Path Integral

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Autumn 2019

1 Before the PI

1.1 Schrödinger, Heisenberg & interaction

We denote $U = \exp(Ht/i\hbar)$, and similarly with $H_0 \to U_0$, $V \to U_V$.

Schrödinger

1. State kets are $\left|\psi(t)\right\rangle = U \left|\psi(t=0)\right\rangle$;
2. observables are $A(t) \equiv A(t=0)$;
3. base kets are defined by $A\left|a\right\rangle = a\left|a\right\rangle$, therefore $\left|a(t)\right\rangle \equiv \left|a(t=0)\right\rangle$.

Heisenberg

1. State kets are $\left|\psi(t)\right\rangle \equiv \left|\psi(t=0)\right\rangle$;
2. observables are $A(t) = U^\dagger A(t=0) U$;
3. base kets are $\left|a(t)\right\rangle = U^\dagger \left|a(t=0)\right\rangle$.

Interaction We denote by a subscript S or I objects in the Schrödinger or interaction system. In the

1. State kets are defined as $\left|\psi(t)\right\rangle_I = U_0^\dagger \left|\psi(t)\right\rangle_S$;
2. observables are defined as $A_I(t) = U_0^\dagger A_S U_0$;
3. as base kets we use eigenstates of H_0: $H_0\left|n\right\rangle = E_n\left|n\right\rangle$. These evolve like $\left|n(t)\right\rangle = U_0\left|n(t=0)\right\rangle$.

Then, we can generically write the evolution of a Schrödinger ket as

$$\left|\psi(t)\right\rangle_S = \sum_n c_n(t)\exp(E_n t/i\hbar)\left|n\right\rangle \,, \tag{1}$$

therefore the evolution of the interaction ket is

$$\left|\psi(t)\right\rangle_I = U_0^\dagger \left|\psi(t)\right\rangle_S = \sum_n c_n(t)\left|n\right\rangle \,. \tag{2}$$

We can write an equation for the evolution of the $c_n(t)$:

$$i\hbar\dot{c_n}(t) = \sum_m V_{nm}\exp(i\omega_{nm}t)c_m(t)\,, \tag{3}$$

where $\omega_{nm} = (E_n - E_m)/\hbar$ and $V_{nm} = \left\langle n\right| V \left|m\right\rangle$. This is a matrix equation for the coefficient vector.

Time-dep perturbations If we define the interaction-picture evolution operator as $\left|\alpha, t\right\rangle = U_I(t)\left|\alpha, 0\right\rangle$ we have its evolution as $i\hbar\partial_t U_I = V_I U_I$.

For small times $U_I \approx \mathbb{1}$, so we can integrate the Schrödinger equation:

$$
\begin{aligned}
U_I &= \mathbb{1} + \frac{1}{i\hbar}\int_0^t V_I(t')U_I(t')\,\mathrm{d}t' && \text{(4a)}\\
&= \mathbb{1} + \frac{1}{i\hbar}\int_0^t V_I(t')\left(\mathbb{1} + \frac{1}{i\hbar}\int_0^{t'} V_I(t'')U_I(t'')\,\mathrm{d}t''\right)\mathrm{d}t' && \text{(4b)}\\
&= \mathbb{1} + \frac{1}{i\hbar}\int_0^t V_I(t')\,\mathrm{d}t' + \frac{1}{(i\hbar)^2}\int_0^t\int_0^{t'} V_I(t')V_I(t'')\,\mathrm{d}t'\,\mathrm{d}t'' + o(V_I^2) && \text{(4c)}
\end{aligned}
$$

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Now, if we start on a base ket $\left|i\right\rangle$, the evolution coefficients $c_n(t)$ will be given by the matrix elements $\left\langle n\right| U_I(t)\left|i\right\rangle$. We can compute these to any order in V_I, by taking the components of the previous equation and applying the following computation any time we have the components of V_I:

$$\left\langle n\right| V_I \left|i\right\rangle = \left\langle n\right| U_0^\dagger V U_0 \left|i\right\rangle = \exp(i\omega_{ni}t)V_{ni}\,, \tag{5}$$

since the $\left|n\right\rangle$ are eigenstates of the unperturbed Hamiltonian.

1.2 The propagator

If $H\left|\alpha'\right\rangle = \alpha'\left|\alpha'\right\rangle$, then the evolution operator can be decomposed as

$$U(t) = \sum_{\alpha'}\exp\left(\frac{E_{\alpha'}t}{i\hbar}\right)\left|\alpha'\middle\rangle\middle\langle\alpha'\right| \,. \tag{6}$$

This can be written in the position basis as a Green function by contracting with two position vectors:

$$\langle x' | U(t) | x'' \rangle = \sum_{\alpha'} \exp\left(\frac{E_{\alpha'} t}{i\hbar}\right) \langle x' | \alpha' \rangle \langle \alpha' | x'' \rangle \stackrel{\text{def}}{=} K(x', x''; t)\,, \tag{7}$$

and with this we can directly compute the evolution at a generic time: $\psi(x'', t) = \int \mathrm{d}^3 x' \, K(x'', x'; t) \psi(x')$. It is effectively the transition amplitude: $K = \langle x'', t | x', 0 \rangle$ when seen in the Heisenberg picture (since we are evolving a base ket).

1. $K(x', x'', t)$ satisfies the Schrödinger equation, since it is a sum of terms which do;
2. $\lim_{t \to 0} K(x', x'', t) = \delta^3(x', x'')$.

1.3 Some useful propagators

Free particle We consider $H = p^2/2m$; the momentum eigenstates are $p |p'\rangle = p' |p'\rangle$, and they are also energy eigenstates with $H |p'\rangle = ((p')^2/2m) |p'\rangle$.

We compute:

$$K(x', x'', t) = \int \mathrm{d}p' \, \langle x'' | p' \rangle \langle p' | x' \rangle \exp\left(\frac{(p')^2 t}{i\hbar 2m}\right), \tag{8}$$

and recall that $\langle x | p \rangle = \exp(-px/i\hbar)/\sqrt{2\pi\hbar}$. We simplify the exponent to get a Gaussian integral: it is known that

$$\int_{\mathbb{R}} \mathrm{d}x \exp\left(-i\alpha x^2\right) = \sqrt{\frac{\pi}{i\alpha}}\,, \tag{9}$$

therefore in the end we get:

$$K(x', x'', t) = \frac{1}{2\pi\hbar} \exp\left(\frac{im(x'' - x')^2}{2\hbar t}\right) \sqrt{\frac{2m\pi\hbar}{it}}\,, \tag{10}$$

which for $t \to 0$ is in the form $\exp\left((x' - x'')^2/t\right)\sqrt{t} \to \delta(x'' - x')$.

Harmonic oscillator We consider $H = p^2/2m + m\omega^2 x^2/2$. It is known that the eigenfunctions are given by the Hermite polynomials:

$$\langle x' | n \rangle = \frac{1}{\pi^{1/4}\sqrt{2^n n!}} \frac{1}{x_0^{1/2}} H_n y \exp\left(-\frac{(x/x_0)^2}{2}\right), \tag{11}$$

where $x_0 = \sqrt{\hbar/(m\omega)}$ (both masses and frequencies are inverse lengths in natural units!). We also know the eigenenergies, $E_n = \hbar\omega(n + 1/2)$. We can then compute away, to finally get:

$$K = \sqrt{\frac{m\omega}{2i\pi\hbar\sin(\omega t))}} \exp\left(\frac{im\omega\Big(\big((x'')^2 + (x')^2\big)\cos(\omega t) - 2x'x''\Big)}{2\hbar\sin(\omega t)}\right). \tag{12}$$

2 The Path Integral

We can time-slice the interval between a certain time $0 = t_0$ and another time $t = t_N$ in N parts. Then, evolving the system with a the propagator for each one, we get:

$$K(x_N, x_0, t) = \int \left(\prod_{i=1}^{N-1} \mathrm{d}x_i\right)\left(\prod_{i=0}^{N-1} \langle x_{i+1}, t_{i+1} | x_i, t_i\rangle\right). \tag{13}$$

We call the time-slice $\epsilon = t/N$. We will expand the in ϵ up to first order the evolution operator $\exp(H\epsilon/i\hbar)$.

The braket $\langle x_{i+1}, t_{i+1} | x_i, t_i\rangle$, if we assume $t_{i+1} - t_i = \epsilon$, can be written as

$$\langle x_{i+1}| \exp\left(\frac{H\epsilon}{i\hbar}\right) |x_i\rangle\ . \tag{14}$$

The first case we consider is a free particle Hamiltonian, $X = p^2/2m + V(x)$; we insert a momentum completeness

$$\langle x_{i+1}| \exp\left(\frac{H\epsilon}{i\hbar}\right) |x_i\rangle = \int \mathrm{d}p' \, \langle x_{i+1}|p'\rangle \, \langle p'| \exp\left(\frac{H\epsilon}{i\hbar}\right) |x_i\rangle\ , \tag{15}$$

and now make a

Claim 1.

$$\langle p'| \exp\left(\frac{H\epsilon}{i\hbar}\right) |x_i\rangle = \exp\left(\frac{\epsilon}{i\hbar}\Big(p'^2/2m + v(x_i)\Big)\right) + O(\epsilon^{3/2})\,. \tag{16}$$

Proof. We rewrite the expression as

$$\big\langle p'\big| \exp\big(\epsilon(T+U)\big) \, |x\rangle\ , \tag{17}$$

where $T = \frac{p^2/2m}{i\hbar}$, $U = \frac{V}{i\hbar}$. If we multiply and divide by $e^{\epsilon U}$ (respectively T) we get that proving our identity is equivalent to proving that:

$$\big\langle p\big| \exp(-\epsilon T)\exp(\epsilon H/i\hbar)\exp(-\epsilon U)\, |x\rangle = \big\langle p'\big|x\big\rangle\ , \tag{18}$$

and we call the product of exponentials $\exp\left(-\epsilon^2 C\right)$.

The CBH formula yields a solution C to the equation $e^C = e^A e^B$ in terms of commutators of A and B. With it, we arrive at:

$$\exp\left(-\epsilon^2 C\right) = \exp\left(-\frac{\epsilon^2}{2}[T,U] + O(\epsilon^3)\right), \tag{19}$$

... $\square$

Then, using the fact that $\langle x|p\rangle = \exp(-xp/i\hbar)/\sqrt{2\pi\hbar}$, we get:

$$\int \mathrm{d}p' \langle x_{i+1}|p'\rangle \langle p'| \exp\left(\frac{H\epsilon}{i\hbar}\right)|x_i\rangle = \tag{20a}$$

$$= \frac{1}{2\pi\hbar}\int \mathrm{d}p' \exp\left(-\frac{(x_{i+1}-x_i)p'}{i\hbar}\right)\exp\left(\frac{\epsilon}{i\hbar}\left(\frac{p'^2}{2m} - V(x_i)\right)\right) \tag{20b}$$

$$= \frac{1}{2\pi\hbar}\int \mathrm{d}p' \exp\left(\frac{\epsilon}{i\hbar}\left(H(p',x) - \dot{x}p'\right)\right), \tag{20c}$$

and now we can complete the square: if we define the new variable $\widetilde{p} = p' - m\dot{x}$ we have $\widetilde{p}^2/2m - m\dot{x}^2/2 = p'^2/2m - \dot{x}p'$, therefore the integral becomes Gaussian in $\widetilde{p}$:

$$\frac{1}{2\pi\hbar}\int \mathrm{d}\widetilde{p}\exp\left(\frac{\epsilon}{i\hbar}\left(\frac{\widetilde{p}^2}{2m} - \frac{m\dot{x}^2}{2} + V(x)\right)\right) = \tag{21a}$$

$$= \frac{1}{2\pi\hbar}\sqrt{\frac{2\pi m\hbar}{i\epsilon}}\exp\left(-\epsilon\frac{L(x,\dot{x})}{i\hbar}\right), \tag{21b}$$

but

2.1 Path integral of a quadratic Lagrangian

Let $L(x,\dot{x})$ be a quadratic Lagrangian:

$$L = a\dot{x}^2 + bx\dot{x} + cx^2 + d\dot{x} + ex + f\,. \tag{22}$$

The propagator for L, computed via path integral, is:

$$K = \int \mathrm{D}[x]\,\exp\left(\frac{i}{\hbar}\int \mathrm{d}t\, L\right) \tag{23a}$$

$$= \int \mathrm{D}[x]\,\exp\left(\frac{i}{\hbar}\int \mathrm{d}t\,(\underbrace{a\dot{x}^2 + bx\dot{x} + cx^2 + d\dot{x} + ex + f}_{F})\right). \tag{23b}$$

Let x_c be the classical path; let's write $x = x_c + y$ and therefore $\mathrm{D}[x] = \mathrm{D}[y]$. Properly replacing x and $\dot{x}$, the propagator can be written as:

$$\begin{aligned}
F &= a(\dot{x}_c^2 + \dot{y}^2 + 2\dot{x}_c\dot{y}) + b(x_c\dot{x}_c + x_c\dot{y} + y\dot{x}_c + y\dot{y}) + c(x_c^2 + y^2 + 2x_c y) + \\
&\quad + d(\dot{x}_c + \dot{y}) + e(x_c + y) + f \qquad (24a) \\
&= (a\dot{x}_c^2 + bx_c\dot{x}_c + cx_c^2 + d\dot{x}_c + ex_c + f) + (a\dot{y}^2 + by\dot{y} + cy^2) + \\
&\quad + \dot{y}(2a\dot{x}_c + bx_c + d) + y(b\dot{x}_c + 2cx_c + e) \qquad (24b) \\
&= L_c + (a\dot{y}^2 + by\dot{y} + cy^2) + \dot{y}\,\frac{\partial L}{\partial \dot{x}}\bigg|_{x_c} + y\,\frac{\partial L}{\partial x}\bigg|_{x_c}, \qquad (24c)
\end{aligned}$$

and so

$$K = \int \mathrm{D}[y]\,\exp\left(\frac{i}{\hbar}\int \mathrm{d}t\left(L_c + (a\dot{y}^2 + by\dot{y} + cy^2) + \dot{y}\,\frac{\partial L}{\partial \dot{x}}\bigg|_{x_c} + y\,\frac{\partial L}{\partial x}\bigg|_{x_c}\right)\right). \qquad (25)$$

Evaluating by parts the last part of the integral:

$$\begin{aligned}
I &= \int \mathrm{d}t\left(\dot{y}\,\frac{\partial L}{\partial \dot{x}}\bigg|_{x_c} + y\,\frac{\partial L}{\partial x}\bigg|_{x_c}\right) \qquad (26) \\
&= y\bigg|_i^f \frac{\partial L}{\partial \dot{x}}\bigg|_{x_c} + \int \mathrm{d}t\left(-y\left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}}\bigg|_{x_c} - \frac{\partial L}{\partial x}\bigg|_{x_c}\right)\right) \qquad (27)
\end{aligned}$$

that, by the equation of motion and the definition of y, is 0. Therefore,

$$K = e^{\frac{i}{\hbar}S_c}\int \mathrm{D}[y]\,\exp\left(\frac{i}{\hbar}\int \mathrm{d}t\,(a\dot{y}^2 + by\dot{y} + cy^2)\right) \qquad (28)$$

Only the quadratic terms contribute to the propagator prefactor; the linear terms affect only the classical action computing.

3 Adding a source term to the action

3.1 The free particle case

Let's suppose to have a free particle, and let's add a source term:

$$L = \frac{m}{2}\dot{x}^2 + Jx \qquad (29)$$

As showed for the quadratic Lagrangians, the source factor affect only the classic action term:

$$K = e^{\frac{i}{\hbar}S_c}\int \mathrm{D}[y]\,\exp\left(\frac{i}{\hbar}\int \mathrm{d}t\,(\frac{m}{2}\dot{y}^2)\right) \qquad (30)$$

and, remembering the already computed path integral for free particle,

$$K = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} e^{\frac{i}{\hbar}S_c} \tag{31}$$

3.2 Generic Lagrangian and functional derivatives

Let L be a generic Lagrangian, and let's add a source term

$$L' = L + Jx \tag{32}$$

where $J = J(t)$. Considering time and space quantized, the propagator is:

$$K = \int \mathrm{d}x_1 \ldots \mathrm{d}x_n \exp\left(\frac{i}{\hbar}\sum_i (L(\dot{x}_i, x_i) + J_i x_i)\right) \tag{33}$$

Deriving K by a generic J_i,

$$\frac{\partial K}{\partial J_i} = \frac{i}{\hbar}\int \mathrm{D}[x]\, x_i \exp\left(\frac{i}{\hbar}\sum_i (L(\dot{x}_i, x_i) + J_i x_i)\right) \tag{34}$$

and going to the continuous limit,

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar}\int \mathrm{D}[x]\, x(t^*) \exp\left(\frac{i}{\hbar}\int \mathrm{d}t\, (L(\dot{x}, x) + Jx)\right) \tag{35}$$

where $\frac{\delta K[J]}{\delta J(t^*)}$ is the functional derivative.

To find the meaning of this expression the path integral can be split in three integral, wrt the position at time t^*. Let $\mathrm{D}[x_{i*}]$ be the differential on all the path from x_i to x^*, and $\mathrm{D}[x_{*f}]$ be the differential on all the path from x^* to x_f. So:

$$\begin{aligned}
\frac{\delta K[J]}{\delta J(t^*)} &= \frac{i}{\hbar}\int \mathrm{D}[x]\, x(t^*) \exp\left(\frac{i}{\hbar}\int \mathrm{d}t\, (L(\dot{x}, x) + Jx)\right) && (36)\\
&= \frac{i}{\hbar}\int \mathrm{D}[x_{i*}]\; \mathrm{d}x^*\, \mathrm{D}[x_{*f}]\, x^* \exp\left(\frac{i}{\hbar}\left(\int_{t_i}^{t^*} + \int_{t^*}^{t_f}\right) \mathrm{d}t\, (L(\dot{x}, x) + Jx)\right) && (37)\\
&= \frac{i}{\hbar}\int \mathrm{d}x^*\, K(f,*) x^* K(*,i) && (38)
\end{aligned}$$

Remembering that $K(f,i) = \left\langle x_f, t_f \middle| x_i, t_i \right\rangle$:

$$\begin{aligned}
\frac{\delta K[J]}{\delta J(t^*)} &= \frac{i}{\hbar}\int \mathrm{d}x^*\, \left\langle x_f, t_f \middle| x^*, t^* \right\rangle x^* \left\langle x^*, t^* \middle| x_i, t_i \right\rangle && (39)\\
&= \frac{i}{\hbar}\int \mathrm{d}x^*\, \left\langle x_f \middle| e^{-\frac{i}{\hbar}H(t_f - t^*)} \middle| x^* \right\rangle x^* \left\langle x_* \middle| e^{-\frac{i}{\hbar}H(t^* - t_i)} \middle| x_i \right\rangle && (40)
\end{aligned}$$

Therefore, having $\int \mathrm{d}x \,|x\rangle\, x\, \langle x| = \hat{x}$:

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar} \left\langle x_f \right| e^{-\frac{i}{\hbar}H(t_f - t^*)} \hat{x}^* e^{-\frac{i}{\hbar}H(t^* - t_i)} \left| x_i \right\rangle \tag{41}$$

$$= \frac{i}{\hbar} \left\langle x_f, t_f \right| \hat{x}(t^*) \left| x_i, t_i \right\rangle \tag{42}$$

that means, the functional derivative allow us to compute the expectation value for $\hat{x}$ at a fixed time t^*.

3.3 Smart way to solve perturbed harmonic oscillator

Let's consider a perturbed harmonic oscillator:

$$L = \underbrace{\frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2}_{L_{HO}} - \lambda x^4 \tag{43}$$

To solve the path integral, let's add a source term to the Lagrangian and compute $K[J]$:

$$K[J] = \int \mathrm{D}[x] \, \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \, (L_{HO} - \lambda x^4 + Jx) \right) \tag{44}$$

$$= \int \mathrm{D}[x] \, \exp\left\{ -\frac{i}{\hbar} \int \mathrm{d}t \, \lambda x^4 \right\} \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \, (L_{HO} + Jx) \right) \tag{45}$$

$$= \int \mathrm{D}[x] \sum_n \frac{1}{n!} \left(-\frac{i\lambda}{\hbar} \int \mathrm{d}t \, x^4 \right)^n \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \, (L_{HO} + Jx) \right) \tag{46}$$

$$= \sum_n \frac{1}{n!} \left(-\frac{i\lambda}{\hbar} \right)^n \int \mathrm{D}[x] \; \mathrm{d}t_1 \ldots \mathrm{d}t_n \, x_1^4 \ldots x_n^4 \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \, (L_{HO} + Jx) \right) \tag{47}$$

$$= \sum_n \frac{1}{n!} \left(-\frac{i\lambda}{\hbar} \right)^n \frac{\hbar^4}{i^4} \frac{\delta^4}{\delta J_1^4} \cdots \frac{\hbar^4}{i^4} \frac{\delta^4}{\delta J_n^4} \int \mathrm{D}[x] \, \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \, (L_{HO} + Jx) \right) \tag{48}$$

where when writing a product that involves a functional derivative the time integral is understood, i.e.

$$\frac{\partial F[J]}{\partial J} y = \int \mathrm{d}t \, \frac{\partial F[J]}{\partial J(t)} y(t) \tag{49}$$

In the equation (48) can be recognized the path integral for the un-perturbed harmonic oscillator:

$$K[J] = \sum_n \frac{1}{n!} \left(-i\lambda\hbar^3 \right)^n \frac{\delta^4}{\delta J_1^4} \cdots \frac{\delta^4}{\delta J_n^4} K_{HO}[J] \qquad = \exp\left(-i\lambda\hbar^3 \frac{\delta^4}{\delta J^4} \right) K_{HO}[J] \tag{50}$$

Finally, to return to the initial problem without source term, is enough to compute everything in $J = 0$:

$$K = \exp\left(-i\lambda\hbar^3 \frac{\delta^4}{\delta J^4}\right) K_{HO}[J]\bigg|_{J=0} \tag{51}$$