Feynman path-integral

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1. Motivation
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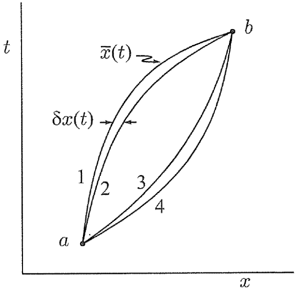
3. Example - Free Particle
4. Wick-Rotation
5. Conclusion

Classical Mechanics - Review

The basics:

- Lagrangian function $L = T - V$
  T : Kinetic energy
  V : Potential energy
- Action $S = \int_{t_0}^{t_1} L \mathrm{d}t$



Hamilton's principle of stationary action:

- $\delta S = 0$
- Euler–Lagrange equations: $\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$

$\Rightarrow$ Equations of motion
$\Rightarrow$ Classical path

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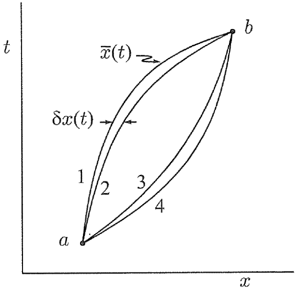

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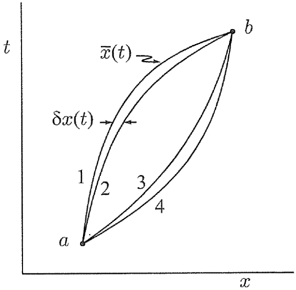

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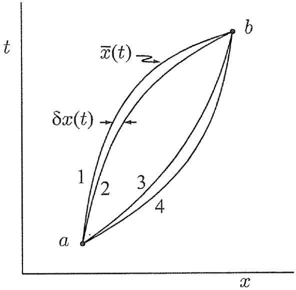

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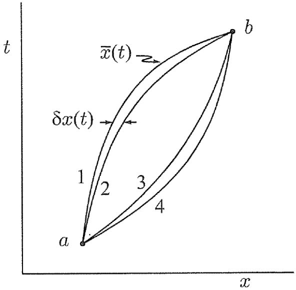

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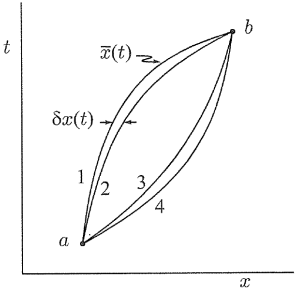

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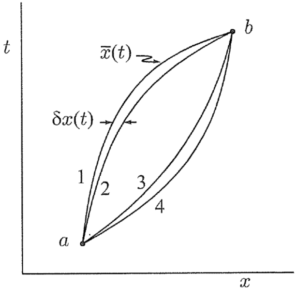

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Concept

Question: Going to QM, can we use the action S, so that in the classical limes, we end up with $\delta S = 0$ again?

- Time evolution of a quantum state vector $\rightarrow$ propagation of an amplitude in configuration space

$$\Psi(x_f, t_f) = \int \langle x_f | U(t_f, t_i) | x_i \rangle \Psi(x_i, t_i) \mathrm{d}x_i$$

- Propagator K^S:

$$K^S(x_f, t_f, x_i, t_i) = \langle x_f | U(t_f, t_i) | x_i \rangle$$

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The time evolution operator

Schrödinger's Equation:

$$i\hbar\ \partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

$$i\hbar\ \partial_t\Psi(\vec{r},t) = \hat{H}\ \Psi(\vec{r},t) \quad \Rightarrow \quad \frac{\partial_t\Psi(\vec{r},t)}{\Psi(\vec{r},t)} = -\frac{i}{\hbar}\hat{H}$$

Time Evolution:

$$\Psi(\vec{r},t) = \hat{U}(t)\ \Psi_0(\vec{r})$$

$$\frac{\partial_t\hat{U}(t)}{\hat{U}(t)} = -\frac{i}{\hbar}\hat{H} \quad \Rightarrow \quad \ln(\hat{U}(t)) = \mathcal{T}\left[-\frac{i}{\hbar}\int_0^t \mathrm{d}t'\ \hat{H}\right]$$

$$\hat{U}(t) = \mathcal{T}\left[\exp\left\{-\frac{i}{\hbar}\int_0^t \mathrm{d}t'\ \hat{H}\right\}\right]$$

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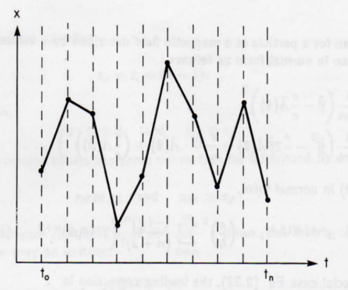

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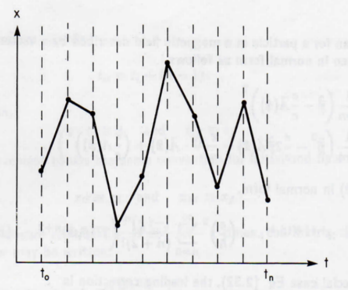

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$$\langle x|\mathrm{e}^{-\frac{i}{\hbar}\hat{H}\Delta t}|x'\rangle$$

$$\approx \langle x|\mathrm{e}^{-\frac{i}{\hbar}\hat{T}\Delta t}\mathrm{e}^{-\frac{i}{\hbar}\hat{V}\Delta t}|x'\rangle$$

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Trotter-Suzuki slicing:

$$\mathrm{e}^{\epsilon(A+B)} = \mathrm{e}^{\epsilon A}\mathrm{e}^{\epsilon B} + \mathcal{O}(\epsilon^2)$$

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Derivation

$$
\begin{aligned}
&\langle x|\mathrm{e}^{-\frac{i}{\hbar}\hat{T}\Delta t}|x'\rangle \\
&\quad= \langle x|\mathrm{e}^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\Delta t}|x'\rangle \\
&\quad= \int \mathrm{d}p\ \langle x|\mathrm{e}^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\Delta t}|p\rangle\langle p|x'\rangle \\
&\quad= \int \mathrm{d}p\ \langle x|p\rangle \mathrm{e}^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t}\langle p|x'\rangle \\
&\quad= \frac{1}{2\pi\hbar}\int \mathrm{d}p\ \mathrm{e}^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t}\mathrm{e}^{\frac{i}{\hbar}p(x-x')} \\
&\quad= \sqrt{\frac{m}{i2\pi\hbar\Delta t}}\ \mathrm{e}^{\frac{im(x-x')^2}{2\hbar\Delta t}}
\end{aligned}
$$

Intermediate steps:

$$\mathbb{1} = \int \mathrm{d}p\ |p\rangle\langle p|$$

$$\langle x|p\rangle = \sqrt{\frac{1}{2\pi\hbar}}\ \mathrm{e}^{\frac{i}{\hbar}px}$$

$$\int_{-\infty}^{\infty} \mathrm{d}y\ \mathrm{e}^{-ay^2+by} = \sqrt{\frac{\pi}{a}}\ \mathrm{e}^{\frac{b^2}{4a}}$$

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$$\Rightarrow K^S(x_f, t_f, x_i, t_i) = \langle x_f| \left(e^{-\frac{i}{\hbar}\hat{H}\Delta t}\right)^N |x_i\rangle$$

$$= \int \prod_{k=1}^{N-1} dx_k \quad \langle x_N|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_{N-1}\rangle \quad \langle x_{N-1}|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_{N-2}\rangle \dots$$

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$$K^F(x_f, t_f, x_i, t_i) = \lim_{N\to\infty} \int \prod_{k=1}^{N-1} dx_k \left(\frac{m}{i2\pi\hbar\Delta t}\right)^{\frac{N}{2}}$$

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Derivation

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$$\approx \int \prod_{k=1}^{N-1} \mathrm{d}x_k \; \sqrt{\alpha}\; e^{\beta(x_N - x_{N-1})^2} e^{\gamma V(x_{N-1})} \langle x_{N-1} | e^{-\frac{i}{\hbar}\hat{H}\Delta t} | x_{N-2} \rangle \ldots$$

$$\ldots \langle x_1 | e^{-\frac{i}{\hbar}\hat{H}\Delta t} | x_0 \rangle$$

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Derivation

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Continuity

$$\sum_{k=1}^{N} \Delta t \frac{m}{2}\left(\frac{x_k - x_{k-1}}{\Delta t}\right)^2 \to \int_{t_i}^{t_f} \mathrm{d}t\ \frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2$$

$$\sum_{k=1}^{N} \Delta t\ V(x_{k-1}) \to \int_{t_i}^{t_f} \mathrm{d}t\ V(x(t))$$

Derivation

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Derivation

Diverential:

$$\lim_{\Delta t \to 0} \frac{x(t + \Delta t) - x(t)}{\Delta t} = \frac{\mathrm{d}x}{\mathrm{d}t}$$

Derivation

Diverential:

$$\lim_{\Delta t \to 0} \frac{x_k(t + \Delta t) - x_{k-1}(t)}{\Delta t} = \frac{\mathrm{d}x}{\mathrm{d}t} \quad ??$$

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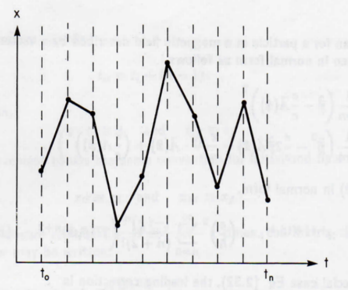

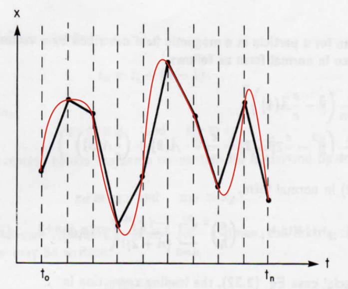

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Derivation

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

with

$$\int \mathcal{D}[x(t)] = \lim_{N\to\infty} \int \prod_{k=1}^{N-1} \mathrm{d}x_k \left(\frac{m}{i2\pi\hbar\Delta t}\right)^{\frac{N}{2}}$$

$$S[x(t)] = \int_{t_i}^{t_f} \mathrm{d}t\ L[x(t)]$$

$$L[x(t)] = \frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x(t))$$

Remarks

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

Remarks

- not only classical path $\delta S = 0$, but all possible paths
- classical limit ($\hbar \to 0$): saddle-point gives only contribution $\to \delta S = 0$
- assumption of continuity
- convergence of the prefactor
- alternative access to QM, without Schrödinger's equation

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The Free Particle

Lagrangian function:

$$L = \frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 \cancel{-V(x)}$$

Propagator:

$$K_0^F(x_f, t_f, x_i, t_i) = \lim_{N\to\infty} \int \prod_{k=1}^{N-1} \mathrm{d}x_k \left(\frac{m}{i2\pi\hbar\Delta t}\right)^{\frac{N}{2}} \times \exp\left\{\frac{im}{2\hbar\Delta t}\sum_{k=1}^{N}(x_k - x_{k-1})^2\right\}$$

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Step-by-step integration

First integral:

$$\left(\frac{m}{i2\pi\hbar\Delta t}\right)^{\frac{2}{2}} \int_{-\infty}^{\infty} \exp\left\{\frac{im}{2\hbar\Delta t}\left[(x_2 - x_1)^2 + (x_1 - x_0)^2\right]\right\} \mathrm{d}x_1$$

$$= \left(\frac{m}{i2\pi\hbar\Delta t \cdot 2}\right)^{\frac{1}{2}} \exp\left\{\frac{im}{2\hbar\Delta t \cdot 2}(x_2 - x_0)^2\right\}$$

Multiply by: $\left(\frac{m}{i2\pi\hbar\Delta t}\right)^{\frac{1}{2}} \exp\left\{\frac{im}{2\hbar\Delta t}(x_3 - x_2)^2\right\}$

Second integral:

$$= \left(\frac{m}{i2\pi\hbar\Delta t \cdot 3}\right)^{\frac{1}{2}} \exp\left\{\frac{im}{2\hbar\Delta t \cdot 3}(x_3 - x_0)^2\right\}$$

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Step-by-step integration

Feynman path-integral

Andreas Topp

Motivation

Derivation

Example - Free Particle

Wick-Rotation

Conclusion

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

After $n-1$ steps:

$$K_0^F(x_f, t_f, x_i, t_i) = \lim_{N\to\infty} \left(\frac{m}{i2\pi\hbar N\Delta t}\right)^{\frac{1}{2}} \exp\left\{\frac{im}{2\hbar N\Delta t}(x_f - x_i)^2\right\}$$

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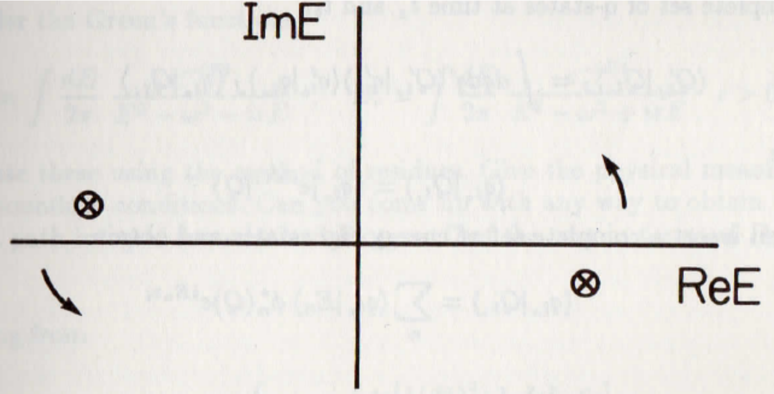
Wick-Rotation

Rotating time-axis $\Rightarrow$ Euclidean definition of the path integral



The Partition Function

Definition:

$$Z(\beta) = \mathrm{tr}\ \mathrm{e}^{-\beta \hat{H}}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x\ \langle x | \mathrm{e}^{-\beta \hat{H}} | x \rangle$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x\ \langle x | \mathrm{e}^{-\frac{i}{\hbar} t \hat{H}} | x \rangle \qquad \hookleftarrow \quad t = -i\beta\hbar$$

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Euclidean Action

What does $t = -i\tau$ in the action mean?

$$\frac{i}{\hbar} S_E[x] = \frac{i}{\hbar} \int \mathrm{d}t \left[\frac{m}{2} \left(\frac{\mathrm{d}x}{\mathrm{d}t} \right)^2 - V(x) \right]$$

$$= \frac{i}{\hbar}(-i) \int \mathrm{d}\tau \left[\frac{m}{2} \left(\frac{1}{-i} \right)^2 \left(\frac{\mathrm{d}x}{\mathrm{d}\tau} \right)^2 - V(x) \right]$$

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Remarks

- purely real $\rightarrow$ computation
- connection to statistical physics in thermal equilibrium

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Recapitulation

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

- another equivalent access for QM
- generality in the derivation
- sum over representative sample of paths $\rightarrow$ practical technique
- imaginary time path integrals are merely a computational device
- real time path integrals ?

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- imaginary time path integrals are merely a computational device
- real time path integrals ?

Recapitulation

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

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The End

Thank you very much for your attention!

Sources

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Appendix - ground state energy

$$Z(\beta) = \mathrm{tr}\ \mathrm{e}^{-\beta\hat{H}}$$
$$= \sum_n \langle n|\mathrm{e}^{-\beta E_n}|n\rangle$$
$$\overset{\beta\to\infty}{=} \langle 0|\mathrm{e}^{-\beta E_0}|0\rangle$$
$$= \mathrm{e}^{-\beta E_0}$$

$$Z(\beta) = \int_{-\infty}^{\infty} \mathrm{d}x\ K(x, t = -i\beta\hbar, x, 0)$$

$$\Rightarrow E_0 = -\lim_{\beta\to\infty} \frac{1}{\beta} \ln \int_{-\infty}^{\infty} \mathrm{d}x\ K(x, t = -i\beta\hbar, x, 0)$$

Appendix - ground state energy

$$Z(\beta) = \mathrm{tr}\ \mathrm{e}^{-\beta \hat{H}} = \sum_n \langle n | \mathrm{e}^{-\beta E_n} | n \rangle \overset{\beta\to\infty}{=} \langle 0 | \mathrm{e}^{-\beta E_0} | 0 \rangle = \mathrm{e}^{-\beta E_0}$$

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Appendix - ground state energy

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Appendix - equivalence to Schrödinger's equation

Concept:

$$\Psi(\vec{x}, t_0 + \Delta t) = \int \mathrm{d}x' K(\vec{x}, t_0 + \Delta t, \vec{x'}, t_0)\Psi(\vec{x'}, t_0)$$
$$= \Psi(\vec{x}, t_0) + \Delta t \partial_t \Psi(\vec{x}, t_0) + \mathcal{O}(\Delta t^2)$$

With:

$$K^F(\vec{x}, t_0 + \Delta t, \vec{x'}, t_0) = \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{\frac{1}{2}}$$
$$\times \exp\left\{\frac{i}{\hbar}\frac{m}{2\Delta t}\sum_{\alpha=1}^{3}\xi_\alpha^2 - \frac{i}{\hbar}\frac{q}{c}\xi_\alpha A_\alpha(\vec{x} + p\vec{\xi}) - \frac{i}{\hbar}\Delta t V(\vec{x} + r\vec{\xi})\right\}$$

Appendix - equivalence to Schrödinger's equation

Identify order of Δt:

$$\Rightarrow \partial_t \Psi(\vec{x}, t_0) = -\frac{i}{\hbar}\,[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) + \frac{q}{c}p(\vec{\nabla}\vec{A})\frac{i\hbar}{m} + \frac{1}{2}\frac{q^2}{mc^2}A^2 + \frac{qi\hbar}{cm}\vec{A}\vec{\nabla}]\ \Psi(\vec{x}, t_0)$$

$$\stackrel{p=\frac{1}{2}}{=} -\frac{i}{\hbar}\left[\frac{\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}(\vec{x})\right)^2}{2m} + V(\vec{x})\right]\ \Psi(\vec{x}, t_0)$$

Appendix - equivalence to Schrödinger's equation

Feynman path-integral

Andreas Topp

Motivation

Derivation

Example - Free Particle

Wick-Rotation

Conclusion

Identify order of Δt:

$$\Rightarrow \partial_t \Psi(\vec{x}, t_0) = -\frac{i}{\hbar}\,[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) + \frac{q}{c}p(\vec{\nabla}\vec{A})\frac{i\hbar}{m} + \frac{1}{2}\frac{q^2}{mc^2}A^2 + \frac{qi\hbar}{cm}\vec{A}\vec{\nabla}]\;\Psi(\vec{x}, t_0)$$

$$\overset{p=\frac{1}{2}}{=} -\frac{i}{\hbar}\left[\frac{\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}(\vec{x})\right)^2}{2m} + V(\vec{x})\right]\;\Psi(\vec{x}, t_0)$$