Aula II:

Queremos calcular: $\hbar i\, G(N,0) = \lim_{N\to\infty} \langle x_N | U(t_N, t_{N-1}) \cdots U(t_1, t_0) | x_0 \rangle$

para realizar esse cálculo introduzimos relações de completeza:

$$\mathbb{1} = \int dx\, |x\rangle\langle x| .$$

$\Rightarrow$

$$= \lim_{N\to\infty} \int dx_1 \cdots dx_{N-1} \langle x_N | U(t_N, t_{N-1}) | x_{N-1}\rangle\langle x_{N-1}| \cdots |x_1\rangle\langle x_1| U(t_1, t_0) | x_0\rangle$$

o k-ésimo termo é: $\langle x_{k+1} | U(t_{k+1}, t_k) | x_k \rangle$

$$= \langle x_{k+1} | U(t_k + \Delta t, t_k) | x_k \rangle$$

$$= \langle x_{k+1} | \exp\left(-\frac{i}{\hbar} H(t_k)\, \Delta t\right) | x_k \rangle$$

forma infinitesimal

★ Exercício: Mostrar $e^{\lambda A + \lambda B} = e^{\lambda A} e^{\lambda B} e^{-\frac{\lambda^2}{2}[A,B]}$ até 2 ordem.

em particular: $e^{\lambda A + \lambda B} = e^{\lambda A} e^{\lambda B} + \mathcal{O}(\lambda^2)$

isto é, para λ pequeno A e B podem serem considerados operadores que comutam. $[A,B] = 0 + \mathcal{O}(\lambda^2)$. Então:

$$\exp\left(-\frac{i}{\hbar} H(t_k)\, \Delta t\right) = \exp\left(-\frac{i}{\hbar}\Delta t \left(\frac{p^2}{2m} + V\right)\right)$$

$$= \exp\left(-\frac{i\Delta t}{\hbar}\frac{p^2}{2m}\right) \exp\left(-\frac{i\Delta t}{\hbar} V\right) + \mathcal{O}(\Delta t^2)$$

Logo, até ordem λ podemos calcular:

$$\langle x_{k+1} | e^{-\frac{i\Delta t}{\hbar} p^2/2m}\, e^{-\frac{i\Delta t}{\hbar} V} | x_k \rangle = \langle x_{k+1} | e^{-\frac{i\Delta t}{\hbar}\frac{p^2}{2m}} | x_k \rangle\, e^{-\frac{i\Delta t}{\hbar} V(x_k)}$$

$$= \langle x_{k+1} | \exp\left(-\frac{i}{\hbar}\Delta t \frac{p^2}{2m}\right) \int dp_k |p_k\rangle\langle p_k | x_k\rangle \, e^{-\frac{i}{\hbar}\Delta t V(x_k)}$$

$$= \int dp_k \langle x_{k+1}| \exp\left(\frac{-i\Delta t}{\hbar}\frac{p^2}{2m}\right)|p_k\rangle \exp\left(-\frac{i}{\hbar}p_k x_k\right) \cdot \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{-i}{\hbar}\Delta t V(x_k)\right)$$

$$= \int dp_k \langle x_{k+1} | p_k\rangle \exp\left(\frac{-i\Delta t \, p_k^2}{2m\hbar}\right) \exp\left(\frac{-i}{\hbar}p_k x_k\right) \exp\left(\frac{-i\Delta t \, V(x_k)}{\hbar}\right) \frac{1}{\sqrt{2\pi\hbar}}$$

$$= \frac{1}{2\pi\hbar}\int dp_k \exp\left(\frac{-i\Delta t}{2\hbar m} p_k^2\right) \exp\left(\frac{i}{\hbar}p_k(x_{k+1}-x_k)\right) \exp\left(-\frac{i\Delta t}{\hbar}V(x_k)\right)$$

$$= \frac{1}{2\pi\hbar}\int dp_k \exp\left(-\frac{i\Delta t}{2\hbar m}\left(p_k^2 - 2m\, p_k \underbrace{\frac{(x_{k+1}-x_k)}{\Delta t}}_{\equiv \dot{x}_k}\right)\right) \exp\left(-\frac{i\Delta t V(x_k)}{\hbar}\right)$$

$$= \frac{1}{2\pi\hbar}\int dp_k \exp\left(-\frac{i\Delta t}{2\hbar m}\left(p_k^2 - 2m\, p_k \dot{x}_k\right)\right) \exp\left(-\frac{i\Delta t}{\hbar} V(x_k)\right)$$

$$= \frac{1}{2\pi\hbar}\int dp_k \exp\left(\frac{i}{\hbar}\Delta t \left(\underbrace{\dot{x}_k p_k - H(x_k,p_k)}\right)\right)$$

Thansformado de legendre

$$x p - H \rightarrow L .$$

Portanto: $$i\hbar G(t_f, t_0) = \lim_{N\to\infty} \int \prod_{j=1}^{N-1} dx_j \int \prod_{k=0}^{N-1} \frac{dp_k}{2\pi\hbar} \times$$

$$\times \exp\left(\frac{i}{\hbar}\Delta t \sum_{k=0}^{N-1} \left(\dot{x}_k p_k - H(x_k,p_k)\right)\right)$$

Integrando apenas o que depende de p:

$$\int dp_k \exp\left(\frac{i\Delta t}{\hbar}\left(\dot{x}_k p_k - H(x_k,p_k)\right)\right)$$

$$= \int dp_k \exp\left(\frac{i\Delta t}{\hbar}\left(\dot{x}_k p_k - p_k^2/2m\right)\right) = \sqrt{\frac{2m\pi\hbar}{i\Delta t}} \exp\left(\frac{i}{\hbar}\Delta t\, m \frac{\dot{x}_k^2}{2}\right)$$

Definimos então:

$$i\hbar\, G(x_f,t_f; x_i,t_i) = \int \mathcal{D}[x] \exp\left(\frac{i}{\hbar} S(x_i,t_i; x_f,t_f)\right)$$

com $\mathcal{D}[x]$ sendo definida como:

$$\mathcal{D}[x] = \lim_{N\to\infty} \left(\frac{m}{2\pi\hbar i\Delta t}\right)^{N/2} \prod_{j=1}^{N-1} dx_j \quad , \quad \text{e } S \text{ sendo:}$$

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

* Exercício: Verificar que a medida é esta.

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* Cálculo para diferentes L.

O chamado limite semi clássico é estabelecido por:

$\frac{S}{\hbar} \gg 1$. Neste caso, como a frequência de oscilação é alta, caminhos que diferem do caminho clássico quando somados anulam suas contribuições.

Queremos calcular o caminho estacionário $\delta S = 0$ que é o que possui maior contribuição para a integral de caminho.

$x = x_{cl} + \eta \quad , \quad \dot{x} = \dot{x}_{cl} + \dot{\eta}$

$\eta(t_f) = \eta(t_i) = 0 .$

$\dot{x}^2 = (\dot{x}_{cl} + \dot{\eta})^2 = \dot{x}_{cl}^2 + \dot{\eta}^2 + 2\dot{x}_{cl}\dot{\eta} = \dot{x}_{cl} + \dot{\eta} 2 \dot{x}_{cl} + \mathcal{O}(\dot{\eta}^2)$

$V(x) = V(x_{cl}) + V'(x_{cl})\,\eta + \mathcal{O}(\eta^2) .$

$$S = \int_{t_i}^{t_f} dt \left[\frac{m}{2}\dot{x}_{cl}^2 - V(x_{cl}) \right] + \int_{t_i}^{t_f} dt \left[m \dot{x}_{cl}\dot{\eta} - V'(x_{cl})\,\eta \right]$$

$$S = S_{cl} + m\dot{x}_{cl}\eta \Big|_{t_i}^{t_f} - \int_{t_i}^{t_f} dt \left[m\ddot{x}_{cl} + V'(x_{cl}) \right] \eta$$

$\Rightarrow \quad \ddot{x}_{cl}\, m = -V'(x_{cl}) .$

As flutuações quânticas são dadas por: $\mathcal{O}(\eta^2, \dot{\eta}^2, \eta\dot{\eta})$

→ Partícula livre: $V(x) = 0$:

$$i\hbar\, G(x_f, t_f; x_i, t_i) = \lim_{N\to\infty} \left(\frac{m}{2\pi\hbar i \Delta t} \right)^{N/2} \int \prod_{j=1}^{N-1} dx_j \exp\left(\frac{i}{\hbar} \sum_{k=0}^{N-1} \frac{m}{2} \frac{(x_{k+1} - x_k)^2}{\Delta t^2} \Delta t \right)$$

$x_k = x_k^{cl} + \eta \Rightarrow (x_{k+1} - x_k)^2 = (x_{k+1\,cl} - x_{k\,cl})^2$

$+ \eta_{k+1}^2 + \eta_k^2 - 2\eta_{k+1}\eta_k$

Termos lineares em η tem contribuição nula na integral.

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$$i\hbar\, G(x_f,t_f;x_i,t_i) = \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{N/2} \exp\left(\frac{i}{\hbar}S_{cl}\right)\int \prod_{j=1}^{N-1} dx_j \exp\left(\frac{i}{\hbar}\sum_{k=1}^{N-1}\frac{m}{2}\frac{(\eta_{k+1}-\eta_k)^2}{\Delta t^2}\Delta t\right)$$

$$= \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{N/2} \exp\left(\frac{i}{\hbar}S_{cl}\right)\int \prod_{j=1}^{N-1} dx_j \exp\left(\frac{i}{\hbar}\sum_{k,l=1}^{N-1}\eta_k M_{kl}\eta_l\right)$$

$$S_{cl} = \frac{m}{2}\frac{(x_f-x_i)^2}{t_f-t_i}$$

→ Matriz M controla as flutuações quânticas, tem dimensão $(N-1)\times(N-1)$

$$M = \frac{m}{2\Delta t\hbar}\begin{pmatrix} 2 & -1 & 0 & \cdots & & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & \cdots & & & & \end{pmatrix}$$

★ Exercício: Verificar!

Integral gaussiana generalizada:

$$\int \prod_{i=1}^{N} dx_i \exp\left(-\sum_{i=1}^{N}\sum_{j=1}^{N} x_i M_{ij} x_j\right) = \pi^{N/2}\left(\sqrt{\mathrm{Det}\, M}\right)^{-1}$$

$$\mathrm{Det}(M) = N$$

Combinando os resultados:

$$i\hbar\, G(x_f,t_f;x_i,t_i) = \boxed{\lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\underbrace{\Delta t N}_{t}}\right)} \exp\left(\frac{i}{\hbar}S_{cl}\right)$$

→ amplitude dependente do tempo (parte quântica)

↳ parte "clássica".