Lecture 6.

Note Title 10/4/2009

Semiclassical asymptotics in quantum mechanics.

$$-i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\Delta + V(q)\right)\psi(x,t),$$

$\psi(x,t)$, $\quad \psi(x,0) = \psi(x)$

As $\hbar \to 0$ let us look for solutions of the form

$$\psi(x,t) = e^{\frac{i}{h}S(x,t)}\left(\psi_0(x,t) + h\,\psi_1(x,t) + \cdots\right)$$

Thm 1 Such formal expression is a solution if

1. $\partial_t S = \frac{1}{2}\sum_a (\partial_a S)^2 + V(q)$
2. $\left(\partial_t + \sum_a \partial_a S\, \partial_a + \frac{1}{2}\Delta S\right)\psi_0 = 0$
3. $\left(\partial_t + \sum_a \partial_a S\, \partial_a + \frac{1}{2}\Delta S\right)\psi_n = \frac{i}{2}\Delta \psi_{n-1}$

Proof (h/w)

Digression: Hamilton - Jacobi action

Let $\gamma_c(t, Q_1, Q_2)$ be a solution to Newton's equations

$$m\ddot{\gamma}_c^a(t) = -\frac{\partial V}{\partial q^a}(\gamma_c(t))$$

with $\gamma_c(t_1) = Q_1$, $\gamma_c(t_2) = Q_2$.

$$S^{(c)}_{t_2,t_1}(Q_2, Q_1) = \int_{t_1}^{t_2} \left(\frac{m}{2}\sum_a \dot{\gamma}_c^a(t)^2 - V(\gamma_c(t))\right)dt$$

Use Legendre transform to pass from the Lagrangian to the Hamiltonian:

$$S^{(c)}_{t_2,t_1}(Q_2, Q_1) = \int_{t_1}^{t_2} p(t)\dot{q}(t) - \int_{t_1}^{t_2} H(p(t), q(t))\,dt$$

This is the Hamilton-Jacobi function. It satisfies the equations

(1) $\frac{\partial S_{t_2 t_1}(q_2, q_1)}{\partial t_2} + H\left(d_{q_2} S_{t_2 t_1}(q_2, q_1), q_2\right) = 0,$

(2) $\frac{\partial S_{t_2 t_1}(q_2, q_1)}{\partial t_1} - H\left(-d_{q_1} S_{t_2 t_1}(q_2, q_1), q_1\right) = 0,$

In addition,

(3) $p(t_2) = d_{q_2} S_{t_2 t_1}(q_2, q_1)$

(4) $p(t_1) = -d_{q_1} S_{t_2 t_1}(q_2, q_1),$

(5) $S_{t_2, t_1}(q_2, q_1) = S_{t_2 - t_1}(q_2, q_1)$

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Proof: (3) Assume $N=1$, i.e. config. space is $\mathbb{R}$

$$\frac{\partial S}{\partial q_2} = \int_{t_1}^{t_2} \left(\frac{\partial \dot{\gamma}}{\partial q_2}\frac{\partial \mathcal{L}}{\partial \xi}(\dot{\gamma}, \gamma) + \frac{\partial \gamma}{\partial q_2}\frac{\partial \mathcal{L}}{\partial q}\right)dt$$

$$= \int_{t_1}^{t_2} \left(-\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \xi}(\dot{\gamma}, \gamma) + \frac{\partial \mathcal{L}}{\partial q}(\dot{\gamma}, \gamma)\right)\frac{\partial \gamma}{\partial q_2}\,dt$$

$$+ \frac{\partial \gamma}{\partial q_2}\frac{\partial \mathcal{L}}{\partial \xi}(\dot{\gamma}, \gamma)\Big|_{t_1}^{t_2},$$

The first term vanishes because we $\{\gamma(t)\}$, by assumption, is a solution to the E.L. equations.

$\gamma(t_2) = q_2$, $\gamma(t_1) = q_1$, and $\frac{\partial \mathcal{L}}{\partial \xi}(\dot{\gamma}(t), \gamma(t)) = p(t)$

$\frac{\partial \gamma(t_2)}{\partial q_2} = 1$, $\frac{\partial \gamma(t_1)}{\partial q_2} = 0$ and $\Rightarrow \frac{\partial S}{\partial q_2} = p_2$

(4) similar to (3)

(1) $$\frac{\partial S}{\partial t_2} = \mathcal{L}(\dot\gamma(t_2), \gamma(t_2)) + \int_{t_1}^{t_2} \left(\frac{\partial \dot\gamma}{\partial t_2} \frac{\partial \mathcal{L}}{\partial \xi}(\dot\gamma,\gamma) + \frac{\partial \gamma}{\partial t_2} \frac{\partial \mathcal{L}}{\partial q}(\dot\gamma,\gamma)\right) dt =$$

$$= \mathcal{L}(\dot\gamma(t_2), \gamma(t_2)) + \int_{t_1}^{t_2} \left(-\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \xi}(\dot\gamma,\gamma) + \frac{\partial \mathcal{L}}{\partial q}(\dot\gamma,\gamma)\right) dt$$

$$+ \frac{\partial \gamma(t)}{\partial t_2} \frac{\partial \mathcal{L}}{\partial \xi}(\dot\gamma(t),\gamma(t)) \Big|_{t_1}^{t_2} = \mathcal{L}(\dot\gamma(t_2),\gamma(t_2)) +$$

$$+ \frac{\partial \gamma(t)}{\partial t_2}\Big|_{t=t_2} p(t_2) - \frac{\partial \gamma(t)}{\partial t_2}\Big|_{t=t_1} p(t_1),$$

$$\gamma(t_2) = q_2 \Rightarrow \frac{d}{dt_2}(\gamma(t_2)) = 0 \Rightarrow$$

$$\Rightarrow \dot\gamma(t_2) + \frac{\partial \gamma(t)}{\partial t_2}\Big|_{t=t_2} = 0, \text{ similarly } \frac{\partial \gamma(t)}{\partial t_2}\Big|_{t=t_1} = 0$$

Taking into account $p(t_2) = \frac{\partial \mathcal{L}}{\partial \xi}(\dot\gamma(t_2), \gamma(t_2))$ we obtain:

$$\frac{\partial S}{\partial t_2} = \mathcal{L}(\dot\gamma(t_2),\gamma(t_2)) - \dot\gamma(t_2)\, p(t_2) =$$

$$= -\mathcal{H}(p(t_2), \gamma(t_2)) = -\mathcal{H}\left(\frac{\partial S}{\partial q_2}, q_2\right)$$

(2) similar to (1)

(5) $$\frac{\partial S}{\partial t_1} + \frac{\partial S}{\partial t_2} = \mathcal{H}(p_1, q_1) - \mathcal{H}(p_2, q_2),$$

But $\mathcal{H}(p(t), q(t)) = \text{const}$ along any flow line of the Ham. vector field generated by H $\Rightarrow \frac{\partial S}{\partial t_1} + \frac{\partial S}{\partial t_2} = 0$

$\Rightarrow S_{t_2, t_1}$ depends only on $t_2 - t_1$

<u>Thm</u>. Let $\gamma_c(t)$ be solutions of E.L. equations with $\gamma_c(t_1) = q_1$, $\gamma_c(t_2) = q_2$. Assume there are finitely many of them. Then as $h \to 0$ the kernel of the propagator has the asymptotical expansion

$$U_t(q_2, q_1) \simeq \sum_{\gamma_c} (2\pi i h)^{-\frac{n}{2}} \exp\left(\frac{i}{h} S^{(c)}_t(q_2,q_1) + \frac{i\pi\mu(\gamma_c)}{4}\right) \left|\det\left(\frac{\partial^2 S^{(c)}_t(q_2,q_1)}{\partial q_2^i \partial q_1^j}\right)\right|^{\frac{1}{2}} \cdot$$

$$\cdot \left(1 + \sum_{n \geq 1} h^n U_c^{(n)}(q_2, q_1)\right),$$

Feynman integral in quantum mechanics

$$\mathcal{U}^{(F)}_t(q_1, q_2) = \int_{\substack{\gamma(t) = q_2 \\ \gamma(0) = q_1}} e^{\frac{i}{h} S[\gamma]} \mathcal{D}\gamma$$

Let us justify this proposal comparing $h \to 0$ asymptotical expansion of both expressions

$\mathcal{U}_t(q_1, q_2)$ we already know

$\mathcal{U}^{(F)}_t(q_1, q_2)$ compute formally

Asymptotical expansions of oscillatory integrals.

$$I_\hbar = \int_{\mathbb{R}^N} e^{i\frac{f(x)}{\hbar}} dx$$

Diverges absolutely, but may converge conditionally

Ex. $\displaystyle\int_{\mathbb{R}} e^{\frac{i}{2}x^2} dx = \lim_{t,t'\to\infty} \int_{-t'}^{t} e^{\frac{i}{2}x^2} dx$

Lemma 1

$$\int_{\mathbb{R}^N} e^{\frac{i}{2}(x,Bx)} d^N x = (2\pi)^{\frac{N}{2}} \frac{e^{\frac{i\pi}{4}\operatorname{sign}(B)}}{\sqrt{|\det(B)|}},$$

Proof. (h/w) Hint: $B^t = B$, use coordinates in which B is diagonal.

Lemma 2

$$\int'_{\mathbb{R}^N} e^{\frac{i}{2}(x,Bx)} x_{i_1}\cdots x_{i_n}\, d^N x =$$
$$= (2\pi)^{\frac{N}{2}}\, i^n \frac{e^{\frac{i\pi}{4}\operatorname{sign}(B)}}{\sqrt{|\det(B)|}} \sum_m (B^{-1})_{i_{m_1} i_{m_2}} (B^{-1})_{i_{m_3} i_{m_4}} \cdots (B^{-1})_{i_{m_{n-1}} i_{m_n}}.$$

Here $\displaystyle\int'_{\mathbb{R}^N} f(x)\, d^N x = \lim_{\varepsilon\to+0} \int_{\mathbb{R}^N} f(x) e^{-\varepsilon|x|^2} d^N x$,

Proof. $$\int'_{\mathbb{R}^N} \cdots = (-i)^n \frac{\partial}{\partial y_{i_1}} \cdots \frac{\partial}{\partial y_{i_n}} \int_{\mathbb{R}^N} e^{\frac{i}{2}(x,Bx)+iyx} d^N x$$
$$= (-i) \frac{\partial}{\partial y_{i_1}} \cdots \frac{\partial}{\partial y_{i_n}} \frac{e^{i\frac{\pi}{4}\operatorname{sign}(B)}}{\sqrt{|\det(B)|}} e^{-\frac{i}{2}(y,B^{-1}y)}$$
$$= \dots$$

Conjecture: approximate the path integral by finite dimensional integrals, then take the limit, the limit exists and is equal to $U_t(q_1, q_2)$.

Thm. This is true for the heat equation. (Wiener integral).

Not known in quantum mech. (no statements that this is not true).