PHASM426 / PHASG426
Advanced Quantum Theory Problem Sheet 3

Deadline: 12th December 2017.

Please hand in your completed work at the **end** of the lecture on that day. Attache the coversheet. If you are unable to attend the lecture, you may scan your work, *save it as a single PDF file* and email it to me **prior** to this lecture. You may also bring the work to me in my office (B12) before the lecture. **Make sure your completed work is clearly labelled with your name and college**. Please note that UCL places severe penalties on late-submitted work.

1. **Generalisation of the Ehrenfest theorem**. The Heisenberg picture leads to equations of motion that are formally similar to those obtained in classical mechanics.

   (a) Consider the Shrödinger picture Hamiltonian of a particle of mass m under the influence of a potential $V(\hat{x})$:

   $$H_S = \frac{1}{2m}\hat{p}^2 + V(\hat{x}).$$

   Show that the Hamiltonian operator in the Heisenberg picture becomes:

   $$H_H(t) = \frac{1}{2m}\hat{p}_H^2(t) + V(\hat{x}_H(t)).$$

   [1]

   Model Answer: In the Heisenber picture

   $$\begin{aligned} H_H(t) &= U^\dagger(t) H_s U(t) \\ &= \frac{1}{2m}U^\dagger\Big(\hat{p}U(t)U^\dagger(t)\hat{p}\Big)U(t) + U^\dagger V(\hat{x})U(t) \\ &= \frac{1}{2m}\hat{p}_H^2(t) + V(\hat{x}_H(t)). \end{aligned}$$

   Marks: **1 mark** for correct answer. Partial mark for partial answer.

   (b) Consider the Heisenberg equation

   $$\frac{\partial}{\partial t}\hat{O}_H(t) = \frac{i}{\hbar}[H_H(t), \hat{O}_H(t)].$$

and the results proved on problem 1 to show that $\hat{x}_H(t)$ and $\hat{p}_H(t)$ satisfy the following differential equations (which are similar in form to those that give the evolution of the classical quantities x and p):

$$\begin{aligned}\frac{\partial}{\partial t}\hat{x}_H(t) =& \frac{1}{m}\hat{p}_H(t)\\ \frac{\partial}{\partial t}\hat{p}_H(t) =& -\frac{\partial}{\partial \hat{x}_H}V(\hat{x}_H(t)).\end{aligned}$$

[1]

Model answer: In order to prove these results we need to compute $[H_H(t), \hat{x}_H(t)]$ and $[H_H(t), \hat{p}_H(t)]$, which involve the commutation relations: $[\hat{p}_H^2(t), \hat{x}_H(t)]$, $[V(\hat{x}_H(t)), \hat{x}_H(t)]$, $[\hat{p}_H^2(t), \hat{p}_H(t)]$ and $[V(\hat{x}_H(t)), \hat{p}_H(t)]$. Using the relations proved in 1(a), we have that in the Shrödinger picture $[\hat{p}^2, \hat{x}] = -i\hbar\hat{p}$ and using the results proved in 1(b) we obtain $[\hat{p}_H^2(t), \hat{x}_H(t)] = -i\hbar\hat{p}_H(t)$. Similarly $[V(\hat{x}), \hat{p}] = i\hbar\frac{\partial}{\partial\hat{x}}V(\hat{x})$ and therefore $[V(\hat{x}_H(t)), \hat{p}_H(t)] = i\hbar\frac{\partial}{\partial\hat{x}_H}V(\hat{x}_H(t))$.
It is straight forward to show that $[V(\hat{x}_H(t)), \hat{x}_H(t)] = 0$ and $[\hat{p}_H^2(t), \hat{p}_H(t)] = 0$.

Marks: **1 mark** for correctly invoking the results of probed in 1.

(c) Consider that the particle of mass m is an electron of charge e under the influence of an electric field of intensity E such that the potential operator is given by $V(\hat{x}) = -eE\hat{x}$. Using the results of 2(b), write an expression for the expected value of $\hat{p}_H(t)$ as a function of time. Assume the particle is initially in a state $|\psi(0)\rangle$. [2]

Model answer: The potential operator in the Heisenberg picture becomes $V(\hat{x}_H(t)) = -eE\hat{x}_H(t)$ and the expected value of $\hat{p}_H(t)$ is given by $\langle\hat{p}_H(t)\rangle = \langle\psi(0)|\hat{p}_H(t)|\psi(0)\rangle$. Then, according to 2(b), this expected value satisfy the differential equation:

$$\frac{\partial}{\partial t}\langle\hat{p}_H(t)\rangle = -\frac{\partial}{\partial\hat{x}_H}\langle V(\hat{x}_H(t))\rangle = eE$$

Therefore

$$\langle\hat{p}_H(t)\rangle = \langle\hat{p}_H(0)\rangle + eEt,$$

where $\langle\hat{p}_H(0)\rangle$ is the expected value of $\hat{p}_H(t)$ at time $t = 0$. Recall that at $t = 0$ the Heisenberg picture operator $\hat{p}_H(0)$ equals the operator $\hat{p}$ in the Shrödinger picture i.e. $\langle\hat{p}_H(0)\rangle = \langle\psi(0)|\hat{p}|\psi(0)\rangle$

Marks: **2 marks.** Deduce 1 mark if $\langle\hat{p}_H(0)\rangle$ has been set to zero.

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2. **Approximations in unitary dynamics**

(a) Prove that for any self-inverse operator $\hat{O}$, i.e. where $\hat{O}^2 = \mathbb{1}$,

$$\exp[i\omega t\hat{O}] = \cos(\omega t)\mathbb{1} + i\sin(\omega t)\hat{O}.$$

[2]

Model Answer:
The proof on this uses the fact that since $\hat{O}^2 = \mathbb{1}$, all even powers of $\hat{O}$ are equal to $\mathbb{1}$, and all odd powers are equal to $\hat{O}$, hence

$$\begin{aligned}\exp[i\omega t\hat{O}] &= \sum_j (i\omega t)^j \hat{O}^j/j! \\ &= \sum_j (i\omega t)^{2j}\hat{O}^{2j}/(2j)! + \sum_j (i\omega t)^{2j+1}\hat{O}^{2j+1}/(2j+1)! \\ &= \sum_j (i\omega t)^{2j}/(2j)!\mathbb{1} + \sum_j (i\omega t)^{2j+1}/(2j+1)!\hat{O} \\ &= \cos(\omega t)\mathbb{1} + i\sin(\omega t)\hat{O}.\end{aligned}$$

Marks: **2 marks**. Partial marks for a partial solution.

(b) Using the result of part 2(a), find the evolution operator for the following Hamiltonian:

$$H = \hbar g\frac{\sigma_x + \sigma_z}{\sqrt{2}}.$$

use it to derive $|\psi(t)\rangle$, for a spin-half particle, initially in state $|\psi(0)\rangle = |\uparrow\rangle$.

[2]

Model Answer:
We use the fact that $(\frac{\sigma_x+\sigma_z}{\sqrt{2}})^2 = \mathbb{1}$, hence the evolution operator for this Hamiltonian is

$$U(t) = \exp[-igt\frac{\sigma_x + \sigma_z}{\sqrt{2}}] = \cos(gt)\mathbb{1} - i\sin(gt)\frac{\sigma_x + \sigma_z}{\sqrt{2}}$$

Recalling that $\sigma_x|\uparrow\rangle = |\downarrow\rangle$ and $\sigma_z|\uparrow\rangle = |\uparrow\rangle$ to write:

$$|\psi(t)\rangle = \cos(gt)|\uparrow\rangle - i\sin(gt)\frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}$$

Marks: **2 marks**. Partial marks for a partial solution.

(c) A first-order Trotter approximation for evolution under this Hamiltonian is

$$U_1 = \exp[-ig\sigma_x t/\sqrt{2}]\exp[-ig\sigma_z t/\sqrt{2}].$$

Calculate the first order approximate solution $|\psi_1(t)\rangle = U_1(t)|\uparrow\rangle$. The error in this computation can be quantified in terms of the norm of the difference between exact $|\psi(t)\rangle$ and approximate solution $|\psi_1(t)\rangle$. By expressing $|\psi(t)\rangle$ and $|\psi_1(t)\rangle$ as a power series in t up to second order, calculate this error, $||\,|\psi(t)\rangle - |\psi_1(t)\rangle||$ to the second order in t.

Hint: Recall that the spin states $|\uparrow\rangle$ and $|\downarrow\rangle$ form an orthonormal basis for the spin-state of a spin-half particle, and that the operators σ_x and σ_z transform these states as follows:

$$\sigma_x|\uparrow\rangle = |\downarrow\rangle \qquad \sigma_x|\downarrow\rangle = |\uparrow\rangle \qquad \sigma_z|\uparrow\rangle = |\uparrow\rangle \qquad \sigma_z|\downarrow\rangle = -|\downarrow\rangle$$

[3]

Model Answer: Under $U_1(t)$ evolution, the state will evolve. Since $\sigma_x^2 = \sigma_z^2 = \mathbb{1}$ the time-evolving state becomes

$$\begin{aligned}
&|\psi_1(t)\rangle = U_1(t)|\uparrow\rangle \\
&= \Big(\cos(gt/\sqrt{2})\mathbb{1} - i\sin(gt/\sqrt{2})\sigma_x\Big)\Big(\cos(gt/\sqrt{2})\mathbb{1} - i\sin(gt/\sqrt{2})\sigma_z\Big) \\
&= \Big(\cos^2(gt/\sqrt{2})\mathbb{1} - i\sin(gt/\sqrt{2})\cos(gt/\sqrt{2})(\sigma_x+\sigma_z) - \sin^2(gt/\sqrt{2})\sigma_x\sigma_z\Big)|\uparrow\rangle \\
&= \Big(\cos^2(gt/\sqrt{2}) - i\sin(gt/\sqrt{2})\cos(gt/\sqrt{2})\Big)|\uparrow\rangle \\
&\qquad + \Big(-i\sin(gt/\sqrt{2})\cos(gt/\sqrt{2}) - \sin^2(gt/\sqrt{2}\Big)|\downarrow\rangle
\end{aligned}$$

Marks: **3 marks**. Partial marks for a partial solution.

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3. The interaction picture is employed to describe the dynamics of a system whose Hamiltonian has the form $H = H_0 + V$, where the eigenstates and eigenenergies of H_0 are known. In this representation, operators take the form $O_I(t) = U_0^\dagger(t) O U_0(t)$ with $U_0(t) = \exp[-iH_0 t/\hbar]$. A Hamiltonian describing the interaction between a pair of two-state atoms takes the form

$$H = \hbar\epsilon_1|A\rangle\langle A| + \hbar\epsilon_2|B\rangle\langle B| + \hbar J\left(|A\rangle\langle B| + |B\rangle\langle A|\right),$$

where $|A\rangle \equiv |e_1, g_2\rangle$; $|B\rangle \equiv |g_1, e_2\rangle$ and $|e_{1(2)}\rangle$ and $|g_{1(2)}\rangle$ are the excited and ground states of atom $1(2)$, respectively.

(a) Show that $V_I(t) = \hbar J\Big(e^{i(\epsilon_1-\epsilon_2)t}|A\rangle\langle B| + e^{-i(\epsilon_1-\epsilon_2)t}|B\rangle\langle A|\Big)$. [4]

Model answer. Identify

$$H_0 = \hbar\epsilon_1|A\rangle\langle A| + \hbar\epsilon_2|B\rangle\langle B|$$

and

$$V = \hbar J\left(|A\rangle\langle B| + |B\rangle\langle A|\right)$$

and define $U_0(t) = e^{-iH_0t} = e^{-i\epsilon_1|A\rangle\langle A|}e^{-i\epsilon_2|B\rangle\langle B|}$ because $|B\rangle\langle B|$ and $|\rangle\langle A|$ commute . Then

$$\begin{aligned}V_I(t) =&\hbar J\Big(e^{i\epsilon_1|A\rangle\langle A|}e^{i\epsilon_2|B\rangle\langle B|}|A\rangle\langle B|e^{-i\epsilon_1|A\rangle\langle A|}e^{-i\epsilon_2|B\rangle\langle B|}\\ &+ e^{i\epsilon_1|A\rangle\langle A|}e^{i\epsilon_2|B\rangle\langle B|}|B\rangle\langle A|e^{-i\epsilon_1|A\rangle\langle A|}e^{-i\epsilon_2|B\rangle\langle B|}\Big)\end{aligned}$$

Notice that

$$e^{i\epsilon_2|B\rangle\langle B|}|A\rangle = (\mathbb{1} + i\epsilon_2 t|B\rangle\langle B| + (i\epsilon_2 t)^2|B\rangle\langle B|/2! + \cdots)|A\rangle = |A\rangle.$$

We also have

$$e^{i\epsilon_1|A\rangle\langle A|}|A\rangle = e^{i\epsilon_1 t}|A\rangle \text{ and } e^{i\epsilon_2 t|B\rangle\langle B|}|B\rangle = e^{i\epsilon_2 t}|B\rangle.$$

Then,

$$V_I(t) = \hbar J\Big(e^{i(\epsilon_1-\epsilon_2)t}|A\rangle\langle B| + e^{-i(\epsilon_1-\epsilon_2)t}|B\rangle\langle A|\Big).$$

Marks: **4 marks**. 1 mark for identifying H_0 and V and writting correctly the form of $U_0(t)$. 3 marks for correctly identifying how each exponential operator acts on each ket. Partial marks for partial answers.

(b) In the interaction picture, the joint state of the atoms at time t can be expressed as $|\Psi(t)\rangle_I = \alpha(t)|A\rangle + \beta(t)|B\rangle$. This state satisfies the differential equation $\frac{d}{dt}|\Psi(t)\rangle_I = (-i/\hbar)V_I(t)|\Psi(t)\rangle_I$. Assume that $\epsilon_1 = \epsilon_2$ and $|\Psi(0)\rangle = |A\rangle$. Show that the state at time t becomes $|\Psi(t)\rangle_I = \cos(Jt)|A\rangle - i\sin(Jt)|B\rangle$ [4]

Model answer. When $\epsilon_1 = \epsilon_2$, we have

$$V_I(t) = \hbar J\Big(|A\rangle\langle B| + |B\rangle\langle A|\Big)$$

. Consider the derivative of $|\Psi(t)\rangle_I$ with respect to time:

$$\frac{d|\Psi(t)\rangle_I}{dt} = -(i/\hbar)V_I|\Psi(t)\rangle_I.$$

The left-had side of this equation becomes

$$\frac{d|\Psi(t)\rangle_I}{dt} = \frac{d\alpha(t)}{dt}|A\rangle + \frac{d\beta(t)}{dt}|B\rangle$$

and the right hand side

$$-(i/\hbar)V_I|\Psi(t)\rangle_I = -iJ(\beta(t)|A\rangle + \alpha(t)|B\rangle).$$

Then

$$\frac{d\alpha(t)}{dt} = -iJ\beta(t) \text{ and } \frac{d\beta(t)}{dt} = -iJ\alpha(t)$$

. Taking the second derivativies we then arrive to the following equations:

$$\frac{d^2\alpha(t)}{dt2} + J^2\alpha(t) = 0 \text{ and } \frac{d^2\beta(t)}{dt2} + J^2\beta(t) = 0$$

with the initial conditions $\alpha(0) = 1$ and $\beta(0) = 0$. Hence $\alpha(t) = \cos(Jt)$ and $\beta(t) = -i\sin(Jt)$.

Marks: **4 marks**. 1 mark for writting the correct left-hand and right-had side expresions, 1 mark for deriving the linear differential equtions of firt-order, 1 mark for deriving the diferential equations of second-order and 1 mark for justifying correctly the solution. partial marks for partial answers.

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4. **Applying time-dependent perturbation theory.** A spin-1 particle is held in a strong magnetic field in the z-direction. Immediately prior to time $t = -t_0$, a measurement of its spin indicates that it is in the state $|s = 1, m_s = 1\rangle$. At $t = -t_0$ the experiment is perturbed by a weak magnetic field in the x-direction which ramps up to a maximum and then decays back down to zero at time $t = t_0$.

   (a) The resulting Hamiltonian is $H = \Omega\hat{S}_z + \lambda(t)\hat{S}_x$ where $\lambda(t) = \lambda_0(1 - |t|/t_0)$ for $|t| < t_0$ and $\lambda(t) = 0$ for $|t| \geq t_0$ and $|\lambda_0| \ll \Omega$. Using perturbation theory, show that (to first-order) the probability that a measurement on the spin at time $t = t_0$ will indicate $m_s = 0$ is:

   $$P^{(1)}_{1\to 0} = 2\left|\frac{\lambda_0}{\Omega^2 t_0}\right|^2 (1 - \cos(\Omega t_0))^2.$$

   You may find the following spin-1 matrix representations of $\hat{S}_z$ and $\hat{S}_x$:

   $$\hat{S}_x = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad \hat{S}_z = \hbar\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

and the following indefinite integral helpful:

$$\int e^{iat}(1-bt)dt = \frac{-e^{iat}}{a^2}(b + ia(1-bt)) + c.$$

[5]

Model Answer: We start by recognising that we are working with transitions between eigenstates of the $\hat{S}_z$ operator. The matrix representation for the $\hat{S}_z$ operator is diagonal and non-degenerate implying that its eigenvectors in this basis are $|s=1, m_s=1\rangle = (1,0,0)^T$, with eigenvalue $\hbar$ $|s=1, m_s=0\rangle = (0,1,0)^T$, with eigenvalue 0 and $|s=1, m_s=-1\rangle = (0,0,1)^T$, with eigenvalue $-\hbar$ (where ^{T} stands for transpose, ie. the column vector which is the transpose of this row vector.) The spin state notation $|s=1, m_s=1\rangle$ etc. you should have encountered in previous courses, (you can refresh this in e.g. Bransden and Joachain chapter 6). We are studying the transition probability from the state with spin $\hbar$ ($m_s=1$) to the state with zero spin ($m_s=0$). Following the method outlined in lectures, we thus first must calculate the first order correction

$$c_0^{(1)} = \frac{1}{i\hbar}\int_{-t_0}^{t_0} dt' e^{i\omega_{01}t'} V_{01}(t')$$

To compute this integral, we need two quantities ω_{01} and $V_{01}(t')$. ω_{01} is derived from the energy difference between states $m=0$ and $m=1$, *before the perturbation was switched on*, ie. the eigenvalues of these states with respect to H_0. Thus, $\omega_{01} = (E_0 - E_1)/\hbar = -\Omega$. $V_{01}(t')$ is the matrix element of $\hat{V}$, i.e.

$$\begin{aligned}
V_{01}(t) &= \lambda(t)\langle s=1, m_s=0|\hat{S}_x|s=1, m_s=0\rangle \\
&= \frac{\lambda(t)\hbar}{\sqrt{2}}\begin{bmatrix}0 & 1 & 0\end{bmatrix}\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{bmatrix}\begin{bmatrix}1 & 0 & 0\end{bmatrix} \\
&= \frac{\lambda(t)\hbar}{\sqrt{2}}
\end{aligned}$$

We thus need to integrate

$$c_0^{(1)} = \frac{1}{i\sqrt{2}}\int_{-t_0}^{t_0} dt' e^{-i\Omega t'}\lambda(t')$$

In this case $\lambda(t) = \lambda_0(1 - |t|/t_0)$ we integrate as follows:

$$\begin{aligned}
c_0^{(1)} &= \frac{\lambda_0}{i\sqrt{2}}\int_{-t_0}^{t_0} dt' e^{-i\Omega t'}\left(1 - \frac{|t'|}{t_0}\right) \\
&= \frac{\lambda_0}{i\sqrt{2}}\int_{-t_0}^{0} dt' e^{-i\Omega t'}\left(1 + \frac{t'}{t_0}\right) + \int_{0}^{t^0} dt' e^{-i\Omega t'}\left(1 - \frac{t'}{t_0}\right)
\end{aligned}$$

We now use the standard integral as given for each of these integrals, after doing so and after cancelling terms, we find

$$\begin{aligned} c_0^{(1)} &= \frac{\lambda_0}{i\sqrt{2}} \frac{-1}{\Omega^2} \left(\frac{-2}{t_0} + \frac{1}{t_0} \left(\exp[i\Omega t_0] + \exp[-i\Omega t_0] \right) \right) \\ &= \frac{\lambda_0 i}{\sqrt{2}\Omega^2 t_0} \left(-2 + 2\cos(\Omega t_0) \right) \end{aligned}$$

Taking the modulus square of this expression, we recover the expression for $|P^{(1)}_{1\to 0}|$.

Marks: 1 mark for setting up the problem correctly and identifying the correct expression for $c_0^{(1)}$. **1 mark** for identifying ω_{01} and $V_{01}(t)$. **1 mark** for splitting the integral range to deal with $|t'|$, **1 mark** for integrating, **1 mark** for squaring and arranging the expression into the desired form.

(b) Without detailed calculation, explain why, in this example, second order perturbation theory is required to see a non-zero transition probability to the state $|s=1, m_s=-1\rangle$. [1]

Model Answer: Second order perturbation theory is required, since to first order this transition has zero probability, since the relevant matrix element $V_{-1,+1} = \lambda(t)\langle s=1, m_s=-1|\hat{S}_x|s+1, m_{s=+1}\rangle$ is zero.

Marks: 1 mark for noting that there is no first order transition and for explaining why (in terms of the matrix element).