Feynman Path Integral in Solid State Physics

A.Lichtenstein@physnet.uni-hamburg.de R.220

Contents

http://www.physnet.uni-hamburg.de/hp/group_magno/pim_10.php

Literature:

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2. N. Nagaosa "Quantum Field Theory in Condensed Matter Physics" (Springer, 1999)
3. A. Altland and B. Simons "Condensed Matter Field Theory" (Cambridge University Press 2006)
   http://www.tcm.phy.cam.ac.uk/~bds10/
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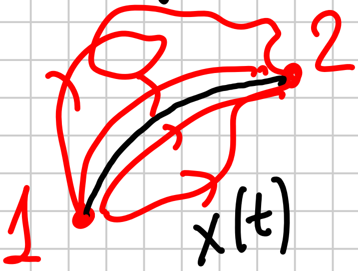
1. Introduction: What is Path Integral?

Proposed by P. Dirac and R. Feynman – very flexible and alternative formulation of QM. Useful – for Many-Body physics and QFT.



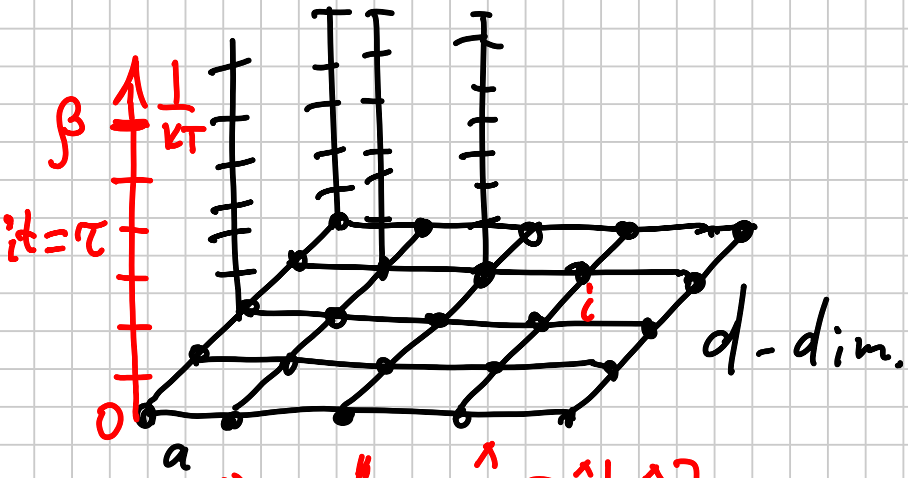
Amplitude for particle travel along path $x(t) \sim e^{iS/\hbar}$

S – classical action

Complex Quantum Amplitude $A \sim \sum_{x(t)} e^{iS[x(t)]/\hbar}$

Sum over all paths $\equiv P\int$

"d+1" Lattice



$c_i^*(\tau),\ c_i(\tau)$

"$x(t)$" $\rightarrow \hat{H}[\hat{c}_i^+, \hat{c}]$

$\Downarrow$ Path Integral

?

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} \equiv \int \mathcal{D}[c^*, c]\, e^{-\int_0^\beta d\tau \left(c^*(\tau) \frac{\partial}{\partial \tau} c(\tau) + \hat{H}[c_i^*] \right)}$$

Reminder: 1-QM, 2QM,

Single-Particle QM:

$|\psi\rangle \in \mathcal{H}$ - state vector in Hilbert-space

$$\langle\phi|\psi\rangle = \int d^3r\, \phi^*(\vec{r})\psi(\vec{r}) = \langle\psi|\phi\rangle^*$$

Norm: $\langle\psi|\psi\rangle = \int d^3r\, |\psi(\vec{r})|^2 < +\infty$

Matrix element:

$$\langle\phi|\hat{A}|\psi\rangle = \int d^3r\, \phi^*(\vec{r})\hat{A}\psi(\vec{r}) \equiv \langle\phi|\hat{A}\psi\rangle$$

Basis $|i\rangle$, $i = 1, 2, 3 \dots$ of $\mathcal{H}$-space

(infinite basis: $\sum \to \int$)

Orthonormal: $\langle i|j\rangle = \delta_{ij}$

Completeness: $\sum_i |i\rangle\langle i| = \hat{1}$

$\forall\, |\phi\rangle, |\psi\rangle \in \mathcal{H}$

$$|\psi\rangle = \sum_i |i\rangle\langle i|\psi\rangle, \quad \langle\psi| = \sum_i \langle\psi|i\rangle\langle i|$$

$$\hat{A}|\psi\rangle = \Big(\underbrace{\sum_i |i\rangle\langle i|}_{\hat{1}}\Big)\hat{A}\Big(\underbrace{\sum_j |j\rangle\langle j|}_{\hat{1}}\Big)|\psi\rangle =$$

$$= \sum_{ij} |i\rangle\langle i|\hat{A}|j\rangle\langle j|\psi\rangle$$

$$\langle\phi|\hat{A}|\psi\rangle = \sum_{ij} \langle\phi|i\rangle\langle i|\hat{A}|j\rangle\langle j|\psi\rangle$$

Hermitian conjugate: $\hat{A}^+$ of $\hat{A}$

$\langle\phi|\hat{A}|\psi\rangle = \langle\hat{A}^+\phi|\psi\rangle$ - holds for $\forall\phi,\psi$

Compare the scalar product of A^+:

$$\hat{A}^+|\phi\rangle = \sum_{j,i} |j\rangle\langle j|\hat{A}^+|i\rangle\langle i|\phi\rangle$$

$$\langle \hat{A}^+\phi|\psi\rangle = \sum_{j,i} \langle\phi|i\rangle\langle j|A^+|i\rangle^*\langle j|\psi\rangle$$

$$\Rightarrow \quad \langle j|\hat{A}^+|i\rangle = \langle i|\hat{A}|j\rangle^*$$

$\hat{A}$: eigenvalue (a) and eigenstate $(|a\rangle)$:

$$\hat{A}|a\rangle = a|a\rangle \qquad \hat{A}^+ = \hat{A} \Rightarrow a = a^* \text{ real.}$$

Position operator: $\vec{r}$

$$\hat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle \leftarrow \text{state with particle located at } \vec{r}$$

$$\langle\vec{r}|\vec{r}\,'\rangle = \delta(\vec{r}-\vec{r}\,')$$

$$\int d^3r\, |\vec{r}\rangle\langle\vec{r}| = \hat{1}$$

Momentum operator: $\vec{p}$

$$\hat{\vec{p}}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle \leftarrow \text{state of particle with momentum } \vec{p}$$

$$\langle\vec{p}|\vec{p}\,'\rangle = \delta(\vec{p}-\vec{p}\,')$$

$$\int d^3p\, |\vec{p}\rangle\langle\vec{p}| = \hat{1}$$

and

$$\langle\vec{r}|\vec{p}\rangle = (2\pi\hbar)^{-3/2} e^{i\vec{p}\vec{r}/\hbar}$$

$\psi(\vec{r}) = \langle\vec{r}|\psi\rangle$ – wave function of particle in the state $|\psi\rangle$ in coordinate representation.

In coordinate representation

$$\langle \vec r|\hat{\vec r}|\psi\rangle = \vec r\langle \vec r|\psi\rangle \equiv \vec r\,\psi(\vec r) \Rightarrow \hat{\vec r} = \vec r$$

$$\langle \vec r|\hat{\vec p}|\psi\rangle = \int d^3p\,\langle \vec r|\hat{\vec p}\underbrace{|\vec p\rangle\langle \vec p|}_{\hat 1}\psi\rangle = \int d^3p\,\vec p\langle \vec r|\vec p\rangle\langle \vec p|\psi\rangle$$

$$= \frac{\hbar}{i}\frac{\partial}{\partial \vec r}\int d^3p\langle \vec r|\vec p\rangle\langle \vec p|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial \vec r}\psi(\vec r) \Rightarrow \hat{\vec p} = \frac{\hbar}{i}\frac{\partial}{\partial \vec r}$$

Hamiltonian for 1-particle: $\hat H = \frac{\hat{\vec p}^2}{2m} + V(\vec r)$

$$\hat H|\psi_\alpha\rangle = \varepsilon_\alpha|\psi_\alpha\rangle$$

State: $|\alpha\rangle = |\vec r, \underset{\text{orbitals}}{m}, \underset{\text{spin}}{\sigma}\rangle$

$$\langle\alpha|\alpha'\rangle = \langle \vec r, m, \sigma|\vec r', m', \sigma'\rangle = \delta_{mm'}\delta_{\sigma\sigma'}\delta(\vec r - \vec r')$$

$$\sum_m \sum_{\sigma=\pm1}\int d^3r\,|\vec r m\sigma\rangle\langle \vec r m\sigma| = \hat 1$$

Many-Particles – 2-Quantization

$$\langle \vec r_1, \dots \vec r_N|\psi\rangle \equiv \psi(\vec r_1, \dots \vec r_N) \begin{cases} \nearrow B \\ \searrow F \end{cases} ?$$

$\hat P = (P_1, \dots, P_N)$ – permutation of the set $(1, 2, \dots N)$

$$\psi(\vec r_{P_1}, \vec r_{P_2}, \dots, \vec r_{P_N}) = \underbrace{(\pm 1)}_{\parallel\ \zeta}{}^{P}\,\psi(\vec r_1, \vec r_2, \dots, \vec r_N)$$

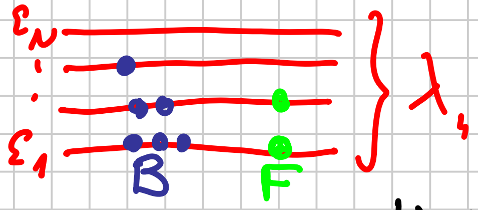
$$\zeta = \begin{cases} +1 & (\text{Boson}, \quad S = 0, 1, 2, \dots) \\ -1 & (\text{Fermion}, \quad S = \frac12, \frac32, \dots) \end{cases}$$

$$[\hat A, \hat B]_\zeta = \begin{cases} [\ ,\ ] & -B \\ \{\ ,\ \} & -F \end{cases} = \hat A\hat B - \zeta\hat B\hat A$$

(Anti-)Symmetrisation operator $\mathcal{P}$

$$\hat{\mathcal{P}}_{\binom{B}{F}} \psi(\vec r_1,\dots,\vec r_N) = \frac{1}{N!}\sum_{P} \xi^{P}\, \psi(\vec r_{P_1},\dots,\vec r_{P_N})$$

N-particle wave function:



$$|\lambda_1\lambda_2\cdots\lambda_N) = \frac{1}{\sqrt{N!\prod_\lambda (n_\lambda)!}} \sum_P \xi^P |\lambda_{P_1})\otimes|\lambda_{P_2})\otimes\cdots\otimes|\lambda_{P_N})$$

n_λ - total number of particle in $|\lambda)$, $(F: n_\lambda \le 1)$

for Fermion: $n_\lambda = \{0,1\}$ – "mod 2" $(1+1=0)$

Fock space: $\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}_N$

$$\mathcal{F}_N = |n_1\, n_2 \cdots n_N) , \quad \sum_i n_i = N$$

occupation number representation

Creation $(\hat a^+_\lambda)$ and annihilation $(\hat a_\lambda)$ operators for single-particle state $|\lambda)$

$$\hat a_i^+ |n_1\cdots n_i\cdots) = (n_i+1)^{1/2}\,\xi^{S_i}\,|n_1,\cdots,n_i+1,\cdots)$$

where $S_i = \sum_{j=1}^{i-1} n_j$

$$(\hat a_i^+)^+ = \hat a_i$$ - Hermitian adjoint

$$\langle n_1\cdots n_i\cdots|\hat a_i^+|n_1'\cdots n_i'\cdots) = \sqrt{n_i'+1}\,\xi^{S_i'}\,\delta_{n_1 n_1'}\cdots\delta_{n_i n_i'+1}\cdots$$

$$\langle n_1'\cdots n_i'\cdots|\hat a_i|n_1\cdots n_i\cdots) = \sqrt{n_i}\,\xi^{S_i}\,\delta_{n_1 n_1'}\cdots\delta_{n_i' n_i-1}$$

$$\Rightarrow \quad \hat a_i|n_1\cdots n_i\cdots) = n_i^{1/2}\,\xi^{S_i}\,|n_1,\cdots,n_i-1,\cdots)$$

Field Operators:

$$\hat{\psi}(\vec{r}) = \sum_i{}' \hat{a}_i \, \phi_i(\vec{r})$$

$$\hat{\psi}^+(\vec{r}) = \sum_i \hat{a}_i^+ \, \phi_i^*(\vec{r})$$

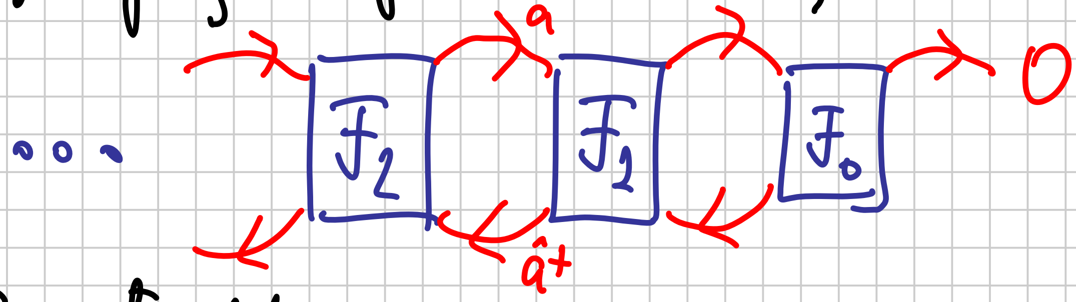
$\{\phi_i\}$ – VONS single particle

Vacuum state $|0\rangle$

$$|n_1 \, n_2 \, \cdots\rangle = \prod_i \frac{(\hat{a}_i^+)^{n_i}}{\sqrt{n_i!}} |0\rangle$$

(Anti-) Commutator: $[\hat{A}, \hat{B}]_\zeta = \hat{A}\hat{B} - \zeta \hat{B}\hat{A}$

$$[\hat{a}_i, \hat{a}_j^+]_\zeta = \delta_{ij} \qquad [\hat{a}_i, \hat{a}_j]_\zeta = [\hat{a}_i^+, \hat{a}_j^+]_\zeta = 0$$



for field-operators:

$$[\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}\,')]_\zeta = \sum_{ij} \underbrace{[\hat{a}_i, \hat{a}_j^+]_\zeta}_{= \delta_{ij}} \phi_i(\vec{r}) \phi_j^*(\vec{r}\,') =$$

$$= \sum_i \phi_i(\vec{r}) \phi_i^*(\vec{r}\,') = \sum_i \langle \vec{r} | i \rangle \langle i | \vec{r}\,' \rangle = \langle \vec{r} | \vec{r}\,' \rangle = \delta(\vec{r} - \vec{r}\,')$$

Representation of Operators

$$\hat{H} = \hat{T} + \hat{V}$$

e.g.

$$\hat{T} = \sum_i \frac{\hat{p}_i^2}{2m} = \sum_i t_i \qquad \text{"Kin"} \quad 1\text{-particle}$$

$$\hat{V} = \frac{1}{2} \sum_{i,j} v(\vec{r}_i - \vec{r}_j) \qquad 2\text{-particle} \quad v_c = \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

In Field operator representation:

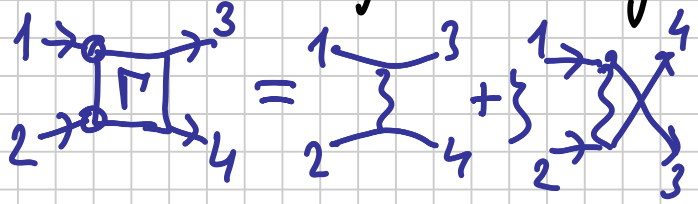
$$\hat{T} = \int \underset{\overset{\shortparallel}{d^3r}}{d\vec{r}}\, \hat{\psi}^{+}(\vec{r})\, t_1\, \psi(\vec{r})$$

$$\hat{V} = \frac{1}{2}\int d\vec{r} \int d\vec{r}\,'\, \hat{\psi}^{+}(\vec{r})\, \hat{\psi}^{+}(\vec{r}\,')\, v(\vec{r}-\vec{r}\,')\, \hat{\psi}(\vec{r}\,')\, \hat{\psi}(\vec{r})$$

Matrix-elements:

$$T_{\lambda\mu} = \langle \lambda | t | \mu \rangle$$

$$U_{\lambda\mu\nu\rho} = \langle \lambda\mu | v | \nu\rho \rangle = \int d\vec{r}_1 \int d\vec{r}_2\, \phi^*_\lambda(\vec{r}_1)\, \phi^*_\mu(\vec{r}_2)\, v_{12}\, \phi_\nu(\vec{r}_1)\, \phi_\rho(\vec{r}_2)$$



Hamiltonian in 2-QM

$$\hat{H} = \sum_{\lambda\mu} T_{\lambda\mu}\, \hat{a}^+_\lambda \hat{a}_\mu + \frac{1}{2}\sum_{\lambda\mu\nu\rho} U_{\lambda\mu\nu\rho}\, \hat{a}^+_\lambda \hat{a}^+_\mu \hat{a}_\rho \hat{a}_\nu$$

!

(Anti)-Symmetrized interaction:

$$\tilde{U}_{\lambda\mu\nu\rho} = U_{\lambda\mu\nu\rho} \mp U_{\lambda\mu\rho\nu}$$

$$\hat{H} = \sum_{\lambda\mu} T_{\lambda\mu}\, \hat{a}^+_\lambda \hat{a}_\mu + \frac{1}{4}\sum_{\lambda\mu\nu\rho} \tilde{U}_{\lambda\mu\nu\rho}\, \hat{a}^+_\lambda \hat{a}^+_\mu \hat{a}_\rho \hat{a}_\nu$$

Quantum Statistical Mechanics

$\beta = \frac{1}{k_B T}$

Partition function:

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H} - \mu \hat{N})}$$

Grand-canonical potential: $\Omega(\mu, V, T)$

$$e^{-\beta\Omega} = Z \Rightarrow \Omega = -\frac{1}{\beta}\ln Z$$

Thermodynamic relation:

$$\frac{\partial \Omega}{\partial \mu} = -N$$

$$\frac{\partial \Omega}{\partial V} = -P$$

$$\frac{\partial \Omega}{\partial T} = -S = \frac{\Omega - U - \mu N}{T}$$

Gibbs-relation:

$$U = TS - PV + \mu N \quad \text{internal energy}$$

Basis (?) $|\alpha\rangle$

$$Z = \sum_\alpha \langle \alpha | e^{-\beta(\hat{H} - \mu\hat{N})} | \alpha \rangle$$

$\Rightarrow$ Path-int. $|\alpha\rangle \equiv$ coherent states

2. Single-particle Path Integral (Feynman)

Formal integration of time-dependent Schrödinger Eq:

$$i\hbar\partial_t |\psi\rangle = \hat{H}|\psi\rangle$$

gives the time evolution operator:

$$|\psi(t')\rangle = \hat{U}(t',t)|\psi(t)\rangle$$

$$\hat{U}(t',t) = e^{-\frac{i}{\hbar}\hat{H}\cdot(t'-t)}\,\theta(t'-t) \leftarrow \text{causality}$$

or: $\left(i\hbar\partial_{t'} - \hat{H}\right)\hat{U}(t'-t) = i\hbar\,\delta(t'-t)\,\hat{\mathbb{1}}$ $\quad \frac{\partial\theta}{\partial t} = \delta$

We choose $t' > t$

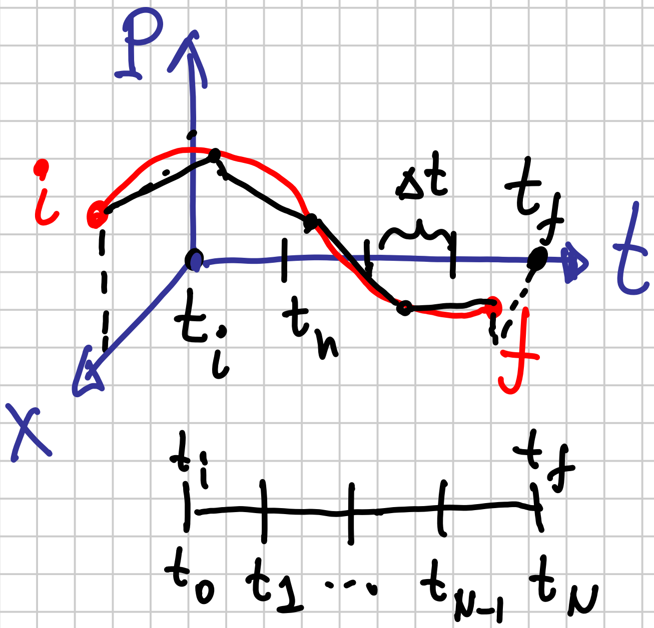
In real space "x"-representation:

$$\psi(x',t') = \int dx\, U(x't', xt)\,\psi(xt)$$

where $U(x't', xt) = \langle x'|e^{-\frac{i}{\hbar}\hat{H}\cdot(t'-t)}|x\rangle$

We choose 1 dim. model $\quad \hat{H} = \frac{p^2}{2m} + V(x) \equiv \hat{T} + \hat{V}$

Time-discretization (Trotter)



N - time-slices

$$\Delta t = \frac{t_f - t_i}{N}$$

$$t_n = t_i + n\cdot\Delta t$$

$$t_0 \equiv t_i \qquad t_N \equiv t_f$$

For $N \gg 1$ $\quad (t_i = 0,\ t_f = t)$

$$e^{-i\hat{H}t/\hbar} = \left[e^{-i\hat{H}\Delta t/\hbar} \right]^N$$

Since $\Delta t \ll 1$, (if $\hat{H} = \hat{T} + \hat{V}$)

$$e^{-i\hat{H}\Delta t/\hbar} = e^{-i\hat{T}\Delta t/\hbar} \cdot e^{-i\hat{V}\Delta t/\hbar} + O(\Delta t^2)$$

$$U(x_f t_f, x_i t_i) = \langle x_f | \left[e^{-i\hat{H}\Delta t/\hbar} \right]^N | x_i \rangle =$$

$$= \int \prod_{n=1}^{N-1} dx_n \, \langle \underset{\substack{\shortparallel \\ x_f}}{x_N} | e^{-\frac{i\Delta t}{\hbar}\hat{H}} | x_{N-1} \rangle \underset{\substack{\shortparallel \\ 1}}{} \langle x_{N-1} | e^{-\frac{i\Delta t}{\hbar}\hat{H}} | x_{N-2} \rangle \cdots \langle x_1 | e^{-\frac{i\Delta t}{\hbar}\hat{H}} | \underset{\substack{\shortparallel \\ x_i}}{x_0} \rangle$$

$\Delta t \ll 1$ – expand – exp

$$\langle x_{n+1} | e^{-\frac{i\Delta t}{\hbar}\hat{H}} | x_n \rangle \approx \langle x_{n+1} | \left(\underset{\substack{\uparrow \\ 1}}{1} - \frac{i\Delta t}{\hbar}\hat{H} \right) | x_n \rangle$$

Using momentum eigenstates (completeness)

$$\langle x_{n+1} | \hat{H} | x_n \rangle = \int dp_n \, \langle x_{n+1} | p_n \rangle \underset{1}{} \langle p_n | \hat{H} | x_n \rangle$$

Since $\hat{H} = H(\hat{p}, \hat{x}) \underset{e.g.}{=} \frac{\hat{p}^2}{2m} + V(x)$

$$\langle p_n | H(\hat{p}, \hat{x}) | x_n \rangle = H(p_n, x_n) \langle p_n | x_n \rangle$$

and $\quad \langle x_{n+1} | p_n \rangle = \dfrac{1}{\sqrt{2\pi\hbar}} \, e^{\frac{i\, p_n x_{n+1}}{\hbar}}$

$$\langle x_{n+1}| e^{-i\frac{\Delta t}{\hbar}\hat{H}} |x_n\rangle = \int dp_n \underbrace{\langle x_{n+1}|p_n\rangle}_{\exp}\underbrace{\langle p_n|x_n\rangle}_{\exp}\underbrace{\left(1-\frac{i\Delta t}{\hbar}H(p_n,x_n)\right)}_{\exp}$$

$$= \int \frac{dp_n}{2\pi\hbar} \exp\left[i\frac{p_n}{\hbar}(x_{n+1}-x_n) - i\frac{\Delta t}{\hbar} H(p_n,x_n)\right]$$

Inserting this for each terms, we obtain

$$\mathcal{U}(x_f t_f, x_i t_i) = \int \frac{dp_{N-1}}{2\pi\hbar} \cdots \int \frac{dp_0}{2\pi\hbar} \int dx_{N-1} \cdots \int dx_1 \, \times$$

$$\times \exp\left\{ \frac{i}{\hbar} \sum_{n=0}^{N-1} \left[p_n (x_{n+1}-x_n) - \Delta t \, H(p_n,x_n) \right] \right\}$$

Continuous limit: $N \to \infty$, $\Delta t \to 0$

$$x_{n+1} - x_n \simeq \underset{\frac{\partial x}{\partial t}}{\dot{x}(t)} \Delta t$$

$$\sum_{n=0}^{N-1} \Delta t \longrightarrow \int_{t_i}^{t_f} dt$$

and introducing "measure":

$$\mathcal{D}[x(t)] \equiv \prod_{n=1}^{N-1} dx_n(t) \quad \text{and} \quad \mathcal{D}[p(t)] = \prod_{n=0}^{N-1} \frac{dp_n(t)}{2\pi\hbar}$$

We get Feynman Path Integral:

$$\mathcal{U}(x_f t_f, x_i t_i) \equiv \langle x_f | e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | x_i \rangle =$$

$$= \int_{\substack{x(t_i)=x_i \\ \forall p}}^{x(t_f)=x_f} \mathcal{D}[p(t)]\mathcal{D}[x(t)] \exp\left\{ \frac{i}{\hbar} \overbrace{\int_{t_i}^{t_f} dt \left[p(t)\frac{\partial}{\partial t}x(t) - H(p(t),x(t)) \right]}^{S} \right\}$$

QM-I without $\hat{p}$, $\hat{x}$, but PI $\forall\, p(t), x(t)$

$p \neq m\dot{x}$

General: $H(\hat p, \hat q)$ $\quad 1 \to 2$

$$\mathcal{U}(2,1) = \int_1^2 \mathcal{D}[p]\,\mathcal{D}[q]\; e^{\frac{i}{\hbar}\int_{t_1}^{t_2} dt\,\underbrace{[p\dot q - H(p,q)]}_{L}}$$

Gaussian Integral

$$\int_{-\infty}^{\infty} dx\, e^{-\frac{a}{2}x^2 + bx} = \sqrt{\frac{2\pi}{a}}\, e^{\frac{b^2}{2a}} \qquad (\mathrm{Re}\, a > 0)$$

Multi-dimensional GI: N-dim:

$$\int d\vec V\, e^{-\frac{1}{2}\vec V^T \cdot \hat M \cdot \vec V + \vec J^T \cdot \vec V} = (2\pi)^{N/2} (\det M)^{-1/2}\, e^{\frac{1}{2}\vec J^T \cdot \hat M^{-1} \cdot \vec J}$$

Since kinetic term: $\hat T = \frac{p^2}{2m}$, it is possible to perform analitical integral over $\int \mathcal{D}[p]$.

1-dim:

$$\int \frac{dp_n}{2\pi\hbar}\, e^{-\frac{i\Delta t}{2m\hbar} p_n^2 + \frac{i}{\hbar}(x_{n+1}-x_n)p_n} = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2} e^{\frac{i}{\hbar}\Delta t \frac{m}{2}\left(\frac{x_{n+1}-x_n}{\Delta t}\right)^2}$$

Continuous limit: $\Delta t \to 0$

$$\Delta t \sum_{n=0}^{N-1} \frac{m}{2}\left(\frac{x_{n+1}-x_n}{\Delta t}\right)^2 \longrightarrow \int^{t_f} dt\, \frac{m}{2}\left(\frac{dx}{dt}\right)^2$$

$$\Delta t \sum_{n=0}^{N-1} V(x_n) \longrightarrow \int^{t_i} dt\, V(x(t))$$

PI-Measure: $\Delta t = \frac{t}{N}$

$$\mathcal{D}[x(t)] = \prod_{n=1}^{N-1} \left(\frac{Nm}{2\pi i t\hbar}\right)^{N/2} dx_n \qquad \to \text{3dim} \Rightarrow \frac{3N}{2}$$

Original Feynman PI:

$$U(x_f t_f, x_i t_i) = \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]} =$$

$$= \int_{x_i t_i}^{x_f t_f} \mathcal{D}[x(t)] \exp\left\{ \frac{i}{\hbar} \int_{t_i}^{t_f} dt \left[\frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x(t)) \right] \right\}$$

Summary: QM is formulate as PI without operators, only with c-numbers

Comments:

a) Normal Ordering (useful for coherent states)

$$\forall\ \hat{O}(\hat{p},\hat{x}) \longrightarrow :\hat{O}(\hat{p},\hat{x}):$$ normal order $\rightarrow$

when all $\hat{p}$ appears to the left of all $\hat{x}$

This "transformation" is always of the order $(\Delta t)^2$

Then, e.g.

$$:e^{-i\frac{\Delta t}{\hbar}\hat{H}(\hat{p},\hat{x})}: = \sum_{n=0}^{\infty} \left(-i\frac{\Delta t}{\hbar}\right)^n \sum_{k=0}^{n} \frac{1}{k!(n-k)!} \left(\frac{\hat{p}^2}{2m}\right)^k \left(V(\hat{x})\right)^{n-k}$$

Useful for particle in EM-field:

$$\hat{H}_{\vec{A}} = \frac{1}{2m}\left(\hat{p} - \frac{e}{c}\vec{A}(\hat{x})\right)^2$$

then: 3dim:

$$\langle x_{n+1} | \hat{1} :e^{-i\frac{\Delta t}{\hbar} H(\hat{p},\hat{x})}: | x_n \rangle =$$

$$= \int d^3p_n \langle x_{n+1}|p_n\rangle\langle p_n| :e^{-i\frac{\Delta t}{\hbar} H(\hat{p},\hat{x})}: |x_n\rangle =$$

$$= \int \frac{d^3p_n}{(2\pi\hbar)^3} \exp\left\{\frac{i p_n}{\hbar}(x_{n+1}-x_n) - \frac{i\Delta t}{\hbar} H(p_n, x_n)\right] x_n\rangle$$

b) Superposition principle: $(x_f t_f) \to (x_1 t_1) \to (x_i t_i)$

$$U(x_f t_f, x_i t_i) = \int dx_1\, U(x_f t_f, x_1 t_1) \cdot U(x_1 t_1, x_i t_i)$$

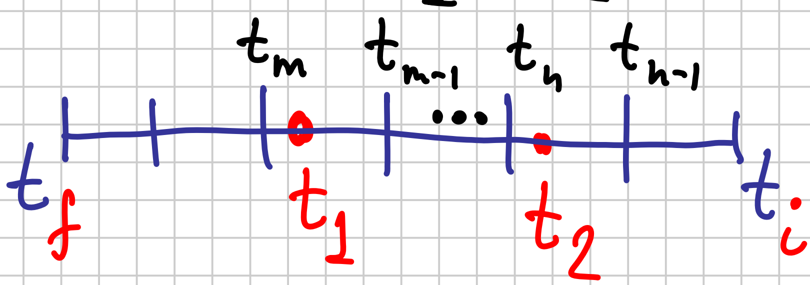
$$\overset{PI}{\Longrightarrow} \int_{(x_i t_i)}^{(x_f t_f)} \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\, L[x(t)]} = \int dx_1 \int_{(x_1 t_1)}^{(x_f t_f)} \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}\int_{t_1}^{t_f} dt\, L[x(t)]} \int_{(x_i t_i)}^{(x_1 t_1)} \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}\int_{t_i}^{t_1} dt\, L[x(t)]}$$

QM-interference $\Longrightarrow$ $\sum$ over all trajectories!

c) Automatic time-ordering

$$\langle \dots | \hat{T}\, \hat{O}_1(\hat{x}, t_1)\, \hat{O}_2(\hat{x}, t_2) | \dots \rangle \overset{PI}{\Longrightarrow} ?$$

consider $t_1 > t_2$



t_m - closest to t_1

t_n - closest to t_2

Then:

$$\langle x_f | \hat{T}\, O_1(\hat{x}, t_1)\, O_2(\hat{x}, t_2)\, e^{-\frac{i}{\hbar}\int_{t_i}^{t_f} \hat{H}(t)\, dt} | x_i \rangle =$$

$$= \langle x_f | \hat{T} e^{-\frac{i}{\hbar}\int_{t_1}^{t_f} H dt}\, O_1(\hat{x}, t_1)\, \hat{T} e^{-\frac{i}{\hbar}\int_{t_2}^{t_1} H dt}\, O_2(\hat{x}, t_2)\, \hat{T} e^{-\frac{i}{\hbar}\int_{t_i}^{t_2} H dt} | x_i \rangle =$$

$$\overset{PI}{=} \lim_{N\to\infty} \int \prod_{k=1}^{N-1} dx_k\, \langle x_f | e^{-\frac{i\Delta t}{\hbar} H} | \dots | x_m \rangle \langle x_m | O_1(x)\, e^{-\frac{i\Delta t}{\hbar} H} | x_{m-1} \rangle \langle x_{m-1} | \dots$$

$$\dots e^{-\frac{i\Delta t}{\hbar} H} | x_n \rangle \langle x_n | O_2(x)\, e^{-i\frac{\Delta t}{\hbar} H} | x_{n-1} \rangle \langle x_{n-1} | \dots e^{-\frac{i\Delta t}{\hbar} H} | x_i \rangle$$

In PI:

$$\Rightarrow \int_{(x_i t_i)}^{(x_f t_f)} \mathcal{D}[x(t)]\, O_1(x(t_1))\, O_2(x(t_2))\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\, L[x(t)]}$$

→ No need of $\hat{T}$-operator!

$O_1(x(t_1))$, $O_2(x(t_2))$ and $H[p(t), x(t)]$ – all acts on complete set of states, introduce at the corresponding discrete time.

d) The role of "$\frac{i}{\hbar} p\dot{x}$"-term: $\rightleftarrows$ $[\hat{x}, \hat{p}] = i\hbar$

Consider path integral of functional $\hat{F}$:

$$\langle \hat{F}(p,x) \rangle \overset{\text{def}}{=} \int \mathcal{D}[p]\mathcal{D}[x]\, F(p(t), x(t))\, e^{\frac{i}{\hbar} S(p(t), x(t))}$$

Discretization: $\int \mathcal{D}[p]\mathcal{D}[x] = \prod_k \int \frac{dp_k}{2\pi\hbar} \int dx_k$

$$\hat{F} \to F(p_k, x_k)$$

Transformation: (variation)

$$p_k \to p_k + \xi_k \quad , \quad |\xi_k| \ll |p_k|$$

$$x_k \to x_k + \eta_k \quad , \quad |\eta_k| \ll |x_k|$$

Then to the 1^{st} order:

$$\langle \hat{F}(p_k, x_k) \rangle = \int \prod_{k'} \frac{dp_{k'}}{2\pi\hbar} dx_{k'} \; F(p_k + \xi_k, x_k + \eta_k) e^{\frac{i}{\hbar} S[p_k+\xi_k, x_k+\eta_k]} =$$

$$= \int \prod_{k'} \frac{dp_{k'}}{2\pi\hbar} dx_{k'} \left(F + \sum_k \xi_k \frac{\partial F}{\partial p_k} + \sum_k \eta_k \frac{\partial F}{\partial x_k} \right) \left(1 + \frac{i}{\hbar} \sum_k \xi_k \frac{\partial S}{\partial p_k} + \frac{i}{\hbar} \sum_k \eta_k \frac{\partial S}{\partial x_k} \right) e^{\frac{i}{\hbar} S} =$$

$$= \langle \hat{F}(p_k, x_k) \rangle + \sum_k \xi_k \underbrace{\left\langle \frac{\partial F}{\partial p_k} + \frac{i}{\hbar} F \frac{\partial S}{\partial p_k} \right\rangle}_{0} + \sum_k \eta_k \underbrace{\left\langle \frac{\partial F}{\partial x_k} + \frac{i}{\hbar} F \frac{\partial S}{\partial x_k} \right\rangle}_{0}$$

Since $\forall\, \xi_k, \eta_k \to 0$

$$\left\langle \frac{\partial F}{\partial x_k} \right\rangle = -\frac{i}{\hbar} \left\langle F \frac{\partial S}{\partial x_k} \right\rangle$$

$$\left\langle \frac{\partial F}{\partial p_k} \right\rangle = -\frac{i}{\hbar} \left\langle F \frac{\partial S}{\partial p_k} \right\rangle$$

Setting: $\hat{F} = \hat{p} \to F[p_k, x_k] = p_{k_0}$

we get (from 2nd Eq.)

$$1 = -\frac{i}{\hbar} \left\langle p_{k_0} \frac{\partial S}{\partial p_{k_0}} \right\rangle$$

Using Action: "on the path"

$$S = \sum_k p_k (x_{k+1} - x_k) - \Delta t \sum_k H(p_k, x_k)$$

We obtain: $\frac{\partial S}{\partial p_{k_0}} = x_{k_0+1} - x_{k_0} - \underbrace{\Delta t}_{\to 0} \sum_k \frac{\partial H}{\partial p_{k_0}}$

$$i\hbar = \langle p_{k_0} (x_{k_0+1} - x_{k_0}) \rangle$$

Order of operator important! $\begin{cases} \langle \hat{p} \cdot \hat{x} \rangle_{t=t_0} \to \langle p_{k_0} x_{k_0} \rangle \\ \langle \hat{x} \cdot \hat{p} \rangle_{t=t_0} \to \langle x_{k_0+1} p_{k_0} \rangle \end{cases}$

then:

$$\langle p_{k_0}(x_{k_0+1}-x_{k_0})\rangle \to \langle \hat{x}\hat{p}-\hat{p}\hat{x}\rangle = \langle[\hat{x},\hat{p}]\rangle_{t=t_0}$$

$$\to \quad i\hbar = [\hat{x},\hat{p}]$$

Variation (Remainder)

def: Functional Differentiation

$$\frac{\delta F[J]}{\delta J(x)} = \lim_{\varepsilon\to 0} \frac{F[J(x')+\varepsilon\delta(x-x')]-F[J(x)]}{\varepsilon}$$

Equivalent definition:

$$F[J+\delta J]-F[J] = \int dx \, \frac{\delta F[J]}{\delta J(x)} \delta J(x) + O(\delta J^2)$$

Then, for example: $F[J]=J$

$$J(x) = \int dx' \, \delta(x-x') \, J(x')$$

$$\leftrightarrow \qquad \frac{\delta J(x)}{\delta J(x')} = \delta(x-x')$$

General: $F[J] = \int dx \, f(x) J(x)$

then $\dfrac{\delta F[J]}{\delta J(x)} = f(x)$

F-equation: $\dfrac{\delta F[J]}{\delta J(x)} = \dfrac{\delta G[J]}{\delta J(x)} F[J]$ has solution: $F[J]=e^{G[J]}$

The chain rule for functional differentiation:

$$\frac{\delta}{\delta g(x)} f(G[g]) = \frac{\partial f(G)}{\partial G} \cdot \frac{\delta G[g]}{\partial g(x)}$$

Of particular important case:

$$F[J] = e^{\int dx\, f(x) J(x)}$$

then $$\frac{\delta F[J]}{\delta J(x)} = f(x) \cdot J(x)$$

Taylor expansion of Functionals:

$$F[f] = F[0] + \int dx_1 \left.\frac{\delta F[f]}{\delta f(x_1)}\right|_{f=0} \cdot f(x_1) +$$

$$+ \frac{1}{2} \int dx_1 dx_2 \left.\frac{\delta^2 F[f]}{\delta f(x_2) \delta f(x_1)}\right|_{f=0} \cdot f(x_1) \cdot f(x_2) + \dots$$

Euler-Lagrange equation: $S[\phi] = \int d^m x\, L(\phi^i, \partial_\mu \phi^i)$

$|\varepsilon| \ll 1$

$$S[\phi + \varepsilon\theta] - S[\phi] = \int_1^2 d^m x \left[L(\phi + \varepsilon\phi, \partial_\mu \phi + \varepsilon \partial_\mu \theta) - L(\phi, \partial_\mu \phi) \right]$$

$$= \int d^m x \left[\frac{\partial L}{\partial \phi^i} \theta^i + \frac{\partial L}{\partial(\partial_\mu \phi^i)} \partial_\mu \theta^i \right] \varepsilon + O(\varepsilon^2) =$$

part. $\int$ $\theta\big|_1^2 = 0$

$$= \int d^m x \left[\frac{\partial L}{\partial \phi^i} - \partial_\mu \frac{\partial L}{\partial(\partial_\mu \phi^i)} \right] \theta^i \varepsilon + O(\varepsilon^2),$$

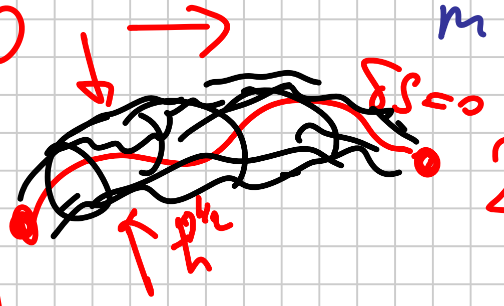
$$\Rightarrow \quad \frac{\delta S[\phi]}{\delta \phi^i(x)} = \frac{\partial L}{\partial \phi^i(x)} - \partial_\mu \frac{\partial L}{\partial(\partial_\mu \phi^i(x))}$$

Variation of Feynman P.I.

$$\delta S[x(t)] = \delta \int_{t_i}^{t_f} dt \left[\frac{m\dot{x}^2}{2} - V(x)\right] =$$

$$= \int_{t_i}^{t_f} dt \, \delta x(t) \left[-m\ddot{x}(t) - V'(x(t))\right]$$

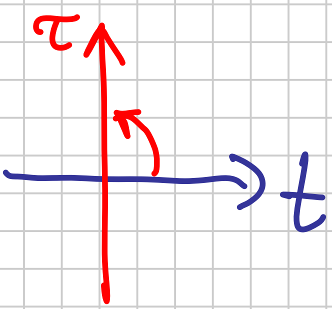
$\delta S = 0 \longrightarrow$ $m\ddot{x} = F = -V'$



$$e^{\frac{i}{\hbar} S[x(t)]}$$

Imaginary time formulation

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \int dx \, \langle x| e^{-\beta H} |x\rangle$$



Wick rotation

$$it = \tau$$

$$\frac{dx}{d\tau} = \frac{dx}{dt}\frac{dt}{d\tau} = -i\frac{dx}{dt}$$

$$\int dt \longrightarrow -i \int d\tau$$

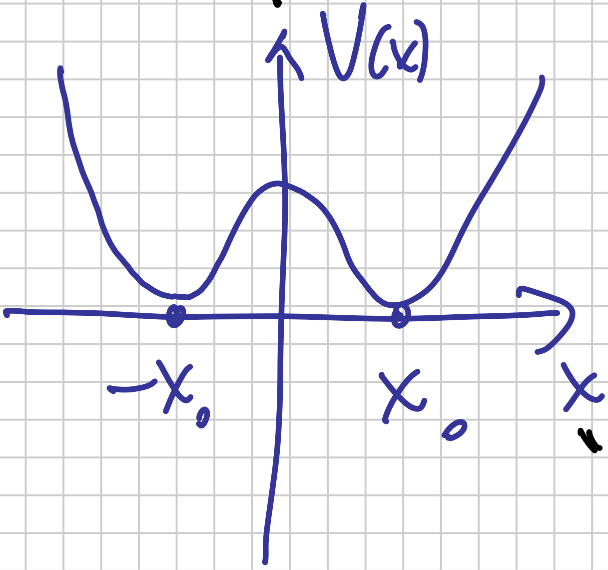
4-dim $\int dt$: Minkowskii $g_{\mu\nu} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$

$\int d\tau$: Euclidian: $g_{\mu\nu} \sim -\mathbb{1}$

Euclidian action (Feynman)

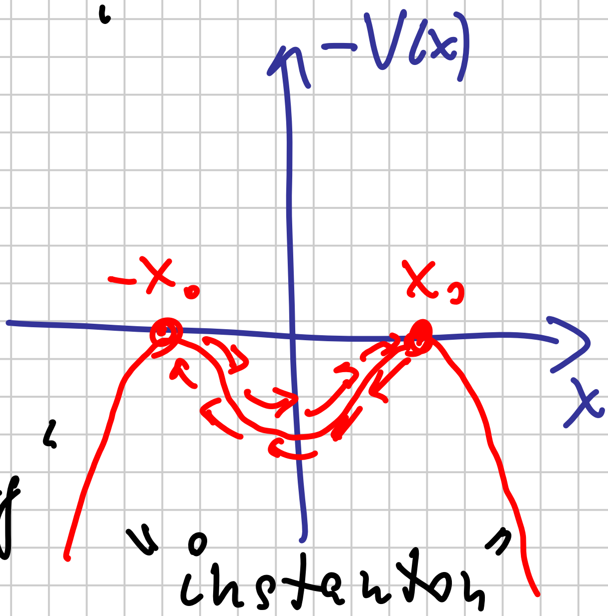
$$\langle x | e^{-\tau \hat{H}} | x \rangle = \int D[x]\, e^{-S}$$

$$S = -\frac{i}{\hbar}\int_{t_i}^{t_f} dt \left[\frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x(t))\right] = \frac{1}{\hbar}\int_{\tau_i}^{\tau_f} d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x(\tau))\right]$$



$t = -i\tau$

$\Longrightarrow$



"Tunneling path"

"instanton"

Generalization of Feynman P.I. for many-particle system

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} v(\hat{x}_i - \hat{x}_j)$$

then Partition function can be written: $(\zeta = \pm 1\ {}^{B}_{F})$

$$Z = \frac{1}{N!}\sum_P \zeta^P \int_{\substack{x_1(\beta) = x_{P_1}(0)\\ \vdots \\ x_N(\beta) = x_{P_N}(0)}} D[x_1(\tau)] \cdots D[x_N(\tau)]\ \times$$

$$\times\ e^{-\int_0^\beta d\tau \left[\sum_{i=1}^{N} \frac{m}{2}\left(\frac{dx_i(\tau)}{d\tau}\right)^2 + \frac{1}{2}\sum_{i\neq j} v(x_i(\tau) - x_j(\tau))\right]}$$

but it is much more efficient to use "coherent states"!