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

Heisenberg

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

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

- 1. State kets are defined as $|\psi(t)\rangle_I = U_0^{\dagger} |\psi(t)\rangle_S$;
- 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 : $H_0 | n \rangle = E_n | n \rangle$. These evolve like $|n(t)\rangle = U_0 | n(t=0) \rangle$.

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

$$|\psi(t)\rangle_{S} = \sum_{n} c_{n}(t) \exp(E_{n}t/i\hbar) |n\rangle ,$$
 (1)

therefore the evolution of the interaction ket is

$$\left|\psi(t)\right\rangle_{I} = U_{0}^{\dagger} \left|\psi(t)\right\rangle_{S} = \sum_{n} c_{n}(t) \left|n\right\rangle.$$
 (2)

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

$$i\hbar\dot{c}_n(t) = \sum_m V_{nm} \exp(i\omega_{nm}t)c_m(t),$$
 (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 $U_I \approx 1$, so we can integrate the Schrödinger equation:

$$U_{I} = 1 + \frac{1}{i\hbar} \int_{0}^{t} V_{I}(t') U_{I}(t') dt'$$
(4a)

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

$$= \mathbb{1} + \frac{1}{i\hbar} \int_0^t V_I(t') dt' + \frac{1}{(i\hbar)^2} \int_0^t \int_0^{t'} V_I(t') V_I(t'') dt' dt'' + o(V_I^2)$$
 (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 :

$$\langle n|V_I|i\rangle = \langle n|U_0^{\dagger}VU_0|i\rangle = \exp(i\omega_{ni}t)V_{ni},$$
 (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

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

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

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

and with this we can directly compute the evolution at a generic time: $\psi(x'',t) = \int d^3x' K(x'',x';t)\psi(x')$. 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

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

therefore in the end we get:

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

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

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

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

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

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:

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

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

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

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

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

and now make a

Claim 1.

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

Proof. We rewrite the expression as

$$\langle p' | \exp(\epsilon(T+U)) | x \rangle$$
, (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:

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

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

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:

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

...

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

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

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

,

2.1 Path integral of a quadratic Lagrangian

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

$$L = a\dot{x}^2 + bx\dot{x} + cx^2 + d\dot{x} + ex + f.$$
 (21)

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

$$K = \int D[x] \exp\left(\frac{i}{\hbar} \int dt L\right)$$
 (22a)

$$= \int D[x] \exp\left(\frac{i}{\hbar} \int dt \left(\underbrace{a\dot{x}^2 + bx\dot{x} + cx^2 + d\dot{x} + ex + f}_{F}\right)\right). \tag{22b}$$

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

$$F = a(\dot{x}_c^2 + \dot{y}^2 + 2\dot{x}_c\dot{y}) + b(x_c\dot{x}_c + x_c\dot{y} + y\dot{x}_c + y\dot{y}) + c(x_c^2 + y^2 + 2x_cy) + d(\dot{x}_c + \dot{y}) + e(x_c + y) + f$$
(23a)

$$= (a\dot{x}_c^2 + bx_c\dot{x}_c + cx_c^2 + d\dot{x}_c + ex_c + f) + (a\dot{y}^2 + by\dot{y} + cy^2) + + \dot{y}(2a\dot{x}_c + bx_c + d) + y(b\dot{x}_c + 2cx_c + e)$$
(23b)

$$= L_c + (a\dot{y}^2 + by\dot{y} + cy^2) + \dot{y} \left. \frac{\partial L}{\partial \dot{x}} \right|_{x_c} + y \left. \frac{\partial L}{\partial x} \right|_{x_c}, \tag{23c}$$

and so

$$K = \int D[y] \exp\left(\frac{i}{\hbar} \int dt \left(L_c + (a\dot{y}^2 + by\dot{y} + cy^2) + \dot{y} \left. \frac{\partial L}{\partial \dot{x}} \right|_{x_c} + y \left. \frac{\partial L}{\partial x} \right|_{x_c}\right)\right). \quad (24)$$

Evaluating by parts the last part of the integral:

$$I = \int dt \left(\dot{y} \frac{\partial L}{\partial \dot{x}} \Big|_{x_c} + y \frac{\partial L}{\partial x} \Big|_{x_c} \right)$$
 (25)

$$=y\Big|_{i}^{f}\frac{\partial L}{\partial \dot{x}}\Big|_{x_{c}}+\int dt\left(-y\left(\frac{d}{dt}\frac{\partial L}{\partial \dot{x}}\Big|_{x_{c}}-\frac{\partial L}{\partial x}\Big|_{x_{c}}\right)\right) \tag{26}$$

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

$$K = e^{\frac{i}{\hbar}S_c} \int D[y] \exp\left(\frac{i}{\hbar} \int dt \left(a\dot{y}^2 + by\dot{y} + cy^2\right)\right)$$
 (27)

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:

$$L = \frac{m}{2}\dot{x}^2 + Jx\tag{28}$$

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

$$K = e^{\frac{i}{\hbar}S_c} \int D[y] \exp\left(\frac{i}{\hbar} \int dt \left(\frac{m}{2}\dot{y}^2\right)\right)$$
 (29)

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

$$K = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} e^{\frac{i}{\hbar}S_c}$$
 (30)

3.2 Generic Lagrangian and functional derivatives

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

$$L' = L + Jx \tag{31}$$

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

$$K = \int dx_1 \dots dx_n \exp\left(\frac{i}{\hbar} \sum_i (L(\dot{x}_i, x_i) + J_i x_i)\right)$$
(32)

Deriving K by a generic J_i ,

$$\frac{\partial K}{\partial J_i} = \frac{i}{\hbar} \int D[x] x_i \exp\left(\frac{i}{\hbar} \sum_i (L(\dot{x}_i, x_i) + J_i x_i)\right)$$
(33)

and going to the continuous limit,

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar} \int D[x] x(t^*) \exp\left(\frac{i}{\hbar} \int dt \left(L(\dot{x}, x) + Jx\right)\right)$$
(34)

where $\frac{\delta K[J]}{\delta I(t^*)}$ 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 $D[x_{i*}]$ be the differential on all the path from x_i to x^* , and $D[x_{*f}]$ be the differential on all the path from x^* to x_f . So:

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

$$= \frac{i}{\hbar} \int D[x_{i*}] dx^* D[x_{*f}] x^* \exp\left(\frac{i}{\hbar} \left(\int_{t_i}^{t^*} + \int_{t^*}^{t_f} dt \left(L(\dot{x}, x) + Jx\right)\right)$$
(36)

$$= \frac{i}{\hbar} \int dx^* K(f, *) x^* K(*, i)$$
 (37)

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

$$\frac{\delta K[J]}{\delta J(t^*)} = \frac{i}{\hbar} \int dx^* \left\langle x_f, t_f \middle| x^*, t^* \right\rangle x^* \left\langle x^*, t^* \middle| x_i, t_i \right\rangle \tag{38}$$

$$= \frac{i}{\hbar} \int dx^* \left\langle x_f \middle| e^{-\frac{i}{\hbar}H(t_f - t^*)} \middle| x^* \right\rangle x^* \left\langle x_* \middle| e^{-\frac{i}{\hbar}H(t^* - t_i)} \middle| x_i \right\rangle \tag{39}$$

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

$$\frac{\delta K[J]}{\delta I(t^*)} = \frac{i}{\hbar} \left\langle x_f \middle| e^{-\frac{i}{\hbar}H(t_f - t^*)} \hat{x}^* e^{-\frac{i}{\hbar}H(t^* - t_i)} \middle| x_i \right\rangle \tag{40}$$

$$= \frac{i}{\hbar} \left\langle x_f, t_f \middle| \hat{x}(t^*) \middle| x_i, t_i \right\rangle \tag{41}$$

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:

$$L = \underbrace{\frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2}_{L_{HO}} - \lambda x^4 \tag{42}$$

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

$$K[J] = \int D[x] \exp\left(\frac{i}{\hbar} \int dt \left(L_{HO} - \lambda x^4 + Jx\right)\right)$$
(43)

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

$$= \int D[x] \sum_{n} \frac{1}{n!} \left(-\frac{i\lambda}{\hbar} \int dt \, x^4 \right)^n \exp\left(\frac{i}{\hbar} \int dt \, (L_{HO} + Jx)\right) \tag{45}$$

$$= \sum_{n} \frac{1}{n!} \left(-\frac{i\lambda}{\hbar} \right)^{n} \int D[x] dt_{1} \dots dt_{n} x_{1}^{4} \dots x_{n}^{4} \exp\left(\frac{i}{\hbar} \int dt \left(L_{HO} + Jx\right)\right)$$
(46)

$$= \sum_{n} \frac{1}{n!} \left(-\frac{i\lambda}{\hbar} \right)^{n} \frac{\hbar^{4}}{i^{4}} \frac{\delta^{4}}{\delta J_{1}^{4}} \dots \frac{\hbar^{4}}{i^{4}} \frac{\delta^{4}}{\delta J_{n}^{4}} \int D[x] \exp\left(\frac{i}{\hbar} \int dt \left(L_{HO} + Jx\right)\right)$$
(47)

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

$$\frac{\partial F[J]}{\partial J}y = \int dt \frac{\partial F[J]}{\partial J(t)}y(t) \tag{48}$$

In the equation (47) can be recognized the path integral for the un-perturbed harmonic oscillator:

$$K[J] = \sum_{n} \frac{1}{n!} \left(-i\lambda \hbar^{3} \right)^{n} \frac{\delta^{4}}{\delta J_{1}^{4}} \dots \frac{\delta^{4}}{\delta J_{n}^{4}} K_{HO}[J] \qquad = \exp\left(-i\lambda \hbar^{3} \frac{\delta^{4}}{\delta J^{4}} \right) K_{HO}[J] \qquad (49)$$

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

$$K = \exp\left(-i\lambda\hbar^3 \frac{\delta^4}{\delta J^4}\right) K_{HO}[J] \bigg|_{I=0}$$
 (50)