Part II: Michaelmas 2021

Advanced Quantum Mechanics Question Sheet 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 $\hat{U}^{-1}(t_2, t_1)$?

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

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

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

$$\hat{U}(t, t_0) = \overrightarrow{\mathcal{T}}\left[\exp\left\{\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t} dt' \hat{H}(t')\right\}\right], \tag{2}$$

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

4. Consider the operator

$$\hat{U} = \exp\left[\hat{\gamma}\right] \exp\left[\hat{\beta}\right] \exp\left[\hat{\alpha}\right], \tag{3}$$

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

$$\hat{U} = \overleftarrow{\mathcal{O}} \left[\exp\left\{\hat{\gamma} + \hat{\beta} + \hat{\alpha}\right\}\right], \tag{4}$$

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

Likewise, demonstrate that

$$\hat{V} = \exp\left[\hat{\alpha}\right] \exp\left[\hat{\beta}\right] \exp\left[\hat{\gamma}\right], \tag{5}$$

motivates

$$\hat{V} = \overrightarrow{\mathcal{O}} \left[\exp\left\{\hat{\gamma} + \hat{\beta} + \hat{\alpha}\right\}\right], \tag{6}$$

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

$$\hat{U} = \overleftarrow{\mathcal{T}} \left[\exp\left\{\sum_n \hat{H}(t_n)\Delta t\right\}\right], \tag{7}$$

leading in principle to the continuous integral form.

Why does the adjoint reverse the process?

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

$$\begin{array}{rcll} \mathrm{Tr}\left[\hat{\rho}\right] & = & 1 & \text{normalisation condition} \\ \hat{\rho}^{\dagger}\hat{\rho} & = & \hat{\rho}\hat{\rho}^{\dagger} & \text{self adjoint} \\ \hat{\rho}\hat{\rho} & = & \hat{\rho} & \text{idempotent for a pure state} \end{array} \tag{8}$$

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

$$\mathrm{Tr}\left[\hat{\rho}^2\right] = 1, \tag{9}$$

whereas for a mixed state

$$\mathrm{Tr}\left[\hat{\rho}^2\right] < 1, \tag{10}$$

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.

7. Suppose that $\hat{\rho}$ is the density operator 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 time variation of the matrix elements are consistent with von Neumann's equation.

8. 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:

$$\langle E \rangle = \hbar\omega \left[\frac{1}{2} + \frac{1}{e^{\hbar\omega/kT} - 1} \right]. \tag{11}$$

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