator”. Clearly $\mathcal{U}(t_2, t_1)$ gives the propagation of the wave function ψ_A in (3) for times subsequent to the support of A : $\psi(\cdot, t_2) = \mathcal{U}(t_2, t_1)\psi(\cdot, t_1)$. It follows in particular that $\mathcal{U}(t_2, t_1)$ must be unitary in order to guarantee that the quantum measure (1) is well-defined, independently of truncation time T (cf. (10) below). Actually, all that is needed for this is that $\mathcal{U}^*\mathcal{U} = 1$,

however in ordinary quantum mechanics we also have $\mathcal{U}\mathcal{U}^* = 1$, so that \mathcal{U}^{-1} exists and is equal to the adjoint \mathcal{U}^* . Then for $s < t$, we can set $\mathcal{U}(s, t) := \mathcal{U}(t, s)^{-1}$. It follows immediately that

$$\mathcal{U}(r, s)\mathcal{U}(s, t) = \mathcal{U}(r, t) \quad (9)$$

for any three times r, s, t , whether they are in sequence or not.

Now let $\psi_0 \in \mathcal{H}_{t_0}$ be a summary of the past, $t < t_0$, in the sense of (3) and (4), and let $B \subseteq \Omega$ be such that $\text{supp } B \subseteq (t_0, t_1)$. If we relativize our quantum measure μ to the initial condition ψ_0 then we can express $\mu(B)$ in terms of the conditional propagator $\mathcal{U}_B(t_1, t_0)$ by a formula that follows directly from the definitions:

$$\mu(B) = \langle \psi_0, \mathcal{U}_B(t_1, t_0)^* \mathcal{U}_B(t_1, t_0) \psi_0 \rangle . \quad (10)$$

It follows from (9) and (10) that $\mu(B)$ is independent of t_1 as long as $t_1 > \text{supp } B$. In much the same manner, we can also define an operator $\widehat{\mathcal{O}}$ associated with a general path-functional \mathcal{O} . Given

$$t_0 < \text{supp } \mathcal{O} < t_1, \quad (11)$$

we put, for arbitrary t ,

$$\widehat{\mathcal{O}}_t = \mathcal{U}(t, t_1) \mathcal{U}_{\mathcal{O}}(t_1, t_0) \mathcal{U}(t_0, t). \quad (12)$$

It is clear that $\widehat{\mathcal{O}}_t$, defined in this way, is independent of the choices of t_0 and t_1 , provided that they respect (11). I will also write $\widehat{\mathcal{O}}$ as ‘**op**(\mathcal{O})’ when the expression \mathcal{O} is too long to accept a “hat” comfortably.

The basic idea of these definitions is that $\widehat{\mathcal{O}}$ expresses the effect on a wave function of re-weighting the path integral with a path-dependent factor $\mathcal{O}(\gamma)$; however, with $\psi = \psi_A$ given by (3), the effect of such a re-weighting will given by (12) only if, for some τ ,

$$\text{supp } A < \tau < \text{supp } \mathcal{O}.$$

In this situation, we evidently can write also, assuming $\tau < t_0 < \text{supp } \mathcal{O} < t_1$,

$$\widehat{\mathcal{O}}_{t_1} \psi_A(q_1, t_1) = \int_{\gamma \in \Omega_{t_0}^{t_1}} d\nu(\gamma) \mathcal{O}(\gamma) e^{iS(\gamma)} \delta(q_1, \gamma(t_1)) \psi_A(\gamma(t_0), t_0) \quad (13)$$

Notice in all this that the subscript t in $\widehat{\mathcal{O}}_t$ refers to the Hilbert space \mathcal{H}_t in which $\widehat{\mathcal{O}}_t$ acts; it has nothing to do with the time at which \mathcal{O} itself is defined. Normally we will be able to omit this t subscript by working within a given “picture”, as explained in the next section.

An important connection between time-order and operator-order follows from the definitions and equation (9):

Ordering rule If there exists a time τ such that

$$\text{supp } \mathcal{O}_1 > \tau > \text{supp } \mathcal{O}_2 ,$$

then

$$\widehat{\mathcal{O}_1 \mathcal{O}_2} = \widehat{\mathcal{O}_1} \widehat{\mathcal{O}_2}$$

where the equation just written is short for $(\widehat{\mathcal{O}_1 \mathcal{O}_2})_t = (\widehat{\mathcal{O}_1})_t (\widehat{\mathcal{O}_2})_t$, t being arbitrary.

By arbitrarily coordinatizing the configuration space at each moment of time (there is in general no natural notion of “time-independent coordinatization”, example: Galilean invariance) we can introduce the so called *position operator*. Pick some t and let the functional $\mathcal{O}(\gamma)$ be defined as the coordinate $q(t)$ of γ at time t . [We might express this more pedantically as $\mathcal{O}(\gamma) = q(t)(\gamma(t))$]. Then we define $(\widehat{q}(t))_s$ to be the operator $\widehat{\mathcal{O}}_s$; in other words we set

$$(\widehat{q}(t))_s := (\widehat{q(t)})_s . \tag{14}$$

Of course, \widehat{q} is really an n -tuple of operators if the configuration space has dimension n . It is immediate from the definitions that $(\widehat{q}(t))_t$ acts in \mathcal{H}_t by multiplying $\psi(q, t)$ by q . (You should prove this to yourself if it’s not obvious to you.) For $t \neq s$ on the other hand, $(\widehat{q}(t))_s$ has no such simple description.

Heisenberg picture, Schrödinger picture

The state vectors ψ_t that we have defined belong not to a single Hilbert space, but to a whole family of them — one space \mathcal{H}_t for each time t (or more generally for each Cauchy surface Σ). Normally it is convenient to eliminate this multiplicity of spaces by identifying the \mathcal{H}_t with each other in order to obtain a single “global” Hilbert space \mathcal{H} .

Depending on how the identification is carried out, one obtains thereby one or another “picture” (“Heisenberg”, “Schrödinger”, “Interaction”, ...). Notice in this connection that the vectors ψ_t are in the first instance functions of position at a given time. Other choices of basis for \mathcal{H}_t are of course possible (momentum basis, energy basis, Fok basis in field theory, etc.), but they appear as subsidiary to the position basis.

Perhaps the most natural identification spaces is that induced by $\mathcal{U}(t, s)$ itself, which leads to the so called Heisenberg picture. Let ‘ \sim ’ denote this equivalence relation: $\psi_t \sim \psi_s \iff \psi_t = \mathcal{U}(t, s)\psi_s$. Thanks to the unitarity of \mathcal{U} , the resulting space \mathcal{H} of equivalence classes inherits a well-defined hermitian metric from the \mathcal{H}_t . For $\psi_t \in \mathcal{H}_t$, let $|\psi_t, t\rangle$ denote $\text{cls}(\psi_t)$, the equivalence class of ψ_t in \mathcal{H} . Then our identification rule can be expressed by

$$|\psi', t'\rangle = |\psi, t\rangle \iff \psi' = \mathcal{U}(t', t)\psi \quad (15a)$$

or equivalently

$$|\mathcal{U}(t', t)\psi, t'\rangle = |\psi, t\rangle. \quad (15b)$$

One advantage of the Heisenberg picture is that the operators $\widehat{\mathcal{O}}_t$ defined in (12) act consistently with (15) and therefore can be interpreted as a single operator acting in \mathcal{H} , namely the operator $\widehat{\mathcal{O}}$ (no more subscript) defined by

$$\widehat{\mathcal{O}}|\psi, t\rangle = |\widehat{\mathcal{O}}_t\psi, t\rangle \quad (16)$$

The self-consistency of this definition should be clear diagrammatically. To check it in formulas, we must show that $|\psi', t'\rangle = |\psi, t\rangle \Rightarrow \widehat{\mathcal{O}}|\psi', t'\rangle = \widehat{\mathcal{O}}|\psi, t\rangle$. But from (12) and (15a,b),

$$\begin{aligned} \widehat{\mathcal{O}}|\psi', t'\rangle &= |\widehat{\mathcal{O}}_{t'}\psi', t'\rangle \\ &= |\mathcal{U}(t', t_1)\mathcal{U}_{\mathcal{O}}(t_1, t_0)\mathcal{U}(t_0, t')\psi', t'\rangle \\ &= |\mathcal{U}_{\mathcal{O}}(t_1, t_0)\mathcal{U}(t_0, t')\psi', t_1\rangle \\ &= |\mathcal{U}_{\mathcal{O}}(t_1, t_0)\mathcal{U}(t_0, t')\mathcal{U}(t', t)\psi, t_1\rangle \\ &= |\mathcal{U}_{\mathcal{O}}(t_1, t_0)\mathcal{U}(t_0, t)\psi, t_1\rangle \\ &= |\mathcal{U}(t, t_1)\mathcal{U}_{\mathcal{O}}(t_1, t_0)\mathcal{U}(t_0, t)\psi, t\rangle \\ &= |\widehat{\mathcal{O}}_t\psi, t\rangle \\ &= \widehat{\mathcal{O}}|\psi, t\rangle \end{aligned}$$

as required.

Another convenient characterization of $\widehat{\mathcal{O}}$ follows from (8). With $t_0 < \text{supp } \mathcal{O} < t_1$, this characterization reads $\langle \psi_1, t_1 | \widehat{\mathcal{O}} | \psi_0, t_0 \rangle = \langle \psi_1, \mathcal{U}_{\mathcal{O}}(t_1, t_0) \psi_0 \rangle$, or

$$\langle \psi_1, t_1 | \widehat{\mathcal{O}} | \psi_0, t_0 \rangle = \int_{\gamma \in \Omega_{t_0}^{t_1}} d\nu(\gamma) e^{iS(\gamma)} \psi_1^*(\gamma(t_1)) \mathcal{O}(\gamma) \psi_0(\gamma(t_0)). \quad (17)$$

proof:

$$\begin{aligned} \langle \psi_1, t_1 | \widehat{\mathcal{O}} | \psi_0, t_0 \rangle &= \langle \psi_1, t_1 | \widehat{\mathcal{O}}_{t_0} \psi_0, t_0 \rangle \\ &= \langle \psi_1, t_1 | \mathcal{U}(t_0, t_1) \mathcal{U}_{\mathcal{O}}(t_1, t_0) \psi_0, t_0 \rangle \\ &= \langle \psi_1, t_1 | \mathcal{U}_{\mathcal{O}}(t_1, t_0) \psi_0, t_1 \rangle \\ &= \langle \psi_1, \mathcal{U}_{\mathcal{O}}(t_1, t_0) \psi_0 \rangle. \end{aligned}$$

This last expression is a scalar product taken in \mathcal{H}_{t_1} . Written out as an integral, it is

$$\begin{aligned} &\int dq_1 \psi_1(q_1)^* [\mathcal{U}_{\mathcal{O}}(t_1, t_0) \psi_0](q_1) \\ &= \int dq_1 \psi_1(q_1)^* \int d\nu(\gamma) \mathcal{O}(\gamma) e^{iS(\gamma)} \delta(q_1, \gamma(t_1)) \psi_0(\gamma(t_0)) \\ &= \int d\nu(\gamma) \mathcal{O}(\gamma) e^{iS(\gamma)} \psi_1(\gamma(t_1))^* \psi_0(\gamma(t_0)), \end{aligned}$$

as claimed. As an example, we can apply (17) to the position functional $q(t)$ and obtain, in view of (14) and for $t_0 < t < t_1$,

$$\langle \psi_1, t_1 | \widehat{q}(t) | \psi_0, t_0 \rangle = \int d\nu(\gamma) e^{iS(\gamma)} \psi_1(\gamma(t_1))^* \gamma(t) \psi_0(\gamma(t_0)).$$

Other pictures are available to the extent that there exist other ways to identify the \mathcal{H}_t than via the path integral itself. For example, in a given spacetime reference frame we can identify the hypersurfaces $t = \text{constant}$ by pure translation in the time direction, giving rise to the so called Schrödinger picture. Such an identification is implicit in (2) for example. Let us introduce the notation $\Xi(t, t') : \mathcal{H}_{t'} \rightarrow \mathcal{H}_t$ for this identification and denote the resulting Hilbert space as \mathcal{H}^{Schr} . Clearly, a general functional $\mathcal{O}(\gamma)$ does *not* induce a consistently defined operator in \mathcal{H}^{Schr} . However, in special cases one can derive Schrödinger picture operators from suitable families of functionals. For example, if we

choose our coordinates $q(t)$ to be independent of time (in our chosen reference frame) then the family of operators $(\widehat{q(t)})_t$ acts coherently in the $\widehat{\mathcal{H}}_t$ because

$$\Xi(t', t) (\widehat{q(t)})_t = (\widehat{q(t')})_{t'} \Xi(t', t),$$

whence it defines in \mathcal{H}^{Schr} the ‘‘Schrödinger position operator’’ \widehat{q} . The difference between this operator and $\widehat{q}(t)$ in the Heisenberg picture is that to define $\widehat{q}(t)$, we held t fixed and varied s in $(\widehat{q(t)})_s$, whereas to define \widehat{q} we vary both t and s , keeping $t = s$.

Henceforth, operators $\widehat{\mathcal{O}}$ without temporal subscripts will always be in the Heisenberg picture, unless stated otherwise.

The equations of motion in operator form

In (17) let us take $\mathcal{O} = 1$ and make a change of variables $\gamma \rightarrow \gamma + \delta\gamma$ where $\delta\gamma$ is a fixed function vanishing at t_1 and t_0 . This yields (since $\delta\gamma(t_1) = \delta\gamma(t_0) = 0$)

$$\langle \psi_1, t_1 | \psi_0, t_0 \rangle = \int_{\gamma \in \Omega_{t_0}^{t_1}} d\nu(\gamma + \delta\gamma) e^{iS(\gamma + \delta\gamma)} \psi_1(\gamma(t_1))^* \psi_0(\gamma(t_0))$$

We now *assume* that the measure-factor $d\nu(\gamma)$ is *translation invariant* in the sense that $d\nu(\gamma + \delta\gamma) = d\nu(\gamma)$. Expanding out $e^{iS(\gamma + \delta\gamma)} = e^{iS + i\delta S} = e^{iS} + i\delta S e^{iS}$ then produces

$$0 = \int d\nu(\gamma) i\delta S e^{iS(\gamma)} \psi_1(\gamma(t_1))^* \psi_0(\gamma(t_0))$$

which, again by (17), says precisely that

$$\langle \psi_1, t_1 | \widehat{\delta S} | \psi_0, t_0 \rangle = 0$$

whence $\widehat{\delta S}$ itself vanishes, since ψ_0 and ψ_1 are arbitrary. For our variation $\delta\gamma$, δS reduces to

$$\delta S = \int \frac{\delta L(t)}{\delta q(t)} \delta\gamma(t) dt \tag{18}$$

whence, since $\delta\gamma$ is also arbitrary, we have

$$\frac{\delta \widehat{L}(t)}{\delta q(t)} = 0 \tag{19}$$

Since $\frac{\delta L}{\delta q}$ is the quantity whose vanishing constitutes the classical equations of motion, we can express (19) by saying that *the classical equations of motion hold in operator form*. For our particle of mass m moving in the potential V ,

$$\frac{\delta L}{\delta q} = -m \frac{d^2 \gamma(t)}{dt^2} - V'(\gamma(t), t)$$

so (19) becomes

$$m \frac{d^2}{dt^2} \widehat{q}(t) + V'(\widehat{q}(t), t) = 0, \quad (20)$$

where, in accord with (14), we have used the definition $\widehat{q}(t) = \widehat{q(t)}$. [As written, (19) is in the Heisenberg picture, but we could free it from any picture by writing it as

$$\left(\frac{\delta \widehat{L}(t)}{\delta q(t)} \right)_s = 0.] \quad (21)$$

The canonical momentum conjugate to $q(t)$

Let $\gamma \rightarrow \gamma + \delta\gamma$ as before, but now drop the assumption that $\delta\gamma = 0$ at the final endpoint. We now have in place of (18), the “Noether identity”

$$\delta S = \int_1^2 \frac{\delta L}{\delta q} \delta\gamma dt + p(t_2) \delta\gamma(t_2), \quad (22)$$

which serves as the *definition* of the momentum functional $p(t)$. Working now with (8), instead of the equivalent (17), and still taking $\mathcal{O} = 1$, we find

$$\begin{aligned} \psi_2(q_2 + \delta\gamma(t_2), t_2) &= \int d\nu(\gamma + \delta\gamma) e^{iS(\gamma + \delta\gamma)} \delta(q_2 + \delta\gamma(t_2), \gamma(t_2) + \delta\gamma(t_2)) \psi_1(\gamma(t_1)) \\ &= \int d\nu(\gamma) [1 + i\delta S(\gamma)] e^{iS(\gamma)} \delta(q_2, \gamma(t_2)) \psi_1(\gamma(t_1)) \\ &= \psi_2(q_2, t_2) + \int d\nu(\gamma) i\delta S(\gamma) e^{iS(\gamma)} \delta(q_2, \gamma(t_2)) \psi_1(\gamma(t_1)) \end{aligned}$$

or by (13),

$$\frac{\partial \psi_2(q_2, t_2)}{\partial q_2} \delta\gamma(t_2) = (i\delta \widehat{S}(\gamma))_{t_2} \psi_2. \quad (23)$$

From (22) and (21) we have

$$\widehat{\delta S} = \widehat{p(t_2)} \delta\gamma(t_2)$$

so that (23) reads

$$\frac{\partial \psi_2(q_2, t_2)}{\partial q_2} \delta \gamma(t_2) = i (\widehat{p(t_2)})_{t_2} \psi_2 \delta \gamma(t_2),$$

or

$$\frac{1}{i} \frac{\partial}{\partial q_2} \psi_2(q_2, t_2) = (\widehat{p(t_2)})_{t_2} \psi_2. \quad (24)$$

This is the familiar fact that the momentum operator acts simply as differentiation with respect to q . In the Heisenberg picture language, it can also be written (with $t_2 = t$) as

$$\widehat{p}(t) |\psi, t\rangle = \left| \frac{1}{i} \frac{\partial \psi}{\partial q}, t \right\rangle \quad (25)$$

where we have defined $\widehat{p}(t) := \widehat{p(t)}$ in analogy with (14). From this, or from (24), it follows immediately that

$$[\widehat{q}(t), \widehat{p}(t)] = i. \quad (26)$$

Notice that from the present point of view, this is a *theorem*, whereas more commonly it is made an assumption (“canonical quantization”) and (25) is derived from it, as its “Schrödinger representation”.

For the Lagrangian (2), or its obvious generalization to more than one particle, (22) implies, as we know,

$$p(t) = m \dot{\gamma}(t) \quad (27)$$

(or $p_i(t) = m_i \dot{\gamma}_i(t)$ if $\gamma_i(t)$ is the i th configuration coordinate at time t and m_i is the mass of the particle whose coordinate γ_i is). Thus we recover the familiar operator equation,

$$\widehat{p}(t) = \widehat{p(t)} = m \widehat{\dot{\gamma}(t)} = m \frac{d}{dt} \widehat{\gamma(t)} = m \frac{d}{dt} \widehat{q}(t) \quad (28)$$

A special case of (24) occurs if $\delta \gamma$ is taken to be an overall spatial translation of all the particles through a displacement δx (recall that γ in general comprises several world lines). In that case (22) reduces to

$$\delta S_1^2 = \int \frac{\delta L}{\delta q} \delta \gamma dt + P(t_2) \delta x_2 \quad (29)$$

where P is the *total* momentum, and (25) then implies that $\widehat{P}(t)$ acts by infinitesimal spatial translation: it is the “generator of spatial translations at time t ”. The final results we want follow from extending these considerations to the case of time-translations.

Further consequences of the Noether identity: the Schrödinger equation

When we generalize $\delta\gamma$ to allow deformation in the time direction, the resulting Noether identity yields an equation (the Schrödinger equation) describing the time dependence of $\mathcal{U}(t, t_0)$. For variety, and also to lighten the notational burden, let's work this out for the concrete Lagrangian (2), rather than in general.

Since we want to vary t as well as q it is useful to regard γ as a *parameterized* path, whose parameter λ runs from 0 to 1. Then, writing $\gamma(\lambda) \equiv (t(\lambda), q(\lambda)) \equiv (\gamma^t(\lambda), \gamma^q(\lambda))$, we have (with $\dot{t} = dt/d\lambda$, $\dot{q} = dq/d\lambda$)

$$S = \int_0^1 d\lambda \left(\frac{m\dot{q}(\lambda)^2}{2\dot{t}} - V(\gamma(\lambda))\dot{t} \right)$$

Taking the variation and integrating by parts as usual produces straightforwardly

$$\delta S = \int_0^1 d\lambda \dot{t} \left(-m \frac{d^2 q}{dt^2} - \frac{\partial V}{\partial q} \right) \delta q + \int_0^1 \left[\frac{dE}{d\lambda} - \frac{\partial V}{\partial t} \frac{dt}{d\lambda} \right] \delta t d\lambda + p \delta q|_0^1 - E \delta t|_0^1$$

with

$$p = m \frac{dq}{dt}$$

and

$$E = \frac{m}{2} \left(\frac{dq}{dt} \right)^2 + V(q, t) \quad (30)$$

Now since we have already studied the effects of δq , we may as well isolate here the effect of δt by setting $\delta q(\lambda) = 0$. (Of course, the meaning of $\delta q = 0$ is frame dependent; with respect to a boosted frame, it would mean something different.) In addition, let's take $\delta t(\lambda)$ to vanish everywhere except near the final endpoint of γ . Then

$$\delta S = \int_0^1 d\lambda \left[\frac{dE}{d\lambda} - \frac{\partial V}{\partial t} \frac{dt}{d\lambda} \right] \delta t - E(1) \delta t(1) \quad (31)$$

Proceeding as before, we have

$$\begin{aligned} \psi(q_1, t_1 + \delta t(1)) &= \int d\nu(\gamma + \delta\gamma) e^{iS(\gamma + \delta\gamma)} \delta(\gamma^q(1), q_1) \\ &= \int d\nu(\gamma) \frac{d\nu(\gamma + \delta\gamma)}{d\nu(\gamma)} (1 + i\delta S) e^{iS(\gamma)} \delta(\gamma^q(1), q_1) \\ &= \int d\nu(\gamma) \left[1 + \left(\frac{d\nu(\gamma + \delta\gamma)}{d\nu(\gamma)} - 1 \right) \right] (1 + i\delta S) e^{iS(\gamma)} \delta(\gamma^q(1), q_1) \\ &= \psi(q_1, t_1) + \int d\nu(\gamma) \left[\left(\frac{d\nu(\gamma + \delta\gamma)}{d\nu(\gamma)} - 1 \right) + i\delta S(\gamma) \right] e^{iS(\gamma)} \delta(\gamma^q(1), q_1) \end{aligned}$$

or

$$\frac{\partial\psi(q_1, t_1)}{\partial t_1} \delta t(1) = \int d\nu(\gamma) \left[\frac{d\nu(\gamma + \delta\gamma)}{d\nu(\gamma)} - 1 + i\delta S(\gamma) \right] e^{iS(\gamma)} \delta(\gamma^q(1), q_1) \quad (32)$$

Now $\delta S(\gamma)$ in (31) has two terms, an integral or “bulk term” and a boundary term. Let us *assume* that

$$J(\gamma) := \frac{d\nu(\gamma + \delta\gamma)}{d\nu(\gamma)} - 1 \quad (33)$$

(the Jacobian of our infinitesimal change of variables $\gamma \rightarrow \gamma + d\gamma$) *also* consists of two such terms:

$$J(\gamma) = \int_0^1 d\lambda J(\lambda) \delta t(\lambda) + J_1 \delta t(1) - J_0 \delta t(0) \quad (34)$$

We will see later to what extent this holds for the measure-factor $d\nu(\gamma)$ appropriate to “skeletonized histories”. Now let us define

$$\mathcal{O}(\gamma) = J(\gamma) + i\delta S(\gamma),$$

so that the right hand side of (32) can be written as

$$\int d\nu(\gamma) \mathcal{O}(\gamma) e^{iS(\gamma)} \delta(\gamma^q(1), q_1) . \quad (35)$$

Given (34), we have for $\mathcal{O}(\gamma)$, with the help also of (31),

$$\mathcal{O}(\gamma) = \int_0^1 d\lambda \delta t(\lambda) \left[J(\lambda) + i \left(\frac{dE}{d\lambda} - \frac{\partial V}{\partial t} \frac{dt}{d\lambda} \right) \right] + (J_1 - iE(1)) \delta t(1) \quad (36)$$

We come now to a subtle but crucial point. In (36) there is no term coming from the initial endpoint, $\lambda = 0$, since we have taken δt to vanish there. If we *also* take $\delta t(1) = 0$, then of course the left hand side of (32) and the boundary contribution to (36) both vanish, whence the remaining integral term in (36) must vanish as well. Hence, since $\delta t(\lambda)$ is still free except at $\lambda = 0, 1$, the integrand itself must contribute zero to (32) (which we could express as $\mathbf{op}(dE/d\lambda - (\partial V/\partial t)(dt/d\lambda) - iJ(\lambda)) = 0$, an equation that logically ought to work out to be conservation of energy in operator form). Without any effect on the result, we may therefore replace $\mathcal{O}(\gamma)$ in (35) by

$$[J_1 - iE(1)]\delta t(1),$$

whereupon (32) becomes

$$\frac{\partial\psi(q_1, t_1)}{\partial t_1} = \int d\nu(\gamma) [J_1 - iE(1)] e^{iS(\gamma)} \delta(\gamma^q(1), q_1) . \quad (37)$$

Finally, if we write

$$H(t_1) := E(1) + iJ_1 \quad (38)$$

then, as before with (24), (37) (with ‘ t_1 ’ simplified to ‘ t ’) says

$$i \frac{\partial\psi(q, t)}{\partial t} = \left(\widehat{H(t)} \right)_t \psi(q, t) \quad (39)$$

Notice that in writing $\partial\psi/\partial t$, we are comparing a vector in \mathcal{H}_t with one in $\mathcal{H}_{t+\delta t}$, in effect using the Ξ introduced earlier to do so; that is, $\partial\psi/\partial t \in \mathcal{H}_t$ really means $(\partial/\partial s)(\Xi(t, s)\psi(s))|_{s=t}$.

At first sight, (38) may look surprising, because it means that our Hamiltonian functional $H(t)$ is not simply the energy as given by (30). However, as we will see, (30) alone would be wrong because of the subtle difference between \widehat{v}^2 and \hat{v}^2 , where $v = dq/dt$ is the velocity. It will turn out, in fact, that iJ_1 will provide exactly the correction needed to turn \widehat{v}^2 into \hat{v}^2 — a correction that is infinite and purely imaginary!

The measure-factor and the quantum measure for skeletonized histories

To evaluate the Jacobian

$$\frac{d\nu(\gamma + \delta\gamma)}{d\nu(\gamma)}$$

we first need to give meaning to the formal integral $\int d\nu(\gamma)$. This is not an easy task, and presents in fact the main mathematical difficulty of the path integral formalism. One way people have proceeded is to discretize time and replace the path γ with a “skeletonized” path consisting of straight line segments between the chosen discrete times. (Mechanical engineers would call this a “finite element” method.) Let the chosen times be

$$0 = t_0, t_1, t_2, \dots, t_N = T$$

and let the path locations at these times be

$$q_0, q_1, q_2, \dots, q_N$$

Then it is natural to take for $d\nu(\gamma)$, the multiple integral

$$d\nu(\gamma) = K dq_0 dq_1 \cdots dq_N = K \prod_{j=0}^N dq_j \quad (40)$$

where K is a normalization factor to be determined that can depend on the times t_j but not on the positions q_j .

For the action-functional itself we may take

$$S(\gamma) = S(q_N, q_{N-1}, \dots, q_1, q_0) = \sum_{j=1}^N S(q_j, q_{j-1})$$

with, say

$$S(q_j, q_{j-1}) = \frac{m}{2} \frac{(q_j - q_{j-1})^2}{t_j - t_{j-1}} + V\left(\frac{q_j + q_{j-1}}{2}, \frac{t_j + t_{j-1}}{2}\right) (t_j - t_{j-1}) \quad (41)$$

which is a discretized version of the continuum action, $\int (m/2) dq^2/dt - V(q, t) dt$. (The midpoint approximation we have used here for the potential is not particularly sacred. Using the exact integral $\int V dt$ along the skeletonized world line would also be possible, as would using the value of V at the final or initial endpoint of each segment. Similarly, some people advocate instead of straight line path segments, segments that are solutions of the classical equations of motion, leading to a more complicated version of the “kinetic energy term” in $S(q_j, q_{j-1})$. For the Lagrangian (2), all these possibilities lead to the same quantum measure in the continuum limit of zero spacing between the t_i .)

Notice here that the q_i are integrated over, but the t_i are not. Thus we actually have defined a large number of skeletonized quantum measures $\mu(\cdot)$, one for each choice of the times t_i . The assumption is that in the limit where the spacings Δt go to zero, all of these skeletonized measures approach the same limit. (There is another approach that does integrate over the t_i , but it introduces a gauge-like over-counting that has to be cancelled out before finite answers can be obtained. The resulting formalism resembles a theory of 0 + 1-dimensional gravity coupled to a scalar field, just as the analogous approach to the dynamics of a spacetime world *sheet* makes string theory look like 1 + 1-dimensional gravity coupled to a scalar field.)

For the normalization factor $K = K(t_N, \dots, t_0)$ the standard choice is

$$K = \prod_{j=1}^N \sqrt{\frac{m}{2\pi i \Delta t_{j,j-1}}} \quad (42)$$

where $\Delta t_{j,j-1} = t_j - t_{j-1}$. With this choice the condition (9) on \mathcal{U} is fulfilled exactly in the special case $V = 0$, and in the limit $\Delta t \rightarrow 0$ generally. Notice that (9) is really two distinct conditions. When $r = t < s$ it reads $\mathcal{U}(r, s)\mathcal{U}(s, r) \equiv \mathcal{U}(s, r)^* \mathcal{U}(s, r) = 1$; that is it asserts that $\mathcal{U}(s, r)$ is *unitary*. When $r > s > t$ on the other hand, (9) merely asserts that propagation is “functorial” in the sense that propagation from t to s followed by propagation from s to r is equivalent to propagation from t to r . Both these properties entail conditions on K . The former determines the absolute value of K , and the latter controls its phase, leaving however the freedom to introduce one arbitrary phase factor for each t_i . Since such an alteration of phase does not affect the quantity of ultimate interest, the quantum measure $\mu(A)$, as given, for example, in (10), it may be regarded as physically meaningless. By availing ourselves of this freedom, we can always bring K to the form (42), which seems the simplest and most convenient.

With this choice, the fundamental combination

$$\int_{\gamma \in \Omega_0^T} d\nu(\gamma) e^{iS(\gamma)}$$

takes on the skeletonized form

$$\prod_{j=1}^N \sqrt{\frac{m}{2\pi i \Delta t_{j,j-1}}} \int \prod_{j=0}^N dq_j \prod_{j=1}^N e^{iS(t_j, q_j; t_{j-1}, q_{j-1})}$$

where $S(,)$ is given by (41). From this, the quantum measure of any set A of histories can be determined: one evaluates the skeletonized version of (1) (which entails deciding what is the skeletonized version of the subset A) and then takes the limit $\Delta t \rightarrow 0$.

The variation of the skeletonized measure-factor $d\nu(\gamma)$

From (40) we see first of all that $d\nu(\gamma)$ is indeed translation invariant with respect to the q_i , a fact we relied on in deriving the operator equations of motion (19) and also the equation (23) for the canonical momentum, together with its consequence (28).

Under variations of the t_i , on the other hand, K (and therefore $d\nu$) is obviously *not* invariant. Rather, we have from (42)

$$\begin{aligned}\log K &= \sum_{j=1}^N [\text{constant} - \frac{1}{2} \log \Delta t_{j,j-1}] \\ \frac{\delta K}{K} &= -\frac{1}{2} \sum_{j=1}^N \frac{\delta \Delta t_{j,j-1}}{\Delta t_{j,j-1}} \\ &= -\frac{1}{2} \sum_{j=1}^N \frac{\delta t_j - \delta t_{j-1}}{\Delta t_{j,j-1}} \\ &= -\frac{1}{2} \sum_{j=1}^N \frac{\delta t_j}{\Delta t_{j,j-1}} + \frac{1}{2} \sum_{j=0}^{N-1} \frac{\delta t_j}{\Delta t_{j+1,j}}\end{aligned}$$

or

$$\frac{\delta K}{K} = -\frac{1}{2} \frac{\delta t_N}{\Delta t_{N,N-1}} + \frac{1}{2} \frac{\delta t_0}{\Delta t_{1,0}} - \frac{1}{2} \sum_{j=1}^{N-1} \delta t_j \frac{t_{j+1} - 2t_j + t_{j-1}}{\Delta t_{j,j-1} \Delta t_{j+1,j}} \quad (43)$$

This same expression is also the infinitesimal Jacobian $J(\gamma)$ appearing in (33) because, for the variations being considered, we clearly have $d\nu(\gamma + \delta\gamma)/d\nu(\gamma) = (K + \delta K)/K$; thus

$$J(\gamma) = \frac{\delta K}{K} .$$

The first thing to notice here is that J does indeed split into a bulk sum plus a boundary term, as assumed in (34). What is more, the bulk sum will indeed go over to a continuum integral as $\Delta t \rightarrow 0$, provided only that $\Delta t_{j,j-1}$ and δt_j are both slowly varying functions of j . Specifically, we find by expanding in powers of Δt that

$$J(\lambda) = -(N/2)\ddot{t}/\dot{t}^2 + O(1/N) .$$

(Conveniently, the term of order N^0 that one might have expected drops out.) And for the boundary term J_1 of interest here, (43) gives us

$$J_1 = \frac{-1}{2\Delta t_{N,N-1}} + O(\Delta t)$$

Putting this together with (38) and (30) yields, finally, the Hamiltonian functional in the skeletonized formulation:

$$H_{skel}(t) = E_{skel}(t) + iJ_1 = \frac{m}{2} \frac{\Delta q^2}{\Delta t^2} + V(q, t) - \frac{i}{2\Delta t} + iO(\Delta t) \quad (44)$$

where $\Delta q := q(t) - q(t - \Delta t)$, $\Delta t = t_N - t_{N-1}$ and $t = t_N$ here is what in (38) was called t_1 . The operator that enters into (39) as the generator of time-translation is then

$$\widehat{H}(t) = \lim_{\Delta t \rightarrow 0} \widehat{H_{skel}}(t) \quad (45)$$

The Hamiltonian operator $\widehat{H}(t)$ as a function of $\widehat{q}(t)$ and $\dot{\widehat{q}}(t)$ (or $\widehat{p}(t)$)

Equations (39), (44) and (45) give us the law of evolution of the wave function ψ as it emerges most naturally from the path integral. In order to connect this result up with the more familiar differential operator form of the Hamiltonian that one encounters in every textbook of quantum mechanics, it remains, in view of (24), only to demonstrate that (45) reduces to $\widehat{p}^2/2m + \widehat{V}(q)$. In light of (44) and (27)–(28), this is the same as showing that

$$\mathbf{op} \left(\frac{m}{2} \frac{\Delta q^2}{\Delta t^2} - \frac{i}{2\Delta t} \right) = \frac{m}{2} \left(\mathbf{op} \left(\frac{\Delta q}{\Delta t} \right) \right)^2,$$

which can also be written as

$$\mathbf{op} \left(\left(\frac{\Delta q}{\Delta t} \right)^2 \right) - \left(\mathbf{op} \left(\frac{\Delta q}{\Delta t} \right) \right)^2 = \frac{i}{m\Delta t} \quad (46)$$

But this is easily seen with the help of (28) and (26). In fact, let $\Delta q = q(t) - q(t - \Delta t) =: a - b$. Then

$$\Delta q^2 = (a - b)^2 = a^2 - 2ab + b^2$$

Remembering our operator ordering rule, we see that, on the other hand,

$$\widehat{\Delta q^2} = \widehat{a^2} - 2\widehat{ab} + \widehat{b^2},$$

which differs from $(\widehat{\Delta q})^2$ by

$$(\widehat{a^2} - 2\widehat{ab} + \widehat{b^2}) - (\widehat{a} - \widehat{b})^2 = -2\widehat{ab} + \widehat{a}\widehat{b} + \widehat{b}\widehat{a} = [\widehat{b}, \widehat{a}]$$

Now from (28), we have

$$\widehat{a} - \widehat{b} = \widehat{q}(t) - \widehat{q}(t - \Delta t) = \widehat{p}\Delta t/m + O(\Delta t^2) \quad (47)$$

whence, by (26),

$$[\widehat{b}, \widehat{a}] = [\widehat{b} - \widehat{a}, \widehat{a}] = -\frac{\Delta t}{m} [\widehat{p}, \widehat{q}] + O(\Delta t^2) = \frac{i\Delta t}{m} + O(\Delta t^2)$$

which exhibits the $\Delta q^2 \sim \Delta t$ dependence familiar from Brownian motion. Hence,

$$\mathbf{op} \left(\left(\frac{\Delta q}{\Delta t} \right)^2 \right) - \left(\mathbf{op} \left(\frac{\Delta q}{\Delta t} \right) \right)^2 = \frac{i}{m\Delta t} + O(\Delta t^0) \quad (48)$$

as anticipated.

This result is almost what we were aiming at, but there is still the final term of order Δt^0 in (48) to account for. That this term also vanishes can be seen by returning to (47) and keeping the next term, $-\ddot{\widehat{q}}\Delta t^2/2$. Given (20), this $O(\Delta t^2)$ term drops out of the commutator $[\widehat{b}, \widehat{a}]$ because of the obvious fact that $\widehat{q}(t) \natural \widehat{q}(t)$. One can easily check that it also drops out when an electromagnetic field is present.

More generally, one can notice that all the corrections we have been worrying about — including iJ_1 itself — are purely imaginary by nature. Thus, they *had* to drop out if the Hamiltonian operator was to come out selfadjoint, or equivalently if the propagator $\mathcal{U}(t_1, t_0)$ was to be unitary as required if the quantum measure is to be well-defined. In a less careful treatment, we might just have discarded all these corrections without doing any work at all, on the grounds that, if they did not vanish, then we would have to modify the measure-factor to make them do so! In this sense, there seems to be no “operator ordering” ambiguity at all in the path integral prescription as applied to (2). (It reappears in a curved configuration space, though.)

Finally, we can notice that the (purely imaginary) discrepancy in the energy that got cancelled by J_1 , namely $i/2\Delta t$ (or $i\hbar/2\Delta t$ if we restore the \hbar) is divergent for small Δt . If we had tried to interpret $\widehat{v}^2 = \mathbf{op}((dq/dt)^2)$ as

$$\lim_{\Delta t \rightarrow 0} \mathbf{op} \left(\left(\frac{\Delta q}{\Delta t} \right)^2 \right)$$

then we would have gotten no finite result at all, not even a wrong one.