22.51 Problem Set 3 (due Fri, Sept. 28)

1 Schrodinger Picture (40 pt)

Question: We are going to fill in the missing steps on lecture and rederive the Schrodinger picture step by step in a rigorous fashion from the three quantum postulates.

(**a**). Prove that,

$$[\hat{A},\ \hat{B}_1\hat{B}_2..\hat{B}_n] \;=\; \sum_{s=0}^{n-1} \hat{B}_1..\hat{B}_s[\hat{A},\hat{B}_{s+1}]\hat{B}_{s+2}..\hat{B}_n. \tag{1}$$

(**b**). By Quantum Postulate 3, any Heisenberg operator must be defined as,

$$\hat{A}(t) \;\equiv\; \sum_n c_n(t)...\hat{q}(t)\hat{p}(t)\hat{q}(t)\hat{q}(t)..., \tag{2}$$

where $...\hat{q}(t)\hat{p}(t)\hat{q}(t)\hat{q}(t)...$ means a certain ordered combination of the elementary Heisenberg operators $\hat{q}(t), \hat{p}(t)$. Also, the partial time-derivative of $\hat{A}(t)$ is defined to be,

$$\frac{\partial\hat{A}(t)}{\partial t} \;\equiv\; \sum_n \dot{c}_n(t)...\hat{q}(t)\hat{p}(t)\hat{q}(t)\hat{q}(t)..., \tag{3}$$

which is equivalent to what we do in classical mechanics. Using the following two axioms,

$$\frac{d\hat{q}(t)}{dt} = \frac{1}{i\hbar}[\hat{q}(t),\hat{\mathcal{H}}(t)], \qquad \frac{d\hat{p}(t)}{dt} = \frac{1}{i\hbar}[\hat{p}(t),\hat{\mathcal{H}}(t)], \tag{4}$$

which relate directly to the classical Hamiltonian dynamics, and (**a**), *prove* that,

$$\frac{d\hat{A}(t)}{dt} \;=\; \frac{1}{i\hbar}[\hat{A}(t),\hat{\mathcal{H}}(t)] \;+\; \frac{\partial\hat{A}(t)}{\partial t}. \tag{5}$$

c. For any $\hat{U}(t)$ that satisfies $\hat{U}^+(t)\hat{U}(t) = \hat{U}(t)\hat{U}^+(t) = \hat{I}$, we may define,

$$\hat{A}_s(t) \;\equiv\; \hat{U}(t)\hat{A}(t)\hat{U}^+(t). \tag{6}$$

Therefore by definition,

$$\hat{q}_s(t) \equiv \hat{U}(t)\hat{q}(t)\hat{U}^+(t), \quad \hat{p}_s(t) \equiv \hat{U}(t)\hat{p}(t)\hat{U}^+(t), \quad \hat{\mathcal{H}}_s(t) \equiv \hat{U}(t)\hat{\mathcal{H}}(t)\hat{U}^+(t). \tag{7}$$

Show that (2) is still satisfied when all the operators have subscript "s" attached. Therefore,

$$\hat{A} \;=\; \sum_n c_n(t)...\hat{q}\hat{p}\hat{q}\hat{q}..., \tag{8}$$

where the operators may or may not depend on t, is considered a *picture-independent* expansion formula.

d. Show that in order for $\hat{q}_s(t)$, $\hat{p}_s(t)$ to be independent of time,

$$\frac{d\hat{q}_s(t)}{dt} \;=\; 0, \quad \frac{d\hat{p}_s(t)}{dt} \;=\; 0, \tag{9}$$

the following would be sufficient,

$$i\hbar\frac{d\hat{U}(t)}{dt} \;=\; \hat{\mathcal{H}}_s(t)\hat{U}(t), \qquad \hat{U}(0) \equiv \hat{I}. \tag{10}$$

Furthermore prove that it guarantees $\hat{U}^+(t)\hat{U}(t) = \hat{U}(t)\hat{U}^+(t) = \hat{I}$ at any t.

e. From now on let $\hat{U}(t)$ satisfies (10). Show that,

$$\frac{d\hat{A}_s(t)}{dt} \;=\; \sum_n \dot{c}_n(t)...\hat{q}_s\hat{p}_s\hat{q}_s\hat{q}_s.... \tag{11}$$

If we define,

$$\frac{\partial\hat{A}_s(t)}{\partial t} \;\equiv\; \sum_n \dot{c}_n(t)...\hat{q}_s\hat{p}_s\hat{q}_s\hat{q}_s..., \tag{12}$$

which is again a *picture-independent* definition if we compare with (3), then we would have,

$$\frac{d\hat{A}_s(t)}{dt} \;=\; \frac{\partial\hat{A}_s(t)}{\partial t} \;=\; \hat{U}(t)\left(\frac{\partial\hat{A}(t)}{\partial t}\right)\hat{U}^+(t). \tag{13}$$

f. Explain why if we define,

$$|\psi_s(t)\rangle \;\equiv\; \hat{U}(t)|\psi\rangle, \tag{14}$$

the two pictures would be equivalent.

g. Show that if $\hat{\mathcal{H}}(t)$ has no explicit dependence on time, meaning that if in its definition (2) all coefficients $c_n(t)$'s are just c_n's, then,

$$\hat{\mathcal{H}}_s(t) \;=\; \hat{\mathcal{H}}_s(0) \;=\; \hat{\mathcal{H}}(t) \;=\; \hat{\mathcal{H}}(0). \tag{15}$$

In summary, there is only one $\hat{\mathcal{H}}$, and,

$$\hat{U}(t) \quad = \quad \exp\left(\frac{t\hat{\mathcal{H}}}{i\hbar}\right), \tag{16}$$

is the solution to (10).

2 Operator Inverse (30 pt)

Question: If $\hat{A}\hat{B} = \hat{B}\hat{A} = \hat{I}$, then $\hat{B}$ is called the inverse of $\hat{A}$ and is denoted by $\hat{A}^{-1}$. Prove by induction that,

$$(\hat{A} - \lambda\hat{B})^{-1} \quad = \quad \hat{A}^{-1} + \lambda\hat{A}^{-1}\hat{B}\hat{A}^{-1} + \lambda^2\hat{A}^{-1}\hat{B}\hat{A}^{-1}\hat{B}\hat{A}^{-1} + ... \tag{17}$$

for small enough $\lambda \in \mathbf{C}$.

3 Operator Trace (30 pt)

Question: Let $\hat{A}$ be Hermitian with $\{|a_n\rangle\}$ as its eigenkets. If we adopt $\{|a_n\rangle\}$ as the basis, then the *matrix representation* of operator $\hat{C}$ would be,

$$C_{nm} \quad \equiv \quad \langle a_n|\hat{C}|a_m\rangle, \tag{18}$$

and we define the *trace* of $\hat{C}$ to be $\mathrm{Tr}_A(\hat{C})$,

$$\mathrm{Tr}_A(\hat{C}) \quad \equiv \quad \sum_n C_{nn} \quad = \quad \sum_n \langle a_n|\hat{C}|a_n\rangle, \tag{19}$$

where the subscript A is used to remind us of the fact that this number may well depend on the choice of $\hat{A}$.

(**a**). Prove that $\mathrm{Tr}_A(\hat{C}) = \mathrm{Tr}_B(\hat{C})$, where $\hat{B}$ can be any Hermitian operator. In other words the trace operation is *representation-independent*, and is an *invariant* of $\hat{C}$ which we shall denote as $\mathrm{Tr}(\hat{C})$.

(**b**). Prove that $\mathrm{Tr}(\hat{C}\hat{D}) = \mathrm{Tr}(\hat{D}\hat{C})$.

(**c**). Calculate $Z(\beta) \equiv \mathrm{Tr}(\exp(-\beta\hat{\mathcal{H}}))$, where $\hat{\mathcal{H}}$ is the simple harmonic oscillator Hamiltonian.

(**d**). Calculate $\bar{E}(\beta) \equiv \mathrm{Tr}(\exp(-\beta\hat{\mathcal{H}})\hat{\mathcal{H}})/Z$ for the simple harmonic oscillator. This is the average energy of an oscillator at finite temperature T with $\beta = 1/k_{\mathrm{B}}T$.