Name:________________________ Date:____________

Time for Completion:____________

Honours QM HW #3

1. Find the differential equation for the time evolution operator $\hat{U}_{\hat{H}}(t,\, t_0)$ using the Schrödinger equation and the definition of the time evolution operator, $|\psi(t)\rangle = \hat{U}_{\hat{H}}(t,\, t_0)|\psi(t_0)\rangle$. Show that if

   (a) $\hat{H}$ is independent of time then $\hat{U}_{\hat{H}}(t,\, t_0) = \exp\big(-i\hat{H}(t-t_0)\big)$ solves the DE you found for $\hat{U}_{\hat{H}}(t,\, t_0)$

   (b) $\hat{H}(t)$ is time dependent but $[\hat{H}(t_1),\, \hat{H}(t_2)] = 0$ then $\hat{U}_{\hat{H}}(t,\, t_0) = \exp\big(-i\int_{t_0}^{t} dt'\, \hat{H}(t')\big)$ solves the DE you found for $\hat{U}_{\hat{H}}(t,\, t_0)$

   (c) $\hat{H}(t)$ is time dependent but $[\hat{H}(t_1),\, \hat{H}(t_2)] \neq 0$ then $\hat{U}_{\hat{H}}(t,\, t_0) = \underleftarrow{T}\exp\big(-i\int_{t_0}^{t} dt'\, \hat{H}(t')\big)$, where, in general, the time-ordered exponential is defined as the Dyson series

$$\underleftarrow{T}\exp\left(\int_{t_0}^{t} dt'\,\hat{A}(t')\right) \equiv \hat{1} + \int_{t_0}^{t} dt_1\,\hat{A}(t_1) + \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\,\hat{A}(t_1)\,\hat{A}(t_2) + \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3\,\hat{A}(t_1)\,\hat{A}(t_2)\,\hat{A}(t_3) + \ldots, \quad (1)$$

   solves the DE you found for $\hat{U}_{\hat{H}}(t,\, t_0)$.

   Note: you might find the Leibniz Rule helpful: for

$$I(\alpha) = \int_{a(\alpha)}^{b(\alpha)} f(x,\, \alpha)\, dx, \quad (2)$$

   we have that

$$\frac{d}{d\alpha}I(\alpha) = \frac{db(\alpha)}{d\alpha}f\big(b(\alpha),\, \alpha\big) - \frac{da(\alpha)}{d\alpha}f\big(a(\alpha),\, \alpha\big) + \int_{a(\alpha)}^{b(\alpha)} \frac{\partial f(x,\, \alpha)}{\partial\alpha}\, dx. \quad (3)$$

2. Prove Ehrenfest's Theorem, that the expectation values of operators evolve as one would expect classically; i.e., show that the expectation values of operators follow Newton's Equation:

$$\frac{d}{dt}\langle\hat{\boldsymbol{p}}\rangle = -\langle\boldsymbol{\nabla}V\rangle \quad (4)$$

   when

$$\hat{H}(t) \;=\; \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{x}}). \quad (5)$$

Show this first using the Heisenberg picture and then again using the Schrödinger picture. Hint: in HW#1 you showed that $[\hat{\boldsymbol{x}}, f(\hat{\boldsymbol{p}})] = i\boldsymbol{\nabla}_{\hat{\boldsymbol{p}}} f(\hat{\boldsymbol{p}})$ holds as an operator equation; you may find it useful to assume that, similarly, $[\hat{\boldsymbol{p}}, g(\hat{\boldsymbol{x}})] = -i\boldsymbol{\nabla}_{\hat{\boldsymbol{x}}}\, g(\hat{\boldsymbol{x}})$

3. The time dependence of the simple harmonic oscillator in the Heisenberg picture. Taking $t_0 = 0$ for simplicity, find $a_H(t)$ and $a_H^\dagger(t)$ using the definition of the Heisenberg operator, $\hat{X}_H(t) \equiv \hat{U}_{\hat{H}}^\dagger(t)\hat{X}_H(0)\hat{U}_{\hat{H}}(t) = \hat{U}_{\hat{H}}^\dagger(t)\hat{X}_S\hat{U}_{\hat{H}}(t)$, and using the Baker-Hausdorff lemma. Recall that $\hat{H} = \omega(\hat{N}+1/2)$, where $\hat{N} = a_H^\dagger(t)a_H(t) = a_S^\dagger a_S = a^\dagger a$ (note that I was able to drop the subscripts in the equation for $\hat{N}$ and $\hat{H}$ because $\hat{H}$ is time independent for the SHO, so the equation holds both when the raising and lowering operators are both taken as in the Heisenberg picture or when both are taken to be in the Schrödinger picture), and

$$[\hat{N},\, \hat{a}] = -\hat{a} \tag{6}$$

$$[\hat{N},\, \hat{a}^\dagger] = \hat{a}^\dagger. \tag{7}$$

Now find $a_H(t)$ and $a_H^\dagger(t)$ using the Heisenberg equations of motion. Recalling that

$$\hat{x}_S = \frac{1}{2m\omega}\left(\hat{a}_S + \hat{a}_S^\dagger\right) \tag{8}$$

$$\hat{p}_S = \frac{m\omega}{2}\left(-\hat{a}_S + \hat{a}_S^\dagger\right), \tag{9}$$

find $\hat{x}_H(t)$ and $\hat{p}_H(t)$ in terms of $\hat{x}_H(0) = \hat{x}_S$ and $\hat{p}_H(0) = \hat{p}_S$.

4. In the last homework set we found $\langle\hat{\boldsymbol{S}}\rangle(t)$ for an electron polarized along the positive x direction at $t = 0$ in a constant, time-independent magnetic field $\boldsymbol{B} = B\hat{z}$ (where the hat on the z refers to a unit vector and not an operator), in the Schrödinger picture. Now let's do the same calculation again in the Heisenberg picture. There are three very nice ways to do this calculation.

   (a) First, use the Baker-Hausdorff lemma to find $\hat{\boldsymbol{S}}_H(t)$.

   (b) Second, use the Heisenberg equations of motion. When you use the HEOM, you should find that

$$\begin{aligned} \frac{d}{dt}\hat{S}_{x,\,H}(t) &= -\,\omega\,\hat{S}_{y,\,H}(t) \\ \frac{d}{dt}\hat{S}_{y,\,H}(t) &= \quad\omega\,\hat{S}_{x,\,H}(t) \\ \frac{d}{dt}\hat{S}_{z,\,H}(t) &= 0, \end{aligned} \tag{10}$$

   where $\hat{H} = -\tilde{\omega}\hat{\boldsymbol{S}}\cdot\boldsymbol{B}$ and $\omega = -\tilde{\omega}B$ as we had from the last time. This is a coupled set of first order ordinary differential equations. The general way to solve a set of coupled first order differential equations, as we know from our extensive manipulations of Lie groups, is to write the equations in matrix form and exponentiate. To wit,

$$\frac{d}{dt}\hat{\boldsymbol{S}}_H(t) = \omega \boldsymbol{M} \cdot \hat{\boldsymbol{S}}_H(t) = \omega \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \hat{\boldsymbol{S}}_H(t), \tag{11}$$

where

$$\hat{\boldsymbol{S}} \equiv \begin{pmatrix} \hat{S}_x \\ \hat{S}_y \end{pmatrix} \tag{12}$$

(the equation for $S_{z,H}(t)$ is trivial). So now exponentiate $\boldsymbol{M}$, and we formally have the solution. We are able to make some additional progress by then Taylor expanding the exponential. Notice something clever about the matrix $\boldsymbol{M}$ (i.e. notice that $\boldsymbol{M}^2 = -\boldsymbol{1}$), then notice something clever about the remaining infinite sums (they should be reminiscent of something you just found using Baker-Hausdorff...). Finally, write down your expressions for $\hat{\boldsymbol{S}}_H(t)$.

(c) For the third and final method (for this HW set, that is), return to Eq. (10). The previous method, that of exponentiating the matrix, is completely general. However we might be clever at an earlier step than from all those manipulations of Taylor expansions. In particular, we might notice that while our HEOM give us a set of coupled, first order ordinary differential equations, if we take the derivative of both sides of the equations in Eq. (10), we find two *uncoupled* secord order ordinary differential equations (the z equation remains trivial). Find these equations, note the boundary conditions (how many do you need?), and solve them. What is $\hat{\boldsymbol{S}}_H(t)$?

Using your expression for $\hat{\boldsymbol{S}}_H(t)$, find $\langle \hat{\boldsymbol{S}} \rangle(t)$ given the above initial conditions and compare it to the quantity found in the previous homework set.