Path Integral

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

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

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

therefore the evolution of the interaction ket is

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

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 $V_{nm} = \langle n| V |m\rangle$. This is a matrix equation for the coefficient vector.

Time-dep perturbations If we define the interaction-picture evolution operator as $|\alpha, t\rangle = U_I(t) |\alpha, 0\rangle$ 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 $|i\rangle$, the evolution coefficients $c_n(t)$ will be given by the matrix elements $\langle n| U_I(t) |i\rangle$. 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:

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

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

1.2 The propagator

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

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

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: $\psi(x'', t) = \int d^3 x' \, K(x'', x'; t) \psi(x')$. 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:

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

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

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

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:

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

3

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:

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

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:

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

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

. . .

> Fill there

2.1 Path integral of a quadratic Lagrangians

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

$$L = a\dot{x}^2 + bx\dot{x} + cx^2 + d\dot{x} + ex + f \tag{14}$$

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

$$K = \int x \exp\left(\frac{i}{\hbar}\int dt\, L\right) \tag{15}$$

$$= \int x \exp\left(\frac{i}{\hbar}\int dt\,(\underbrace{a\dot{x}^2 + bx\dot{x} + cx^2 + d\dot{x} + ex + f}_{F})\right) \tag{16}$$

Let x_c be the classical path; let's write $x = x_c + y$ and therefore $x = y$. Properly

4

replacing x and $\dot{x}$, the propagator can be written as:

$$F = a(\dot{x}_c^2 + \dot{y}^2 + 2\dot{x}_c\dot{y}) + b(x_c\dot{x}_c + x_c\dot{y} + y\dot{x}_c + y\dot{y}) + c(x_c^2 + y^2 + 2x_cy) + \\ + d(\dot{x}_c + \dot{y}) + e(x_c + y) + f \tag{17}$$

$$= (a\dot{x}_c^2 + bx_c\dot{x}_c + cx_c^2 + d\dot{x}_c + ex_c + f) + (a\dot{y}^2 + by\dot{y} + cy^2) + \\ + \dot{y}(2a\dot{x}_c + bx_c + d) + y(b\dot{x}_c + 2cx_c + e) \tag{18}$$

$$= L_c + (a\dot{y}^2 + by\dot{y} + cy^2) + \dot{y} \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} + y \left.\frac{\partial L}{\partial x}\right|_{x_c} \tag{19}$$

and so

$$K = \int y \exp\left(\frac{i}{\hbar} \int dt \left(L_c + (a\dot{y}^2 + by\dot{y} + cy^2) + \dot{y} \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} + y \left.\frac{\partial L}{\partial x}\right|_{x_c} \right) \right) \tag{20}$$

Evaluating by parts the last part of the integral:

$$I = \int dt \left(\dot{y} \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} + y \left.\frac{\partial L}{\partial x}\right|_{x_c} \right) \tag{21}$$

$$= y \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c}\Big|_i^f + \int dt \left(-y \left(\frac{d}{dt} \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_c} - \left.\frac{\partial L}{\partial x}\right|_{x_c} \right) \right) \tag{22}$$

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

$$K = e^{\frac{i}{\hbar}S_c} \int y \exp\left(\frac{i}{\hbar} \int dt \, (a\dot{y}^2 + by\dot{y} + cy^2) \right) \tag{23}$$

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:

$$L = \frac{m}{2}\dot{x}^2 + Jx \tag{24}$$

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

$$K = e^{\frac{i}{\hbar}S_c} \int y \exp\left(\frac{i}{\hbar} \int dt \left(\frac{m}{2}\dot{y}^2\right) \right) \tag{25}$$

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

$$K = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} e^{\frac{i}{\hbar}S_c} \tag{26}$$

5

3.2 Generic Lagrangian and functional derivatives

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

$$L' = L + Jx \tag{27}$$

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

$$K = \int dx_1 \dots dx_n \exp\left(\frac{i}{\hbar} \sum_i (L(\dot{x}_i, x_i) + J_i x_i)\right) \tag{28}$$

Deriving K by a generic J_i,

$$\frac{\partial K}{\partial J_i} = \frac{i}{\hbar} \int x x_i \exp\left(\frac{i}{\hbar} \sum_i (L(\dot{x}_i, x_i) + J_i x_i)\right) \tag{29}$$

and going to the continuous limit,

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar} \int x x(t^*) \exp\left(\frac{i}{\hbar} \int dt \, (L(\dot{x}, x) + Jx)\right) \tag{30}$$

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 x_{i*} be the differential on all the path from x_i to x^*, and x_{*f} be the differential on all the path from x^* to x_f. So:

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar} \int x x(t^*) \exp\left(\frac{i}{\hbar} \int dt \, (L(\dot{x}, x) + Jx)\right) \tag{31}$$

$$= \frac{i}{\hbar} \int x_{i*} \, dx^* \, x_{*f} x^* \exp\left(\frac{i}{\hbar} \left(\int_{t_i}^{t^*} + \int_{t^*}^{t_f}\right) dt \, (L(\dot{x}, x) + Jx)\right) \tag{32}$$

$$= \frac{i}{\hbar} \int dx^* \, K(f, *) x^* K(*, i) \tag{33}$$

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

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar} \int dx^* \langle x_f, t_f | x^*, t^* \rangle x^* \langle x^*, t^* | x_i, t_i \rangle \tag{34}$$

$$= \frac{i}{\hbar} \int dx^* \langle x_f | e^{-\frac{i}{\hbar} H(t_f - t^*)} | x^* \rangle x^* \langle x_* | e^{-\frac{i}{\hbar} H(t^* - t_i)} | x_i \rangle \tag{35}$$

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

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar} \langle x_f | e^{-\frac{i}{\hbar} H(t_f - t^*)} \hat{x}^* e^{-\frac{i}{\hbar} H(t^* - t_i)} | x_i \rangle \tag{36}$$

$$= \frac{i}{\hbar} \langle x_f, t_f | \hat{x}(t^*) | x_i, t_i \rangle \tag{37}$$

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:

$$L = \underbrace{\frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2}_{L_{HO}} - \lambda x^4 \tag{38}$$

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

$$K[J] = \int x \exp\left(\frac{i}{\hbar}\int dt\,(L_{HO} - \lambda x^4 + Jx)\right) \tag{39}$$

$$= \int x \exp\left\{-\frac{i}{\hbar}\int dt\,\lambda x^4\right\}\exp\left(\frac{i}{\hbar}\int dt\,(L_{HO} + Jx)\right) \tag{40}$$

$$= \int x \sum_n \frac{1}{n!}\left(-\frac{i\lambda}{\hbar}\int dt\,x^4\right)^n \exp\left(\frac{i}{\hbar}\int dt\,(L_{HO} + Jx)\right) \tag{41}$$

$$= \sum_n \frac{1}{n!}\left(-\frac{i\lambda}{\hbar}\right)^n \int x\,dt_1\ldots dt_n\,x_1^4\ldots x_n^4 \exp\left(\frac{i}{\hbar}\int dt\,(L_{HO} + Jx)\right) \tag{42}$$

$$= \sum_n \frac{1}{n!}\left(-\frac{i\lambda}{\hbar}\right)^n \frac{\hbar^4}{i^4}\frac{\delta^4}{\delta J_1^4}\cdots\frac{\hbar^4}{i^4}\frac{\delta^4}{\delta J_n^4}\int x \exp\left(\frac{i}{\hbar}\int dt\,(L_{HO} + Jx)\right) \tag{43}$$

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

$$\frac{\partial F[J]}{\partial J}y = \int dt\,\frac{\partial F[J]}{\partial J(t)}y(t) \tag{44}$$

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

$$K[J] = \sum_n \frac{1}{n!}\left(-i\lambda\hbar^3\right)^n\frac{\delta^4}{\delta J_1^4}\cdots\frac{\delta^4}{\delta J_n^4}K_{HO}[J] \qquad = \exp\left(-i\lambda\hbar^3\frac{\delta^4}{\delta J^4}\right)K_{HO}[J] \tag{45}$$

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

$$K = \exp\left(-i\lambda\hbar^3\frac{\delta^4}{\delta J^4}\right)K_{HO}[J]\Big|_{J=0} \tag{46}$$