Assignment 5

OPTI 570 Quantum Mechanics

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Problem I

Part 1.

We define the effective state in the second frame $|\psi_E(t)\rangle = \mathbb{F}(t)|\psi(t)\rangle$, where $\mathbb{F}(t)$ is some unitary time-dependend operator. Substituting $|\psi(t)\rangle = \mathbb{F}^\dagger(t)|\psi_E(t)\rangle$ into the Schrodinger equation yields:

$$
\begin{aligned}
i\hbar\partial_t \left[\mathbb{F}^\dagger(t)|\psi_E(t)\rangle\right] &= H(t)\left[\mathbb{F}^\dagger(t)|\psi_E(t)\rangle\right] \\
i\hbar\left[\partial_t\mathbb{F}^\dagger(t)|\psi_E(t)\rangle + \mathbb{F}^\dagger(t)\partial_t|\psi_E(t)\rangle\right] &= H(t)\mathbb{F}^\dagger(t)|\psi_E(t)\rangle \\
i\hbar\mathbb{F}^\dagger(t)\partial_t|\psi_E(t)\rangle &= \left[H(t)\mathbb{F}^\dagger(t) - i\hbar\partial_t\mathbb{F}^\dagger(t)\right]|\psi_E(t)\rangle \Big/ \mathbb{F}(t) \\
i\hbar\partial_t|\psi_E(t)\rangle &= \left[\mathbb{F}(t)H(t)\mathbb{F}^\dagger(t) - i\hbar\mathbb{F}(t)\partial_t\mathbb{F}^\dagger(t)\right]|\psi_E(t)\rangle \\
i\hbar\partial_t|\psi_E(t)\rangle &= H_E(t)|\psi_E(t)\rangle,
\end{aligned}
$$

where $H_E(t)$ is the effective Hamiltonian:

$$
H_E(t) = \mathbb{F}(t)H(t)\mathbb{F}^\dagger(t) - i\hbar\mathbb{F}(t)\partial_t\mathbb{F}^\dagger(t).
$$

Part 2.

We know that

$$
|\psi_I(t)\rangle = \mathbb{U}_0^\dagger(t,t_0)|\psi_S(t)\rangle, \quad \text{with} \quad \mathbb{U}_0(t,t_0) = e^{-i(t-t_0)H_0/\hbar}.
$$

Then,

$$
\begin{aligned}
i\hbar\partial_t\left[\mathbb{U}_0^\dagger|\psi_S(t)\rangle\right] &= i\hbar\partial_t\mathbb{U}^\dagger|\psi_S(t)\rangle + i\hbar\mathbb{U}_0^\dagger\partial_t|\psi_S(t)\rangle \\
&= i\hbar\partial_t\mathbb{U}_0^\dagger|\psi_S(t)\rangle + \mathbb{U}_0^\dagger H_S(t)|\psi_S\rangle \\
&= \left[i\hbar(\partial_t\mathbb{U}_0^\dagger)\mathbb{U}_0 + \mathbb{U}_0^\dagger H_S(t)\mathbb{U}_0\right]|\psi_I(t)\rangle \\
&= \left[-\mathbb{U}_0^\dagger H_0\mathbb{U}_0 + \mathbb{U}_0^\dagger(H_0 + W(t))\mathbb{U}_0\right]|\psi_I(t)\rangle \quad (i\hbar\partial_t\mathbb{U}_0^\dagger = -\mathbb{U}_0^\dagger H_0) \\
i\hbar\partial_t|\psi_I(t)\rangle &= \left[\mathbb{U}_0(t,t_0)^\dagger W(t)\mathbb{U}_0(t,t_0)\right]|\psi_I(t)\rangle \\
i\hbar\partial_t|\psi_I(t)\rangle &= H_E(t)|\psi_I(t)\rangle,
\end{aligned}
$$

where $H_E(t)$ is the effective Hamiltonian:

$$H_E(t) = \mathbb{U}_0(t,t_0)^\dagger W(t)\mathbb{U}_0(t,t_0).$$

Problem II

1. The probability for energies greater than $2\hbar\omega$ is then

$$P(E > 2\hbar\omega) = \sum_{n\geq 2} |c_n|^2, \quad c_n = \langle n|\psi(t)\rangle.$$

If $P = 0$, then all $c_n = 0,\ n \geq 2$. Only c_0 and c_1 may be non-zero.

2. The normalization condition means that

$$\sum_{n<2} |c_n|^2 = 1 \Longrightarrow |c_0|^2 + |c_1|^2 = 1.$$

The mean value of the energy is

$$\langle H\rangle = \langle\psi|H|\psi\rangle = |c_0|^2 E_0 + |c_1|^2 E_1 = \frac{1}{2}\hbar\omega|c_0|^2 + \frac{3}{2}\hbar\omega|c_1|^2.$$

If $\langle H\rangle = \hbar\omega$, we have a system of equation composed of the normalization and mean value expression:

$$\left.\begin{array}{l}\frac{1}{2}\hbar\omega|c_0|^2 + \frac{3}{2}\hbar\omega|c_1|^2 = \hbar\omega \\ |c_0|^2 + |c_1|^2 = 1\end{array}\right] \longrightarrow |c_0|^2 = |c_1|^2 = \frac{1}{2}.$$

3. First, we develop the mean value of X:

$$\langle X\rangle = \langle\psi|X|\psi\rangle = \frac{1}{2}(\langle 0| + e^{-i\theta_1}\langle 1|)X(|0\rangle + e^{i\theta_1}|1\rangle) = \frac{1}{2}\left[\langle 0|X|0\rangle + e^{i\theta_1}\langle 0|X|1\rangle + e^{-i\theta_1}\langle 1|X|0\rangle + \langle 1|X|1\rangle\right].$$

The last result is due to the result we have obtained in the previous incise. Now, we use the matrix element of X of the harmonic oscillator:

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \quad \text{where} \quad a|n\rangle = \sqrt{n}|n-1\rangle,\ \ a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

We compute the terms separately,

$$\begin{aligned}
\langle 0|X|0\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle 0|(a + a^\dagger)|0\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\langle 0|a|0\rangle + \langle 0|a^\dagger|0\rangle\right] = \sqrt{\frac{\hbar}{2m\omega}}\left[\langle 0|0\rangle + \langle 0|1\rangle\right] = 0,\\
\langle 1|X|1\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left[\langle 1|a|1\rangle + \langle 1|a^\dagger|1\rangle\right] = \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{1}\langle 1|0\rangle + \sqrt{2}\langle 1|2\rangle\right] = 0,\\
\langle 0|X|1\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left[\langle 0|a|1\rangle + \langle 0|a^\dagger|1\rangle\right] = \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{1}\langle 0|0\rangle + \sqrt{2}\langle 0|2\rangle\right] = \sqrt{\frac{\hbar}{2m\omega}},\\
\langle 1|X|0\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left[\langle 1|a|0\rangle + \langle 1|a^\dagger|0\rangle\right] = \sqrt{\frac{\hbar}{2m\omega}}\left[\langle 1|0\rangle + \sqrt{1}\langle 1|1\rangle\right] = \sqrt{\frac{\hbar}{2m\omega}}.
\end{aligned}$$

We put these results in $\langle X\rangle$:

$$\langle X\rangle = \sqrt{\frac{\hbar}{2m\omega}}\frac{e^{i\theta_1} + e^{i\theta_1}}{2} = \sqrt{\frac{\hbar}{2m\omega}}\cos\theta_1 = \frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}.$$

The last relation means that

$$\cos\theta_1 = \frac{\sqrt{2}}{2} \longrightarrow \theta_1 = \pm\frac{\pi}{4} \quad \text{(inside one period)}.$$

4. The time evolution is:

$$|\psi(t)\rangle = \sum_{n=0}^{1} c_n e^{-iE_n t/\hbar}|n\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\omega t/2}|0\rangle + e^{i\theta_1}e^{-i3\omega t/2}|1\rangle\right)$$

We can factor out the common phase that translates to global phase factor so that we have

$$|\psi(t)\rangle \propto \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i(\theta_1-\omega t)|1\rangle}\right) \longrightarrow \theta_1(t) = \theta_1 - \omega t.$$

We use our previous result of $\langle X\rangle$ and replace θ_1 by $\theta_1(t)$:

$$\langle X\rangle(t) = \sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t - \theta_1).$$

The argument of the cosine is reversed as the one in part c) due to the restriction of $\cos\theta_1 = 1/\sqrt{2}$.

Problem III

We know that we can express the density operator in an orthogonal basis

$$\rho = \sum_i \pi_i|\chi_i\rangle\langle\chi_i|, \quad \pi_i \geq 0,\ \sum_i \pi_i = 1.$$

Then squaring ρ affect only to the π_i elements:

$$\rho^2 = \sum_i \pi_i^2|\chi_i\rangle\langle\chi_i|.$$

In a pure state, $\rho = |\psi(t)\rangle\langle\psi(t)|$ behaves as a projector, and its eigenvalues are therefore $\{1, 0, 0, \cdots\}$. Thus, in the $\{|\chi_i\rangle\}$ basis,

$$[\rho]_\chi = \mathrm{diag}(1, 0, 0, \cdots), \quad [\rho^2]_\chi = [\rho]_\chi.$$

However, in the statistical mixture, more than one eigenvalue is non-zero, with $0 < \pi_i < 1$ for at least two indices. Then $[\rho]_\chi$ has several diagonal elements between 0 and 1, and $[\rho^2]_\chi$ has those entries squared.

Since we initially had $\sum_i \pi_i = 1,\ \pi_i \geq 0$, we have that $\sum_i \pi_i \leq 1$ with the equality if one $\pi_i = 1$ and all others are 0. So, the trace will indicate when we are in a pure state or a statistical mixture:

$$\rho \text{ is pure} \iff \mathrm{Tr}[\rho^2] = 1.$$

The inequality between statistical mixture and pure state is that in the latter we can interpret the density operator as a projector whereas in the first case not. This is expressed with the inequality of the idempotency property of any projector:

$$\rho^2 \neq \rho.$$

which translates to a trace les or equal than unity:

$$\mathrm{Tr}[\rho^2] \leq 1.$$

Problem IV

a) We use the definition of the trace

$$\mathrm{Tr}[P_{\psi(t)}] = \sum_j \langle\phi_j|P_{\psi(t)}|\phi_j\rangle = \sum_j \langle\phi_j|\psi(t)\rangle\langle\psi(t)|\phi_j\rangle = \sum_j \langle\psi(t)|\phi_j\rangle\langle\phi_j|\psi(t)\rangle = \langle\psi(t)|\psi(t)\rangle.$$

We now replace the relation with the time-evolution operator, which preserves the norm,

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|U^\dagger(t,0)U(t,0)|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle = 1.$$

Then,

$$\mathrm{Tr}[P_{\psi(t)}] = 1, \quad \forall t.$$

b) We use the expansion of $|\psi(t)\rangle$ to show that the projector at $t = 0$ is

$$[P_{\psi(0)}]_{mn} = \langle u_m|P_{\psi(0)}|u_n\rangle = \langle u_m|\psi(0)\rangle\langle\psi(0)|u_n\rangle = c_m c_n^*.$$

So, iterating over m, n we construct the matrix:

$$P_{\psi(0)} = \begin{bmatrix} |c_1|^2 & c_1 c_2^* & c_1 c_3^* \\ c_2 c_1^* & |c_2|^2 & c_2 c_3^* \\ c_3 c_1^* & c_3 c_2^* & |c_3|^2 \end{bmatrix}$$

We can see directly that the trace (sum of diagonal element) is unitary:

$$\mathrm{Tr}[P_{\psi(0)}] = |c_1|^2 + |c_2|^2 + |c_3|^2 = 1.$$

c) if the first element if $|u_1\rangle = |\psi(0)\rangle$, then the projector will only consider this element

$$P_{\psi(0)} = |\psi(0)\rangle\langle\psi(0)| = \begin{bmatrix} 1 & 0 & \cdots \\ 0 & 0 & \\ \vdots & & \ddots \end{bmatrix}.$$

We can see that the trace is 1 sa is the only element in the diagonal.

d) Let define another projector $P_m = |w_m\rangle\langle w_m|$. The probability of obtaining λ_m is

$$p_m(t) = \langle\psi(t)|P_m|\psi(t)\rangle = \sum_j \langle\psi(t)|u_j\rangle\langle u_j|P_m|\psi(t)\rangle = \sum_j \langle u_j|P_m|\psi(t)\rangle\langle\psi(t)|u_j\rangle$$

$$p_m(t) = \mathrm{Tr}[P_m|\psi\rangle\langle\psi|] = \mathrm{Tr}[P_m P_{\psi(t)}].$$

We use cyclic property of the trace to interchange the order of the argument and finally obtain

$$p_m(t) = \mathrm{Tr}[P_m P_{\psi(t)}] = \mathrm{Tr}[P_{\psi(t)} P_m].$$

e) The derivative ot $P_{\psi(t)}$ is

$$\begin{aligned} \frac{d}{dt}P_{\psi(t)} &= \frac{d}{dt}|\psi\rangle\langle\psi| \\ &= \frac{d}{dt}|\psi\rangle\langle\psi| + |\psi\rangle\frac{d}{dt}\langle\psi| \\ &= \frac{1}{i\hbar}H|\psi\rangle\langle\psi| - \frac{1}{i\hbar}|\psi\rangle\langle\psi|H \qquad \left(i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle\right) \\ &= \frac{1}{i\hbar}(HP_{\psi(t)} - P_{\psi(t)}H) \\ \frac{d}{dt}P_{\psi(t)} &= \frac{1}{i\hbar}[H, P_{\psi(t)}]. \end{aligned}$$