Path Integral

Alessandro Lovo, Alberto Facheris, Francesco Gentile,
Giorgio Mentasti, Jacopo Tissino, Leonardo Zampieri

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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:

$$U_I = \mathbb{1} + \frac{1}{i\hbar} \int_0^t V_I(t') U_I(t') \, \mathrm{d}t' \tag{4a}$$

$$= \mathbb{1} + \frac{1}{i\hbar} \int_0^t V_I(t') \left(\mathbb{1} + \frac{1}{i\hbar} \int_0^{t'} V_I(t'') U_I(t'') \, \mathrm{d}t'' \right) \mathrm{d}t' \tag{4b}$$

$$= \mathbb{1} + \frac{1}{i\hbar} \int_0^t V_I(t') \, \mathrm{d}t' + \frac{1}{(i\hbar)^2} \int_0^t \int_0^{t'} V_I(t') V_I(t'') \, \mathrm{d}t' \, \mathrm{d}t'' + o(V_I^2) \tag{4c}$$

.

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

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

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

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

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: $K = \left\langle x'', t \middle| x', 0 \right\rangle$ 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 $p \left| p' \right\rangle = p' \left| p' \right\rangle$, and they are also energy eigenstates with $H \left| p' \right\rangle = ((p')^2/2m) \left| p' \right\rangle$.

We compute:

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

and recall that $\left\langle x \middle| p \right\rangle = \exp(-px/i\hbar)/\sqrt{2\pi\hbar}$. 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:

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

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:

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

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

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

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:

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

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:

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

but the term $[T,U]$ is not of constant order with respect to ϵ: the range of p which must be considered when integrating is of the order $\epsilon^{-1/2}$, and $[T,U] \sim p$. So the term is actually of order $\exp\left(-\epsilon^{3/2}\right)$. When raising it to the power $N \sim 1/\epsilon$ we get

$$\left(1+\epsilon^{3/2}\right)^{1/\epsilon} \sim 1\,, \tag{20}$$

□

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

$$\int \mathrm{d}p' \left\langle x_{i+1}|p'\right\rangle \left\langle p'\right| \exp\left(\frac{H\epsilon}{i\hbar}\right)|x_i\rangle = \tag{21a}$$

$$= \frac{1}{2\pi\hbar}\int \mathrm{d}p' \exp\left(-\frac{(x_{i+1}-x_i)p'}{i\hbar}\right)\exp\left(\frac{\epsilon}{i\hbar}\left(\frac{p'^2}{2m} - V(x_i)\right)\right) \tag{21b}$$

$$= \frac{1}{2\pi\hbar}\int \mathrm{d}p' \exp\left(\frac{\epsilon}{i\hbar}\left(H(p',x) - \dot{x}p'\right)\right), \tag{21c}$$

and now we can 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 $\widetilde{p}$:

$$\frac{1}{2\pi\hbar}\int \mathrm{d}\widetilde{p} \exp\left(\frac{\epsilon}{i\hbar}\left(\frac{\widetilde{p}^2}{2m} - \frac{m\dot{x}^2}{2} + V(x)\right)\right) = \tag{22a}$$

$$= \frac{1}{2\pi\hbar}\sqrt{\frac{2\pi m\hbar}{i\epsilon}}\exp\left(-\epsilon\frac{L(x,\dot{x})}{i\hbar}\right) \tag{22b}$$

$$= \sqrt{\frac{m}{2\pi i\hbar\epsilon}}\exp\left(-\epsilon\frac{L(x,\dot{x})}{i\hbar}\right) = \langle x_{i+1}, t_{i+1}|x_i, t_i\rangle\ , \tag{22c}$$

but

2.1 Path integral of a quadratic Lagrangian

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

$$L = a\dot{x}^2 + bx\dot{x} + cx^2 + d\dot{x} + ex + f\,. \tag{23}$$

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

$$K = \int \mathrm{D}[x] \, \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \, L\right) \tag{24a}$$

$$= \int \mathrm{D}[x] \, \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \, (\underbrace{a\dot{x}^2 + bx\dot{x} + cx^2 + d\dot{x} + ex + f}_{F})\right). \tag{24b}$$

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:

$$\begin{aligned} F &= a(\dot{x}_c^2 + \dot{y}^2 + 2\dot{x}_c\dot{y}) + b(x_c\dot{x}_c + x_c\dot{y} + y\dot{x}_c + y\dot{y}) + c(x_c^2 + y^2 + 2x_c y) + \\ &\quad + d(\dot{x}_c + \dot{y}) + e(x_c + y) + f \end{aligned} \tag{25a}$$

$$\begin{aligned} &= (a\dot{x}_c^2 + bx_c\dot{x}_c + cx_c^2 + d\dot{x}_c + ex_c + f) + (a\dot{y}^2 + by\dot{y} + cy^2) + \\ &\quad + \dot{y}(2a\dot{x}_c + bx_c + d) + y(b\dot{x}_c + 2cx_c + e) \end{aligned} \tag{25b}$$

$$= L_c + (a\dot{y}^2 + by\dot{y} + cy^2) + \dot{y} \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} + y \left.\frac{\partial L}{\partial x}\right|_{x_c}, \tag{25c}$$

and so

$$K = \int \mathrm{D}[y] \, \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \left(L_c + (a\dot{y}^2 + by\dot{y} + cy^2) + \dot{y} \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} + y \left.\frac{\partial L}{\partial x}\right|_{x_c}\right)\right). \tag{26}$$

Evaluating by parts the last part of the integral:

$$I = \int \mathrm{d}t \left(\dot{y} \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} + y \left.\frac{\partial L}{\partial x}\right|_{x_c}\right) \tag{27}$$

$$= y\Big|_i^f \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} + \int \mathrm{d}t \left(-y \left(\frac{\mathrm{d}}{\mathrm{d}t} \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} - \left.\frac{\partial L}{\partial x}\right|_{x_c}\right)\right) \tag{28}$$

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

$$K = e^{\frac{i}{\hbar} S_c} \int \mathrm{D}[y] \, \exp\left(\frac{i}{\hbar} \int \mathrm{d}t \, (a\dot{y}^2 + by\dot{y} + cy^2)\right) \tag{29}$$

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:

$$L = \frac{m}{2}\dot{x}^2 + Jx \tag{30}$$

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

$$K = e^{\frac{i}{\hbar}S_c} \int \mathrm{D}[y] \, \exp\left(\frac{i}{\hbar}\int \mathrm{d}t \, (\frac{m}{2}\dot{y}^2)\right) \tag{31}$$

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

$$K = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} e^{\frac{i}{\hbar}S_c} \tag{32}$$

3.2 Generic Lagrangian and functional derivatives

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

$$L' = L + Jx \tag{33}$$

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

$$K = \int \mathrm{d}x_1 \ldots \mathrm{d}x_n \exp\left(\frac{i}{\hbar}\sum_i (L(\dot{x}_i, x_i) + J_i x_i)\right) \tag{34}$$

Deriving K by a generic J_i,

$$\frac{\partial K}{\partial J_i} = \frac{i}{\hbar}\int \mathrm{D}[x] \, x_i \exp\left(\frac{i}{\hbar}\sum_i (L(\dot{x}_i, x_i) + J_i x_i)\right) \tag{35}$$

and going to the continuous limit,

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar}\int \mathrm{D}[x] \, x(t^*) \exp\left(\frac{i}{\hbar}\int \mathrm{d}t \, (L(\dot{x}, x) + Jx)\right) \tag{36}$$

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:

$$
\begin{aligned}
\frac{\delta K[J]}{\delta J(t^*)} &= \frac{i}{\hbar}\int \mathrm{D}[x]\, x(t^*) \exp\left(\frac{i}{\hbar}\int \mathrm{d}t\,(L(\dot{x},x)+Jx)\right) && (37)\\
&= \frac{i}{\hbar}\int \mathrm{D}[x_{i*}]\ \mathrm{d}x^*\,\mathrm{D}[x_{*f}]\, x^* \exp\left(\frac{i}{\hbar}\left(\int_{t_i}^{t^*} + \int_{t^*}^{t_f}\right)\mathrm{d}t\,(L(\dot{x},x)+Jx)\right) && (38)\\
&= \frac{i}{\hbar}\int \mathrm{d}x^*\, K(f,*)x^*K(*,i) && (39)
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{\delta K[J]}{\delta J(t^*)} &= \frac{i}{\hbar}\int \mathrm{d}x^* \left\langle x_f, t_f \middle| x^*, t^* \right\rangle x^* \left\langle x^*, t^* | x_i, t_i \right\rangle && (40)\\
&= \frac{i}{\hbar}\int \mathrm{d}x^* \ \left\langle x_f \middle| e^{-\frac{i}{\hbar}H(t_f-t^*)} \middle| x^* \right\rangle x^* \left\langle x_* | e^{-\frac{i}{\hbar}H(t^*-t_i)} | x_i \right\rangle && (41)
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{\delta K[J]}{\delta J(t^*)} &= \frac{i}{\hbar}\left\langle x_f \middle|\, e^{-\frac{i}{\hbar}H(t_f-t^*)}\hat{x}^* e^{-\frac{i}{\hbar}H(t^*-t_i)}\, | x_i \right\rangle && (42)\\
&= \frac{i}{\hbar}\left\langle x_f, t_f \middle|\, \hat{x}(t^*)\, | x_i, t_i \right\rangle && (43)
\end{aligned}
$$

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:

$$
L = \underbrace{\frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2}_{L_{HO}} - \lambda x^4 \tag{44}
$$

To solve the path integral, let's add a source term to the Lagrangian and compute

$K[J]$:

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

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

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

$$= \sum_n \frac{1}{n!}\left(-\frac{i\lambda}{\hbar}\right)^n \int \mathrm{D}[x] \; \mathrm{d}t_1 \ldots \mathrm{d}t_n \, x_1^4 \ldots x_n^4 \exp\left(\frac{i}{\hbar}\int \mathrm{d}t \, (L_{HO} + Jx)\right) \tag{48}$$

$$= \sum_n \frac{1}{n!}\left(-\frac{i\lambda}{\hbar}\right)^n \frac{\hbar^4}{i^4}\frac{\delta^4}{\delta J_1^4} \cdots \frac{\hbar^4}{i^4}\frac{\delta^4}{\delta J_n^4} \int \mathrm{D}[x] \, \exp\left(\frac{i}{\hbar}\int \mathrm{d}t \, (L_{HO} + Jx)\right) \tag{49}$$

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

$$\frac{\partial F[J]}{\partial J} y = \int \mathrm{d}t \, \frac{\partial F[J]}{\partial J(t)} y(t) \tag{50}$$

In the equation (49) can be recognized the path integral for the un-perturbed harmonic oscillator:

$$K[J] = \sum_n \frac{1}{n!}\left(-i\lambda\hbar^3\right)^n \frac{\delta^4}{\delta J_1^4} \cdots \frac{\delta^4}{\delta J_n^4} K_{HO}[J] \qquad = \exp\left(-i\lambda\hbar^3 \frac{\delta^4}{\delta J^4}\right) K_{HO}[J] \tag{51}$$

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

$$K = \exp\left(-i\lambda\hbar^3 \frac{\delta^4}{\delta J^4}\right) K_{HO}[J]\bigg|_{J=0} \tag{52}$$