AQT; Sheet 6; Marc Hauer, Angelo Bradei   12.11.2023

Quickies:

Q1: $\psi(x,t) = \int dx' U(x,x',t,t_0)\psi(x',t_0)$ ✓

Q2: $U(x_N,x_0,t_N,t_0) = A\int \mathcal{D}x(t)\, e^{\frac{i}{\hbar}S(x(t))}$ ✓

Q3: i) $\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')dt'}$ is unitary.

ii) $U(x_N,x_0,t_N,t_0)$ is the time evolution operator for any path from x_0 to x_N. In the Schrödinger picture we do not look at multiple paths, thus the propagator (in S.P.: time evolution operator) is only time dependent: $\hat{U}(t,t_0)$. ✓

Exercise 1:

1.: $e^{\hat{A}}\cdot e^{-\hat{A}} = \left(\sum_{n=0}\frac{\hat{A}^n}{n!}\right)\cdot\left(\sum_{n=0}\frac{(-\hat{A})^n}{n!}\right) \Bigg| \left(\sum_{i=0} a_i\right)\cdot\left(\sum_{j=0} b_j\right) = \sum_{k=0}^{\infty}\sum_{l=0}^{k} a_l b_{k-l}$

$= \sum_{k=0}^{\infty}\sum_{l=0}^{k}\frac{\hat{A}^l}{l!}\frac{(-\hat{A})^{k-l}}{(k-l)!}$

$= \quad (-1)^{k-l}\cdot\hat{A}^k$

$e^{\hat{A}}\cdot e^{-\hat{A}} = \left(\sum_{n=0}\frac{\hat{A}^n}{n!}\right)\left(\sum_{n=0}\frac{(-\hat{A})^n}{n!}\right)$

$= \left(1+\sum_{n=1}\frac{\hat{A}^n}{n!}\right)\cdot\left(1+\sum_{n=1}\frac{(-\hat{A})^n}{n!}\right)$

$= 1+\sum_{n=1}\frac{(-\hat{A})^n}{n!}+\sum_{n=1}\frac{\hat{A}^n}{n!}+\left(\sum_{n=1}\frac{\hat{A}^n}{n!}\right)\left(\sum_{n=1}\frac{(-\hat{A})^n}{n!}\right)$

$= 1+\sum_{n=1}\frac{1}{n!}\left[(-\hat{A})^n+\hat{A}^n\right]+\sum_{n=0}^{\infty}\sum_{l=0}^{n+1}\frac{\hat{A}^{l+1}}{(l+1)!}\frac{(-\hat{A})^{n-l}}{(n-l)!}$

$= 1+\sum_{n=1}\frac{\hat{A}^n}{n!}\left[1+(-1)^n\right]+\sum_{n=0}^{\infty}\sum_{l=0}^{n+1}\hat{A}^{n+1}\frac{(-1)^{n-l}}{(l+1)!(n-l)!}$

$= 1+\sum_{n=0}\frac{\hat{A}^{n+1}}{(n+1)!}\left[1+(-1)^{n+1}\right]+\sum_{n=0}^{\infty}\hat{A}^{n+1}\sum_{l=0}^{n+1}\frac{(-1)^{n-l}}{(l+1)!(n-l)!}$

$\overset{!}{=} 1$

$\Rightarrow \sum_{n=0}^{\infty}\frac{\hat{A}^{n+1}}{(n+1)!}\left[1+(-1)^{n+1}\right]+\sum_{n=0}^{\infty}\hat{A}^{n+1}\sum_{l=0}^{n+1}\frac{(-1)^{n-l}}{(l+1)!(n-l)!} = 0$

$\Rightarrow \frac{1+(-1)^{n+1}}{(n+1)!}+\sum_{l=0}^{n+1}\frac{(-1)^{n-l}}{(l+1)!(n-l)!} = 0$

1) Exponentiating Operators

$$e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{1}{n!} \hat{A}^n$$

1) Show: $e^{\hat{A}} e^{-\hat{A}} = 1$

- $$e^{\hat{A}} \cdot e^{-\hat{A}} = \left(\sum_{n=0}^{\infty} \frac{1}{n!} \hat{A}^n \right) \left(\sum_{m=0}^{\infty} \frac{1}{m!} (-\hat{A})^m \right)$$
$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{n! m!} \hat{A}^n (-\hat{A})^m$$
$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^m}{n! m!} \hat{A}^{(n+m)} \qquad \Big| \; p = n+m$$
$$= \sum_{p=0}^{\infty} \sum_{n=0}^{p} \frac{(-1)^{p-n}}{n!(p-n)!} \hat{A}^p$$
$$= 1 + \sum_{p=1}^{\infty} \frac{(-\hat{A})^p}{p!} \sum_{n=0}^{p} (-1)^n \binom{p}{n} \quad \text{with} \quad \binom{p}{n} = \frac{p!}{n!(p-n)!} \qquad \Big| \; 0 = (1-1)^p = \sum_{n=0}^{p} \binom{p}{n} 1^{p-n} (-1)^n = \sum_{n=0}^{p} \binom{p}{n} (-1)^n$$

$$\Rightarrow e^{\hat{A}} \cdot e^{-\hat{A}} = 1 + 0 = 1 \qquad \square$$

✓

#2 ?

3) Show: $e^{\hat{A}} \hat{B} e^{-\hat{A}} = \sum_{n=0}^{\infty} \frac{1}{n!} [\hat{A}, \hat{B}]_n$

- $$e^{\hat{A}} \hat{B} e^{-\hat{A}} = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{1}{i! j!} \hat{A}^j \hat{B} (-\hat{A})^i \qquad \Big| \; n = i+j$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\sum_{i=0}^{n} \frac{n!}{i!(n-i)!} \hat{A}^{(n-i)} \hat{B} (-\hat{A})^i \right)$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} [\hat{A}, \hat{B}]_n \qquad \square$$

Show: $[\hat{A}, \hat{B}]_n = \sum_{i=0}^{n} \frac{n!}{i!(n-i)!} \hat{A}^{n-i} \hat{B} (-\hat{A})^i$

- $\boxed{n=0}$: $[\hat{A}, \hat{B}]_0 = \hat{A}^0 \hat{B} (-\hat{A})^0 = \hat{B}$
- $\boxed{n+1}$: $$[\hat{A}, \hat{B}]_{n+1} = [\hat{A}, [\hat{A}, \hat{B}]_n]$$
$$= \left[\hat{A}, \sum_{i=0}^{n} \frac{n!}{i!(n-i)!} \hat{A}^{n-i} \hat{B} (-\hat{A})^i \right]$$
$$= \sum_{i=0}^{n} \frac{n!}{i!(n-i)!} [\hat{A}, \hat{A}^{n-i} \hat{B} (-\hat{A})^i]$$
$$= \sum_{i=0}^{n} \frac{n!}{i!(n-i)!} \left(\hat{A}^{n+1-i} \hat{B} (-\hat{A})^i + \hat{A}^{n-i} \hat{B} (-\hat{A})^{i+1} \right)$$
$$= (\ldots)$$

3) Perturbed Harmonic Oscillator

2) $$|A_{fi}^{(1)}|^2 = \delta_{fi} - \frac{i}{\hbar} \int_{t_0}^{t} dt' \exp[i\omega_{fi}(t'-t_0)] \langle f^{(0)} | \hat{H}_{1,s} | i^{(0)} \rangle$$

- $$\langle f^0 | \hat{H}_{1,s} | i^{(0)} \rangle = \langle f^0 | a \hat{x}^p e^{-t^2/\tau^2} | i^{(0)} \rangle$$
$$= a e^{-\frac{t^2}{\tau^2}} \int_{\mathbb{R}} dx \; x^p \; \psi_f(x) \psi_i(x)$$
$$= \frac{ab}{\sqrt{\pi}} \frac{e^{-\frac{t^2}{\tau^2}}}{\sqrt{2^f f!}} \int_{\mathbb{R}} dx \; \underbrace{x^p}_{f(x)} \underbrace{e^{-b^2 x^2}}_{g(x)} \underbrace{H_f(bx)}_{h(x)}$$

$$\Big| \; \psi_n(x) = \left(\frac{b^2}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{1}{2^n n!}} H_n(bx) e^{-\frac{1}{2} b^2 x^2} \quad \text{where} \quad b = \sqrt{\frac{m\omega}{\hbar}}$$

- Assume: $|i\rangle = |n=0\rangle \Rightarrow \psi_i = \left(\frac{b^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2} b^2 x^2}$

- $f(-x) = (-1)^p f(x)$
- $g(-x) = g(x)$
- $h(-x) = H_f(-x) = (-1)^f H(x) = (-1)^f h(x)$

$$\begin{cases} \text{for even } p: & P_{if} \sim \int dx \, f(x) g(x) h(x) = 0 \text{ for even } f \;\rightarrow \text{accessible for odd } f \\ \text{for odd } p: & P_{if} \sim \int dx \, f(x) g(x) h(x) = 0 \text{ for odd } f \;\rightarrow \text{accessible for even } f \end{cases}$$

✓

3) $$P_{1,0} = |A_{10}|^2 = \left| -\frac{i}{\hbar} \int_{t_0}^{t} dt' \exp[i\omega_{fi}(t'-t_0)] \langle 1 | \hat{H}_1 | 0 \rangle \right|^2$$
$$= \left| -\frac{i}{\hbar} \int_{t_0}^{t} dt' \exp[i\omega_{fi}(t'-t_0)] \int_{\mathbb{R}} dx \; a \exp\left[-\frac{t'^2}{\tau^2}\right] x^p \psi_0(x) \psi_1(x) \right|^2 \quad \Big| \; \psi_0(x) = \left(\frac{b^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2} b^2 x^2} \wedge \psi_1(x) = \left(\frac{b^2}{\pi}\right)^{\frac{1}{4}} bx e^{-\frac{1}{2} b^2 x^2} \quad (p=1)$$
$$= \left| -\frac{i}{\hbar} \frac{ab}{\sqrt{\pi}} \int_{t_0}^{t} dt' \exp\left[i\omega_{fi}(t'-t_0) - \frac{t'^2}{\tau^2}\right] \int_{\mathbb{R}} dx \; x^2 \exp[-b^2 x^2] \right|^2 \quad \Big| \; \int_{\mathbb{R}} dx \, x^2 \exp(-b^2 x^2) = -\frac{\partial}{\partial b} \int_{\mathbb{R}} dx \exp(-b^2 x^2) = -\frac{\partial}{\partial b} \sqrt{\frac{\pi}{b^2}} = \frac{\sqrt{\pi}}{b^2}$$
$$= \left| -\frac{i}{\hbar} \frac{a}{b} \exp(-ut_0) \int_{t_0}^{t} dt' \exp(ut' - vt'^2) \right|^2 \quad \text{where} \quad u = i\omega \wedge v = \tau^{-2} \quad \Big| \; t_0 \to -\infty \wedge t \to \infty$$
$$= \left| -\frac{i}{\hbar} \frac{a}{b} \exp(-ut_0) \exp\left(\frac{u^2}{4v}\right) \sqrt{\frac{\pi}{v}} \right|^2$$
$$= \left| -ia\tau \sqrt{\frac{\pi}{\hbar m \omega}} \exp(-i\omega t_0) \exp\left(-\frac{1}{4}\omega^2 \tau^2\right) \right|^2$$
$$= \frac{a^2 \pi \tau^2}{\hbar m \omega} \exp\left(-\frac{1}{2}\omega^2 \tau^2\right)$$

✓

$\hookrightarrow$ for $\tau \to 0$:

i) $a = \text{const.} \Rightarrow P_{1,0} \to 0$

ii) $a \sim \frac{1}{\sqrt{\tau}} \Rightarrow P_{1,0} \to 0$

✓

Exercise 2:

1.: $c_f(t)$ is the coefficient, that „says" how much of $|f\rangle$, $|\psi(t)\rangle$ has:

I: $|\psi(t)\rangle = \sum_n c_n(t)|n\rangle = \sum_{n\neq f} c_n(t)|n\rangle + c_f(t)|f^{(0)}\rangle$

Starting from $|i^{(0)}\rangle = \sum_n c_n(t)|n^{(0)}\rangle = \sum_n \delta_{in}|n^{(0)}\rangle$

$|\psi(t_0)\rangle = |i^{(0)}\rangle \rightsquigarrow |\psi(t)\rangle = |f^{(0)}\rangle$

$\Rightarrow P_{fi}(t) = |\underline{\langle f^{(0)}|i^{(0)}\rangle}|^2$ | (I)

$= |c_f(t)|^2$

2.:

$$|\psi(t)\rangle = \sum_n d_n(t)\,|\psi_n^{(0)}(t)\rangle$$
$$= \sum_n d_n(t)\,\hat{U}(t,t_0)|\psi_n^{(0)}(t_0)\rangle$$
$$= \sum_n d_n(t)\,\hat{U}(t,t_0)|n^{(0)}\rangle$$

$|\psi(t)\rangle = \sum_n c_n(t)|n^{(0)}\rangle$, thus:

$$c_n(t) = d_n(t)\,\hat{U}(t,t_0)$$
$$= d_n(t)\,e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}$$

3.: $E_k^{(0)}|k\rangle = \hat{H}_0|k\rangle$

What is $\dot{d}_f$? $= \frac{d(d_f(t))}{dt}$? yes

$$\langle f^{(0)}|\hat{H}_1(t)|\psi(t)\rangle = \sum_n \langle f^{(0)}|\hat{H}_1(t)\cdot d_n(t)\,e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}|n^{(0)}\rangle$$

$$\hat{H}(t)|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

$$\Rightarrow \hat{H}(t)\,d_n(t)\,e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}|n^{(0)}\rangle = i\hbar\frac{\partial}{\partial t}\left(d_n(t)\,e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}|n^{(0)}\rangle\right)$$ why?

$$\Rightarrow (\hat{H}_1(t)+\cancel{\hat{H}_0})\,d_n(t)\,e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}|n^{(0)}\rangle = i\hbar\, e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}\left(\dot{d}_n(t)|f^{(0)}\rangle + \frac{1}{i\hbar}\hat{H}_0\,d_n(t)\,|n^{(0)}\rangle\right)$$
$$= e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}\left(i\hbar\,\dot{d}_n(t)|f^{(0)}\rangle + \hat{H}_0\,d_n(t)\right)|n^{(0)}\rangle)$$

$$\Rightarrow \hat{H}_1(t)\,d_n(t)\,e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}|n^{(0)}\rangle = i\hbar\,\dot{d}_n(t)\,e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}|f^{(0)}\rangle$$
$$\Rightarrow \hat{H}_1(t)\,d_n(t)\,e^{-\frac{i}{\hbar}E_n^{(0)}(t-t_0)}|n^{(0)}\rangle = i\hbar\,\dot{d}_n(t)\,e^{-\frac{i}{\hbar}E_f^{(0)}(t-t_0)}|f^{(0)}\rangle$$
$$\Rightarrow i\hbar\,\dot{d}_n = \sum_n \langle f^{(0)}|\hat{H}_1(t)|n^{(0)}\rangle\,d_n(t)\,e^{-i\omega_f(t-t_0)} \quad \text{with } \omega_f = \frac{E_f^{(0)}-E_n^{(0)}}{\hbar}$$ $\square$

4.: