Path Integral for QM and QSM

Definitions, in Schrödinger picture

References

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BenTov's Review on QBM
Feynman's original paper
Feynman Vernon original paper
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Schrödinger equation and evolution operator

Evolution of the quantum state

$$i\hbar \frac{d}{dt} \left| \psi(t) \right\rangle = H \mid \psi(t) \rangle \rightarrow \mid \psi(t) \rangle = e^{-i t H/\hbar} \mid \psi(0) \rangle$$

Define evolution operator

$$U(t) \equiv e^{-i t H/\hbar}$$

Probability amplitude or wave function

Expanded in terms of a complete set of eigenfunctions

$$\begin{aligned}\psi(q,\ t) &\equiv \langle q \mid \psi(t) \rangle \\ &= \textstyle\sum_k \langle q \mid u_k \rangle \left\langle u_k \left| e^{-i t H/\hbar} \right| \psi(0) \right\rangle \\ &\equiv \textstyle\sum_k a_k(t)\ u_k(q)\end{aligned}$$

Feynman path integral and generating functional

$$\begin{aligned}\psi(q,\ t) \equiv \langle q \mid \psi(t) \rangle = \langle q \mid U(t - t_0) \mid \psi(t_0) \rangle \\ &= \int dq_0 \langle q \mid U(t - t_0) \mid q_0 \rangle \langle q_0 \mid \psi(t_0) \rangle \\ &= \int dq_0 \langle q \mid U(t - t_0) \mid q_0 \rangle\, \psi(q_0,\ t_0)\end{aligned}$$

`BenTov's Review on QBM` in page 13, shows that the source-free Feynman path integral is the evolution operator in coordinate basis:

$$\begin{aligned}K(q,\ t \mid q_0,\ t_0) \equiv \langle q \mid U(t - t_0) \mid q_0 \rangle = \left\langle q \mid U(t)\, U^\dagger(t_0) \mid q_0 \right\rangle \\ = \int_{w(t_0)=q_0}^{w(t)=q} \mathrm{Dw}\ \mathrm{Exp}\left[\frac{i}{\hbar} \int_{t_0}^{t} ds\, L[w,\ s]\right]\end{aligned}$$

The generating functional

$$Z(q_0, q_f)[J] \equiv Z(q_0, t_0; q_f, t_f)[J(t)] \equiv \int_{w(t_0)=q_0}^{w(t_f)=q_f} \mathrm{Dw}\, \mathrm{Exp}\left[\frac{i}{\hbar} \int_{t_0}^{t} \mathrm{ds}\,(L[w(s), s] + J(s)\, w(s))\right]$$

$$Z(q_0, q)[J=0] = K(q, t \mid q_0, t_0)$$

$$\frac{\delta}{\delta J(t_1)} Z(q_0, q)[J] \mid_{J=0} = \frac{i}{\hbar} \int_{w(t_0)=q_0}^{w(t)=q} \mathrm{Dw}\, w(t_1)\; \mathrm{Exp}\left[\frac{i}{\hbar} \int_{t_0}^{t} \mathrm{ds}\, L[w(s), s]\right] = \left\langle q \mid U(t)\, \hat{q}(t_1)\, U^\dagger(t_0) \mid q_0 \right\rangle$$

Density matrix: $\rho(t) = \int \mathrm{dq}\, \mathrm{dq}'\, \rho(q, q', t) \mid q\rangle\langle q' \mid$

In coordinate basis:

$$\rho(t) = \frac{1}{N} \sum_{n=1}^{N} p_n \mid \psi_n(t)\rangle\langle\psi_n(t) \mid$$

$$= \frac{1}{N} \sum_{n=1}^{N} p_n \int \mathrm{dq}\, \mathrm{dq}' \mid q\rangle\langle q \mid \psi_n(t)\rangle\langle\psi_n(t) \mid q'\rangle\langle q' \mid$$

$$= \int \mathrm{dq}\, \mathrm{dq}'\, \rho(q, q', t) \mid q\rangle\langle q' \mid$$

where we defined

$$\rho(q, q', t) \equiv \frac{1}{N} \sum_{n=1}^{N} p_n\, \psi_n(q, t)\, \psi_n(q', t)^*$$

$Z = \mathrm{Tr}\, \rho(t) = \int \mathrm{dq}\, \rho(q, q, t) = 1$

$$\mathrm{Tr}\, \rho(t) = \int \mathrm{dq}\, \rho(q, q, t)$$

$$= \int \mathrm{dq}\, \frac{1}{N} \sum_{n=1}^{N} p_n \mid \psi_n(q, t) \mid^2$$

$$= \frac{1}{N} \sum_{n=1}^{N} p_n \int \mathrm{dq} \mid \psi_n(q, t) \mid^2$$

$$= \frac{1}{N} \sum_{n=1}^{N} p_n = 1$$

$$\int \mathrm{dq} \mid \psi_n(q, t) \mid^2 = \int \mathrm{dq} \sum_k a_k(t)\, u_k(q) \sum_j a^*{}_j(t)\, u^*{}_j(q)$$

$$\left\{\int \mathrm{dq}\; u_k(q)\; u^*{}_j(q) = \delta_{\mathrm{kj}}\right\}$$

$$= \sum_k \mid a_k(t) \mid^2 = 1$$

`Density matrix in Schroedinger picture` comments.

Keldysh path integral and the Keldysh evolution operator

$$\rho(q, q', t) \equiv \frac{1}{N} \sum_{n=1}^{N} p_n\, \psi_n(q, t)\, \psi_n(q', t)^*$$
$$= \frac{1}{N} \sum_{n=1}^{N} p_n \langle q \mid U(t) \mid \psi_n(0)\rangle \langle \psi_n(0) \mid U^\dagger(t) \mid q'\rangle$$
$$= \frac{1}{N} \sum_{n=1}^{N} p_n \int dq_0 \int dq_0' \langle q \mid U(t) \mid q_0\rangle \langle q_0 \mid \psi_n(0)\rangle \langle \psi_n(0) \mid q_0'\rangle \langle q_0' \mid U^\dagger(t) \mid q'\rangle$$
$$= \int dq_0 \int dq_0'\, J(q, q', t \mid q_0, q_0', 0)\, \rho(q_0, q_0', 0)$$

$$J(q, q', t \mid q_0, q_0', 0) = \langle q \mid U(t) \mid q_0\rangle \langle q_0' \mid U^\dagger(t) \mid q'\rangle$$
$$= K(q, t \mid q_0, 0)\, K(q', t \mid q_0', 0)^*$$
$$= \int_{q_0}^{q} Dw \int_{q_0'}^{q'} Dw' \,\mathrm{Exp}\left[\frac{i}{\hbar} (S[w] - S[w'])\right]$$

$$Z[J, J'] \equiv \int dq_0 \int dq_0'\, Z(q_0, q)[J]\, Z(q_0', q')[J']^*\, \rho(q_0, q_0', 0)$$
$$Z[J = 0, J' = 0] = \int dq\, \rho(q, q, t)$$

Physical observables: correlation functions

Ensemble average

Ensemble average of the expectation value of a quantum operator, as a function of time,

$$\langle O\rangle (t) = \mathrm{Tr}\,[O\, \rho(t)]$$
$$= \frac{1}{N} \sum_{n=1}^{N} p_n \,\mathrm{Tr}\,[O \mid \psi_n(t)\rangle \langle \psi_n(t) \mid]$$
$$= \frac{1}{N} \sum_{n=1}^{N} p_n \,\langle \psi_n(t) \mid O \mid \psi_n(t)\rangle$$

For pure states: $\rho(t) = \mid \psi(t)\rangle \langle \psi(t) \mid$

$$\langle O\rangle (t) = \mathrm{Tr}\,[O\, \rho(t)] = \langle \psi(t) \mid O \mid \psi(t)\rangle$$

Operator insertions interpretation

Assume $t_0 < t < t_*$

$\mathrm{Tr}\,[O\, \rho(t)] = \mathrm{Tr}\left[O\, U(t - t_0)\, \rho(t_0)\, U^\dagger(t - t_0)\right]$

$= \mathrm{Tr}\left[U^\dagger(t - t_0)\, O\, U(t - t_0)\, \rho(t_0)\right] = \mathrm{Tr}[O\,(t - t_0)\, \rho(t_0)]$ (Heisenberg picture)

(1) $= \mathrm{Tr}[U(t_0 - t_*)\, U(t_* - t)\, O\, U(t - t_0)\, \rho(t_0)]$ (Operator inserted in the forward branch at time t)

(2) $= \mathrm{Tr}[U(t_0 - t)\, O\, U(t - t_*)\, U(t_* - t_0)\, \rho(t_0)]$ (Operator inserted in the backward branch at time t)

(3) $= \frac{1}{2}\{(1) + (2)\}$

(1) Operator inserted in the forward branch at time t

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                 O
t0 ------------- t -------->-------- t*
t0 ----------------<---------------- t*
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(2) Operator inserted in the forward branch at time t

t_0 ----------------->-------------- t_*

t_0 ------------- t ------<---------- t_*

O

Assume $t_0 < t_1 < t_2 < t_*$

$$\mathrm{Tr}\left[\, U^{\dagger}(t_2 - t_1)\, O\, U(t_2 - t_1)\, O\, \rho(t_1)\right]$$
$$= \mathrm{Tr}\,[\, O(t_2 - t_1)\, O(t_1 - t_0)\, \rho(t_0)] \quad \text{(Heisenberg picture)}$$
$$= \mathrm{Tr}\,[U(t_0 - t_1)\, U(t_1 - t_*)\, U(t_* - t_2)\, O\, U(t_2 - t_1)\, O\, U(t_1 - t_0)\, \rho(t_0)]$$

Forward branch:

O O

t_0 ------------- t_1 -------->--- t_2 ---->--- t_*

t_0 ---------------<----------------------- t_*

We can have all possible different combinations for the operator insertions.

Transition amplitudes

$$\langle \psi'(t') \mid O \mid \psi(t)\rangle = \langle \psi'(0) \mid U^{\dagger}(t')\, O\, U(t) \mid \psi(0)\rangle$$
$$= \int dq_0 \int dq_0' \langle q_0' \mid U^{\dagger}(t')\, O\, U(t) \mid q_0\rangle\, \psi(q_0, 0)\, \psi'(q_0', 0)^*$$
$$= \int dq \int dq' \int dq_0 \int dq_0' \langle q_0' \mid U^{\dagger}(t') \mid q'\rangle \langle q' \mid O \mid q\rangle \langle q \mid U(t) \mid q_0\rangle\, \psi(q_0, 0)\, \psi'(q_0', 0)^*$$
$$= \int dq \int dq' \int dq_0 \int dq_0' \langle q' \mid O \mid q\rangle\, K(q, t \mid q_0, 0)\, K(q', t' \mid q_0', 0)^*\, \psi(q_0, 0)\, \psi'(q_0', 0)^*$$

Special case: position operator

For the special case of $O = \hat{q} \to \langle q' \mid \hat{q} \mid q\rangle = q\, \delta_{q q'}$

$$\mathrm{Tr}\, \hat{q}\, \rho(t) = \int dq\, dq'\, q\, \delta(q', q)\, \rho(q, q', t)$$
$$= \int dq\, q\, \rho(q, q, t)$$

$$\langle \psi'(t') \mid \hat{q} \mid \psi(t)\rangle = \int dq_0 \int dq_0' \langle q_0' \mid U^{\dagger}(t')\, \hat{q}\, U(t) \mid q_0\rangle\, \psi(q_0, 0)\, \psi'(q_0', 0)^*$$

According to `BenTov's Review on QBM`, and thinking in Heisenberg picture:

Transition amplitude $\langle q' \mid U^{\dagger}(t')\, \hat{q}\, U(t) \mid q_0\rangle$ can be generated using a Feynman path integral generating function.

Expectation values $\langle q_0 \mid U^{\dagger}(t)\, \hat{q}\, U(t) \mid q_0\rangle$ cannot be, would be trivial equal to 1.

In QFT

The QM discussion can be generalized to QFT (there are subtleties though, due to infinite dimensional Hilbert space, see discussion in `Physics stack exchange`). The Gaussian density matrix for mixed quantum field states are discussed in `Quantum Fields Information Theory`.

Schrödinger wave functional is analogous to the wave function.

Some extracts from Feynman-Vernon paper

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Feynman Vernon original paper
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$$\rho(Q, X; Q', X') = \langle \psi(Q, X)\psi^*(Q', X')\rangle_{\text{av}}$$

$$\operatorname{Tr} \rho(Q, X; Q', X') = \iint \rho(Q, X; Q, X)\, dQ\, dX$$

$$\langle A\rangle = \iiint \rho(Q, X; Q', X)A(Q, Q')\, dQ\, dQ'\, dX$$

$$A(Q', Q) = \sum_{i,j} A_{ij}\phi_i^*(Q)\phi_j(Q')$$

$$A_{ij} = \int \phi_i^*(Q)A\phi_j(Q)\, dQ,$$

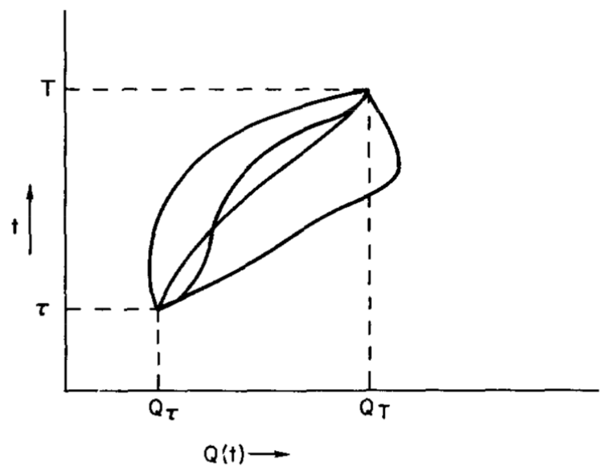
ϕ_i eigenfunction basis

Since $K(Q_T, Q_\tau)$ is the amplitude to go from coordinate Q_τ to Q_T, it f
that at $t = T$ the amplitude that the system is in a state designated by ϕ
when initially in a state $\phi_n(Q_\tau)$ is given by

$$A_{mn} = \int \phi_m{}^*(Q_T)K(Q_T, Q_\tau)\phi_n(Q_\tau)\, dQ_T$$

$$K(Q_T, T; Q_\tau, \tau) = \int \exp[(i/\hbar)S(Q)]\mathfrak{D}Q(t)$$

$$P_{mn} = |A_{mn}|^2$$

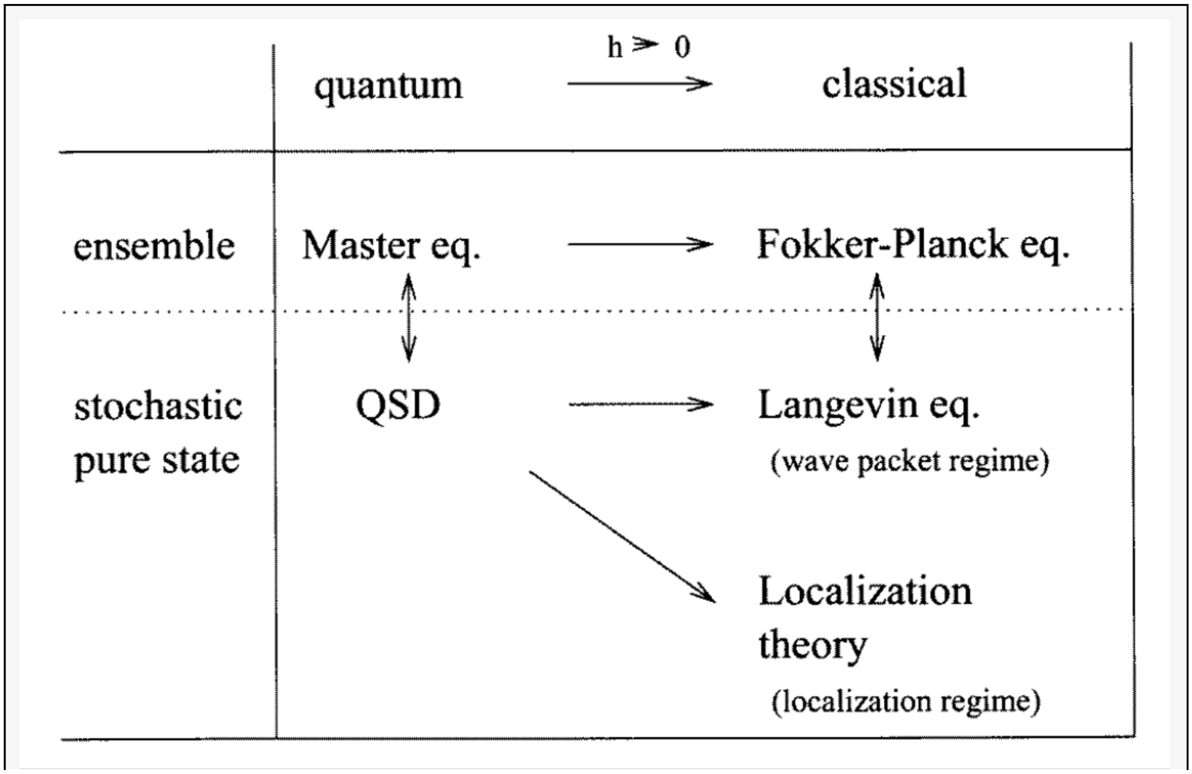


Fokker-Planck <-> Langevin

Book: The Fokker-Planck Equation Methods of Solution and Applications, by Hannes Risken,

Article: `Classical mechanics from quantum state diffusion- a phase-space approach`

Quantum equations relationship



Drift vector and diffusion matrix

Fokker-Planck for the probability density, with many variables:

$$\partial W(\{x\}, t)/\partial t = L_{\mathrm{FP}}(\{x\}, t)\, W(\{x\}, t)$$

$$L_{\mathrm{FP}}(\{x\}, t) = -\frac{\partial}{\partial x_i} D_i(\{x\}, t) + \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(\{x\}, t)$$

Stochastic variables:

$$\{\xi\} = \xi_1, \xi_2, \ldots, \xi_N$$

drift vector

$$D_i(\{x\},t) = \lim_{\tau\to 0}\frac{1}{\tau}\langle \xi_i(t+\tau)-\xi_i(t)\rangle\Big|_{\xi_k(t)=x_k},$$

diffusion matrix

$$D_{ij}(\{x\},t) = D_{ji}(\{x\},t)$$
$$= \frac{1}{2}\lim_{\tau\to 0}\frac{1}{\tau}\langle [\xi_i(t+\tau)-\xi_i(t)][\xi_j(t+\tau)-\xi_j(t)]\rangle\Big|_{\xi_k(t)=x_k}$$

Non-linear Langevin from Fokker Planck, general

From Risken’s book chapter 3.4:

Nonlinear Langevin eqs:

$$\dot{\xi}_i = h_i(\{\xi\},t) + g_{ij}(\{\xi\},t)\,\Gamma_j(t)$$

$$\langle \Gamma_i(t)\rangle = 0\,, \qquad \langle \Gamma_i(t)\,\Gamma_j(t')\rangle = 2\delta_{ij}\,\delta(t-t')$$

$$D_i(\{x\},t) = h_i(\{x\},t) + g_{kj}(\{x\},t)\,\frac{\partial}{\partial x_k}\,g_{ij}(\{x\},t)$$

$$D_{ij}(\{x\},t) = g_{ik}(\{x\},t)\,g_{jk}(\{x\},t)$$

As shown in Chap. 4, the drift and diffusion coefficients determine the Fokker-Planck equation which describes the evolution of the probability density. The drift and diffusion coefficients D_i and D_{ij} are uniquely determined by the functions h_i and g_{ij} of the Langevin equation as given by (3.118, 119) in the Stratonovich sense. The question now arises whether the Langevin equations, i.e., h_i and g_{ij}, are uniquely determined by the drift and diffusion coefficients D_i and D_{ij}. For N variables we have N equations (3.118) and, because of the symmetry of $D_{ij} = D_{ji}$, $\frac{1}{2}N(N+1)$ equations (3.119) for matrices D_{ij} being positive definite. The number of unknown elements h_i is N and the number of unknown elements g_{ij} is N^2. The degree of freedom f is given by

$$f = \text{total number of unknown elements} - \text{total number of equations}$$
$$= N + N^2 - N - \tfrac{1}{2}N(N+1) = \tfrac{1}{2}N(N-1)\,.$$

One way is:

$$g_{ij} = (D^{1/2})_{ij} = (D^{1/2})_{ji}$$
$$h_i = D_i - (D^{1/2})_{kj} \frac{\partial}{\partial x_k} (D^{1/2})_{ij}$$

Kramer’s equation

For a Brownian particle moving in a potential $m\, f(x)$:

$$\dot{v}(t) = -\gamma v(t) - f'(x(t)) + \Gamma(t)$$
$$\dot{x}(t) = v(t)$$

where Γ(t) is the Gaussian noise. The above eq can be written as a single eq:

$$\ddot{x}(t) + \gamma \dot{x}(t) + f'(x(t)) = \Gamma(t)$$

Its corresponding Fokker Planck equation (aka Kramer’s equation in this specific case) is:

$$\frac{\partial W(x,v,t)}{\partial t} = \left\{ -\frac{\partial}{\partial x} v + \frac{\partial}{\partial v} [\gamma v + f'(x)] + \frac{\gamma k T}{m} \frac{\partial^2}{\partial v^2} \right\} W(x,v,t)$$

Linear Langevin -> Path Integral

References

`Path integral solutions for non-Markovian processes` (The Jacobian computation is not clear)

`The functional formalism of classical statisticaldynamics`

Steps

Given a Langevin eq, e.g.:

Linear: $\frac{dx}{dt} = f(x) + g(x)\, \xi(t)$

1. Discretize the eq
2. Compute the conditional probability:

   $R(x \equiv x_n \mid x_0) = \int dx_1 \ldots dx_{n-1}\; p(x_1, \ldots, x_n \mid x_0)$

   Observables can be computed as:

   $\langle F(x_1, \ldots, x_n) \rangle = \frac{\int dx_1 \ldots dx_{n-1}\; F(x_1, \ldots, x_n)\, p(x_1, \ldots, x_n \mid x_0)}{R(x \mid x_0)}$
3. Write the probability density in terms of the one for the noise:

   $p(x_1, \ldots, x_n \mid x_0) = \rho(\xi_1, \ldots, \xi_n)\, J\left[\frac{\partial \xi}{\partial x}\right]$

   RHS in terms of {x}.
4. The noise pdf can be written in terms of the characteristic function:

   $\rho(\xi_1, \ldots, \xi_n) = \int dz_1 \ldots dz_n\; \chi(z_1, \ldots, z_n)\, e^{-i\, z_k\, \xi^k}$
5. The continuum limit is taken, and we obtain the functional integral:

   $\langle F[x] \rangle = \frac{\int Dx\, Dz\, \chi[z] \times F[x] \times A[z, x]}{R(x \mid x_0)}$

   $A[z, x] = J\left[\frac{\partial \xi}{\partial x}\right] e^{-i\, z_k\, \xi^k(\{x\})}$

The procedure can be generalized to multiple (linear) noise terms.

Coupled linear Langevin equations --> nonlinear Langevin

$\dot{x}_1 = x_2 + x_1\, \xi \;\rightarrow\; x_2 = \dot{x}_1 - x_1\, \xi$

$\dot{x}_2 = x_1 + x_2\, \xi$

$$\begin{aligned}\ddot{x}_1 &= \dot{x}_2 + \dot{x}_1\, \xi + x_1\, \dot{\xi} \\ &= x_1 + (\dot{x}_1 - x_1\, \xi)\, \xi + \dot{x}_1\, \xi + x_1\, \dot{\xi} \\ &= x_1 - x_1\, \xi^2 + 2\, \dot{x}_1\, \xi + x_1\, \dot{\xi}\end{aligned}$$

Non-linear Langevin case?

Example: $\frac{dx}{dt} = f(x) + g(x)\, \xi(t)^2 + h(x)\, \xi(t)$

Would the process still apply though?

Can we just define new noises, e.g. $\eta(t) := \xi(t)^2$