Part IB Physics A: Michaelmas 2021

Advanced QUANTUM PHYSICS Questions II

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1. If $\hat{U}(t, t_0)$ is the time shift operator of a quantum system having a time-independent Hamiltonian, verify the following:

1. Identity: $\hat{U}(t, t) = \hat{I}$.
2. Composition: $\hat{U}(t_2, t_1)\hat{U}(t_1, t_0) = \hat{U}(t_2, t_0)$.
3. Time reversal: $\hat{U}^\dagger(t_2, t_1) = \hat{U}^{-1}(t_2, t_1) = \hat{U}(t_1, t_2)$.
4. Unitarity: $\hat{U}(t_2, t_1)\hat{U}^\dagger(t_2, t_1) = \hat{U}^\dagger(t_2, t_1)\hat{U}(t_2, t_1) = \hat{I}$.

What do each of these expressions mean physically?

Suppose, erroneously, that the time evolution operator is not unitary, such that $\hat{U}(t, t) \neq \hat{I}$; what happens in each case, and in particular what is the difference between $\hat{U}^\dagger(t_2, t_1)$ and $\hat{U}^{-1}(t_2, t_1)$?

Answer 1.

$$\begin{aligned}\hat{U}(t_2, t_1) &= \sum_n e^{-iE_n(t_2-t_1)/\hbar}|\phi_n\rangle\langle\phi_n| \\ \hat{U}(t, t) &= \sum_n |\phi_n\rangle\langle\phi_n| = \hat{I}.\end{aligned} \tag{1}$$

The state does not change over over small periods of time, depending on the highest frequency present in the spectrum.

$$\begin{aligned}\hat{U}(t_2, t_1)\hat{U}(t_1, t_0) &= \sum_{mn} e^{-iE_m(t_2-t_1)/\hbar}e^{-iE_n(t_1-t_0)/\hbar}|\phi_m\rangle\langle\phi_m|\phi_n\rangle\langle\phi_n| \\ &= \sum_n e^{-iE_n(t_2-t_1)/\hbar}e^{-iE_n(t_1-t_0)/\hbar}|\phi_n\rangle\langle\phi_n| \\ &= \sum_n e^{-iE_n(t_2-t_0)/\hbar}|\phi_n\rangle\langle\phi_n| \\ &= \hat{U}(t_2, t_0).\end{aligned} \tag{2}$$

Two time shifts are equivalent to a single time shift.

$$\begin{aligned}\hat{U}^\dagger(t_2,t_1) &= \sum_n e^{+iE_n(t_2-t_1)/\hbar}|\phi_n\rangle\langle\phi_n| \\ &= \hat{U}(t_1,t_2).\end{aligned} \tag{3}$$

$$\begin{aligned}\hat{U}^{-1}(t_2,t_1) &= \sum_n e^{+iE_n(t_2-t_1)/\hbar}|\phi_n\rangle\langle\phi_n| \\ &= \hat{U}(t_1,t_2).\end{aligned} \tag{4}$$

The adjoint time reverses a forward shift, and for a complete set of states the inverse and adjoint are the same.

$$\begin{aligned}\hat{U}(t_2,t_1)\hat{U}^\dagger(t_2,t_1) &= \sum_{mn} e^{-iE_m(t_2-t_1)/\hbar}e^{+iE_n(t_2-t_1)/\hbar}|\phi_m\rangle\langle\phi_m|\phi_n\rangle\langle\phi_n| \\ &= \sum_n e^{-iE_n(t_2-t_1)/\hbar}e^{+iE_n(t_2-t_1)/\hbar}|\phi_n\rangle\langle\phi_n| \\ &= \hat{I}.\end{aligned} \tag{5}$$

A forward and reverse shift leave the state unchanged.

If the system is not unitary, say $\hat{V}(t_2,t_1)$, and has state $|\phi_i\rangle$ missing,

$$\begin{aligned}\hat{V}(t_2,t_1) &= \sum_{n\neq i} e^{-iE_n(t_2-t_1)/\hbar}|\phi_n\rangle\langle\phi_n| \\ \hat{V}^\dagger(t_2,t_1) &= \sum_{n\neq i} e^{+iE_n(t_2-t_1)/\hbar}|\phi_n\rangle\langle\phi_n|\end{aligned} \tag{6}$$

$\hat{V}^{-1}(t_2,t_1)$ does not exist, however, because the inverse attempts to restore the information in the state that goes missing when $\hat{V}(t_2,t_1)$ is applied. The adjoint continues to ignore the state, but the inverse attempts to restore the state.

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2. Show that the time shift operator of a time-independent Hamiltonian preserves the following:

1. Inner products.
2. Normalisation.
3. The trace of an operator in the Heisenberg picture.

Likewise show that

$$\left[\hat{U},\hat{H}\right] = \hat{0}.$$

What does this say about the eigenstates of $\hat{H}$ and $\hat{U}$, and what is the physical interpretation.

Additionally, show that

$$\frac{\partial}{\partial t} e^{+i\hat{H}_0(t-t_0)/\hbar} = i\frac{1}{\hbar}\hat{H}_0 e^{+i\hat{H}_0(t-t_0)/\hbar} = i\frac{1}{\hbar} e^{+i\hat{H}_0(t-t_0)/\hbar}\hat{H}_0. \tag{7}$$

Answer 2.

$$\begin{aligned} \langle A(t_2)|B(t_2)\rangle &= \langle A(t_1)|\hat{U}^\dagger(t_2,t_1)\hat{U}(t_2,t_1)|B(t_1)\rangle \\ &= \langle A(t_1)|B(t_1)\rangle, \end{aligned} \tag{8}$$

and similarly

$$\begin{aligned} \langle A(t_2)|B(t_2)\rangle &= \langle A(t_1)|\hat{U}^\dagger(t_2,t_1)\hat{U}(t_2,t_1)|B(t_1)\rangle \\ &= \langle A(t_1)|A(t_1)\rangle. \end{aligned} \tag{9}$$

$$\begin{aligned} \mathrm{Tr}\left[\hat{A}^H(t)\right] &= \mathrm{Tr}\left[\hat{U}^\dagger(t,t_0)\hat{A}^S\hat{U}(t,t_0)\right] \\ &= \mathrm{Tr}\left[\sum_{mn} e^{+iE_m(t-t_0)/\hbar}e^{-iE_n(t-t_0)/\hbar}|\phi_m\rangle\langle\phi_m|\hat{A}^S|\phi_n\rangle\langle\phi_n|\right] \\ &= \sum_i \langle\phi_i|\left[\sum_{mn} e^{+iE_m(t-t_0)/\hbar}e^{-iE_n(t-t_0)/\hbar}|\phi_m\rangle\langle\phi_m|\hat{A}^S|\phi_n\rangle\langle\phi_n|\right]|\phi_i\rangle \\ &= \sum_i \left[\sum_{mn} e^{+iE_m(t-t_0)/\hbar}e^{-iE_n(t-t_0)/\hbar}\langle\phi_m|\hat{A}^S|\phi_n\rangle\delta_{in}\delta_{im}\right] \\ &= \sum_i \langle\phi_i|\hat{A}^S|\phi_i\rangle \\ &= \mathrm{Tr}\left[\hat{A}^S\right]. \end{aligned} \tag{10}$$

$$\begin{aligned} \hat{U}(t_2,t_1)\hat{H} &= \sum_n e^{-iE_n(t_2-t_1)/\hbar}|\phi_n\rangle\langle\phi_n|\sum_m E_m|\phi_m\rangle\langle\phi_m| \\ &= \sum_{mn} E_m e^{-iE_n(t_2-t_1)/\hbar}|\phi_m\rangle\langle\phi_m|\phi_n\rangle\langle\phi_n| \\ &= \hat{H}\hat{U}(t_2,t_1) \\ \left[\hat{U},\hat{H}\right] &= \hat{0}. \end{aligned} \tag{11}$$

$\hat{U}$ and $\hat{H}$ share the same eigenstates, and so each energy eigenstate is associated with a specific phase factor.

$$\begin{aligned}\frac{\partial}{\partial t}e^{+i\hat{H}_0(t-t_0)/\hbar} &= \frac{\partial}{\partial t}\sum_n e^{iE_n(t-t_0)/\hbar}|\phi_n\rangle\langle\phi_n| \\ &= i\frac{1}{\hbar}\sum_n E_n e^{iE_n(t-t_0)/\hbar}|\phi_n\rangle\langle\phi_n| \\ &= i\frac{1}{\hbar}\sum_{mn} E_m e^{iE_n(t-t_0)/\hbar}|\phi_m\rangle\langle\phi_m|\phi_n\rangle\langle\phi_n| \\ &= i\frac{1}{\hbar}\hat{H}_0 e^{+i\hat{H}_0(t-t_0)/\hbar} = i\frac{1}{\hbar}e^{+i\hat{H}_0(t-t_0)/\hbar}\hat{H}_0.\end{aligned} \tag{12}$$

3. If $\hat{H}(t')$ is a time-dependent Hamiltonian, show that the state propagator, when $t < t_0$ is given by

$$\hat{U}(t,t_0) = \overrightarrow{\mathcal{T}}\left[\exp\left\{\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t} dt'\hat{H}(t')\right\}\right], \tag{13}$$

where $\overrightarrow{\mathcal{T}}$ is the anti-time-ordering operator.

Consider the operator

$$\hat{U} = \exp\left[\hat{\gamma}\right]\exp\left[\hat{\beta}\right]\exp\left[\hat{\alpha}\right], \tag{14}$$

where $\hat{\alpha}, \hat{\beta}, \hat{\gamma}$ is a set of non-commuting observables. By considering the first few terms in each of the expansions, or otherwise, demonstrate the plausibility of the identity

$$\hat{U} = \overleftarrow{\mathcal{O}}\left[\exp\left\{\hat{\gamma} + \hat{\beta} + \hat{\alpha}\right\}\right], \tag{15}$$

where $\overleftarrow{\mathcal{O}}$ is an ordering operator that always forces the ordering $\hat{\gamma}, \hat{\beta}, \hat{\alpha}$.

Likewise, demonstrate that

$$\hat{V} = \exp\left[\hat{\alpha}\right]\exp\left[\hat{\beta}\right]\exp\left[\hat{\gamma}\right], \tag{16}$$

motivates

$$\hat{V} = \overrightarrow{\mathcal{O}}\left[\exp\left\{\hat{\gamma} + \hat{\beta} + \hat{\alpha}\right\}\right], \tag{17}$$

where $\overleftarrow{\mathcal{O}}$ is an anti-ordering operator that always reverses the sequence $\hat{\gamma}, \hat{\beta}, \hat{\alpha}$.

This shows that a product of exponentials can be replaced by an exponential of the sums, as long as the appropriate ordering operator is used. The identity does not hold without $\mathcal{O}$, and so is not true for a general sum of exponentials, unlike scalar arguments.

If the operators correspond to a discrete set of Hamitonians at different times, $\hat{H}(t_n)$, explain why this motivates the identity

$$\hat{U} = \overleftarrow{\mathcal{T}}\left[\exp\left\{\sum_n \hat{H}(t_n)\Delta t\right\}\right], \tag{18}$$

leading in principle to the the continuous integral form.

Answer 3.
First part is a repeat of Handout II in time reversed case.
The second part is shown by expanding each exponential to second or third order.

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4. If $\hat{\rho}$ is the density operator, prove the following:

$$\begin{aligned} \mathrm{Tr}\left[\hat{\rho}\right] &= 1 && \text{normalisation condition} \\ \hat{\rho}^{\dagger}\hat{\rho} &= \hat{\rho}\hat{\rho}^{\dagger} && \text{self adjoint} \\ \hat{\rho}\hat{\rho} &= \hat{\rho} && \text{idempotent for a pure state} \end{aligned} \tag{19}$$

Answer 4.

$$\begin{aligned} \mathrm{Tr}\left[\hat{\rho}\right] &= \sum_{mn} P_n \langle\phi_m|\phi_n\rangle\langle\phi_n|\phi_m\rangle \\ &= \sum_n P_n \\ &= 1. \end{aligned} \tag{20}$$

The second identity is obvious.
The third identity follows because

$$\begin{aligned} \hat{\rho}^2 &= |\psi\rangle\langle\psi|\psi\rangle\langle\psi| \\ &= \hat{\rho}. \end{aligned} \tag{21}$$

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5. Prove that for a pure state the following identity must hold

$$\mathrm{Tr}\left[\hat{\rho}^2\right] = 1, \tag{22}$$

whereas for a mixed state

$$\mathrm{Tr}\left[\hat{\rho}^2\right] < 1, \tag{23}$$

where $\hat{\rho}$ is any normalised density operator.

Using this result,show that for both time dependent and time independent Hamiltonians, a pure state can only evolve into a pure state, and a mixed state can only evolve into a mixed state.

Can time evolution result in decoherence, or is something else needed?

Answer 5.

First part follows from previous question.

For a mixed state there must be at least two terms in the density operator; say

$$
\begin{aligned}
\hat{\rho} &= \sum_{n}^{N>1} P_n |\phi_n\rangle\langle\phi_n| \\
\hat{\rho}^2 &= \sum_{m,n}^{M,N>1} P_n P_m |\phi_n\rangle\langle\phi_n|\phi_m\rangle\langle\phi_m| \\
&= \sum_{n}^{N>1} P_n^2 |\phi_n\rangle\langle\phi_n| \\
\mathrm{Tr}\left[\hat{\rho}^2\right] &= \sum_{n}^{N>1} P_n^2 \quad \text{because} \quad \sum P_n = 1.
\end{aligned} \tag{24}
$$

To prove that the 'purity' of a state does not change, work in the Schrödinger picture:

$$
\begin{aligned}
\hat{\rho}(t_0) &= \sum_n P_n |\phi_n(t_0)\rangle\langle\phi_n(t_0)| \\
\hat{\rho}(t) &= \sum_n P_n \hat{U}(t,t_0)|\phi_n(t_0)\rangle\langle\phi_n(t_0)|\hat{U}^\dagger(t,t_0) \\
&= \hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t,t_0)
\end{aligned} \tag{25}
$$

To test for purity

$$
\begin{aligned}
\mathrm{Tr}\left[\hat{\rho}^2(t)\right] &= \mathrm{Tr}\left[\hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t,t_0)\right] \\
&= \mathrm{Tr}\left[\hat{U}(t,t_0)\hat{\rho}^2(t_0)\hat{U}^\dagger(t,t_0)\right] \\
&= \mathrm{Tr}\left[\hat{\rho}^2(t_0)\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)\right] \\
&= \mathrm{Tr}\left[\hat{\rho}^2(t_0)\right].
\end{aligned} \tag{26}
$$

Because the trace is preserved, the purity must also be preserved.

A system cannot decorrelate through unitary time evolution alone.

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6. Suppose that $\hat{\rho}$ is the density matrix of a pure state. Show that for a time independent Hamiltonian the off diagonal matrix elements, in the energy eigenstate basis at $t = 0$, oscillate in time with a frequency that is given by the energy difference between the most extreme energies in the pure state.

Also show that fastest rate of change of any expectation value is given by the difference between the highest and lowest energy levels in the state, or between the highest and lowest energy levels to which the measurement is sensitive, whichever is the smallest.

Why is this also true for a mixed state?

Show that for a pure state, the matrix elements are consistent with von Neumann's equation.

Answer 6.

$$\begin{aligned}\rho_{ij}(t) &= \langle\phi_i|\hat{\rho}(t)|\phi_j\rangle \\ &= \langle\phi_i|\hat{U}(t,t_0)\hat{\rho}(0)\hat{U}^\dagger(t,t_0)|\phi_j\rangle \\ &= \sum_{mn} e^{-iE_m t/\hbar}e^{+iE_n t/\hbar}\langle\phi_i|\phi_m\rangle\langle\phi_m|\psi\rangle\langle\psi|\phi_n\rangle\langle\phi_n|\phi_j\rangle \\ &= e^{-i(E_i-E_j)t/\hbar}\langle\phi_i|\psi\rangle\langle\psi|\phi_j\rangle \\ &= e^{-i(E_i-E_j)t/\hbar}\rho_{ij}(0).\end{aligned} \tag{27}$$

In the Schrödinger picture:

$$\begin{aligned}\langle\hat{A}\rangle(t) &= \mathrm{Tr}\left[\hat{\rho}(t)\hat{A}\right] \\ &= \sum_{ij} e^{-i(E_i-E_j)t/\hbar}\rho_{ij}(0)A_{ji} \\ \frac{d\langle\hat{A}\rangle(t)}{dt} &= \sum_{ij}\frac{-i(E_i-E_j)t}{\hbar}e^{-i(E_i-E_j)t/\hbar}\rho_{ij}(0)A_{ji}\end{aligned} \tag{28}$$

The off-diagonal terms come in pairs, and so the expectation value is always real, as needed.

The fastest rate of change comes from those terms that are farthest apart in energy, the most off-diagonal terms for which both $\rho_{ij}(0)$ and A_{ij} are nonzero. This translates into the biggest energy difference in the pure state, and the dependency of the measurement on two energy components. Both the original state and the measurement control the rate of change of the expectation value.

For a mixed state, we just get a weighted sum, and so the same reasoning applied.

von Neumann's equation is

$$i\hbar\frac{\partial\rho(t)}{\partial t} = \left[\hat{H},\rho(t)\right], \tag{29}$$

and we need

$$\begin{aligned}
\langle\phi_i|\frac{\partial\rho(t)}{\partial t}|\phi_j\rangle &= \frac{-i}{\hbar}\langle\phi_i|\left[\hat{H},\rho(t)\right]|\phi_j\rangle, \\
\frac{\partial\rho_{ij}(t)}{\partial t} &= \frac{-i}{\hbar}\left\{\langle\phi_i|\left[\hat{H},U(t)\rho(0)U^{\dagger}(t)\right]|\phi_j\rangle\right\} \\
&= \frac{-i}{\hbar}(E_i-E_j)e^{-i(E_i-E_j)t/\hbar}\rho_{ij}(0),
\end{aligned} \tag{30}$$

which is consistent with the matrix elements derived earlier.

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7. If a simple harmonic system is described by the thermal density operator $\hat{\rho}(T)$, which is a function of temperature, show that the average energy is given by:

$$\langle E\rangle = \hbar\omega\left[\frac{1}{2}+\frac{1}{e^{\hbar\omega/kT}-1}\right]. \tag{31}$$

Calculate an expression for the variance in the energy, and comment on the terms.