PHYS851 Quantum Mechanics I, Fall 2009
HOMEWORK ASSIGNMENT 5

1. In problem 4.3, we used a change of variables to map the equations of motion for a sinusoidally driven two-level system onto the time-independent Rabi model. Here we will investigate how this change of variables can be treated more formally as a unitary transformation.

   Unitary operators are those which, when acting on (transforming) any state, always preserve the norm of the state. Any Hermitian operator, G can be used to generate a unitary transformation, via the Unitary operator $U_G = e^{iG}$. The Unitary transformation is then defined by $|\psi'(t)\rangle = U_G|\psi(t)\rangle$, where $|\psi(t)\rangle$ is the original state-vector, and $|\psi'(t)\rangle$ is the state vector in the new 'frame of reference'.

   For the case of a time-dependent Hamiltonian, $H(t)$ and a time-dependent generator $G(t)$, we would like to determine the effective Hamiltonian, $H'(t)$, which governs the evolution of the state $|\psi'(t)\rangle$.

   (a) Begin by differentiating both sides of the equation $|\psi'(t)\rangle = U_G(t)|\psi(t)\rangle$ with respect to time. Use Schrödinger's equation to eliminate $\frac{d}{dt}|\psi(t)\rangle$.
   (Tip: keep in mind that in general $[H(t), G(t)] \neq 0$)

$$|\dot{\psi}'\rangle = \dot{U}_G|\psi\rangle + U_G|\dot{\psi}\rangle \tag{1}$$
$$= \dot{U}_G|\psi\rangle - \frac{i}{\hbar}U_G H|\psi\rangle \tag{2}$$

   (b) The effective Hamiltonian in the new 'frame of reference' must satisfy the equation:

$$i\hbar\frac{d}{dt}|\psi'(t)\rangle = H'(t)|\psi'(t)\rangle.$$

   Use the fact that $U_G^\dagger U_G = I$, and your result from 1a, to give an expression for $H'(t)$ in terms of $H(t)$ and $G(t)$.

$$\frac{d}{dt}|\psi'\rangle = \dot{U}_G U_G^\dagger\left(U_G|\psi\rangle\right) - \frac{i}{\hbar}U_G H U_G^\dagger\left(U_G|\psi\rangle\right) \tag{3}$$
$$= -\frac{i}{\hbar}\left[U_G H U_G^\dagger + i\hbar\dot{U}_G U_G^\dagger\right]|\psi'\rangle \tag{4}$$

   Thus we see that

$$H' = U_G H U_G^\dagger + i\hbar\dot{U}_G U_G^\dagger \tag{5}$$

   (c) What is $H'(t)$ in the special case where G is not explicitly time-dependent? What is H' in the case where H and G are both time-independent and $[H, G] = 0$?
   If G is not time-dependent, then $\dot{U}_G = 0$, so that

$$H' = U_G H U_G^\dagger \tag{6}$$

   If $[H, G] = 0$, then it follows that $[U_G, H] = 0$, so that

$$H' = U_G H U_G^\dagger = H U_G U_G^\dagger = H \tag{7}$$

(d) By definition, $H(t) \neq H'(t)$ is defined as the energy operator. In general, would it be safe to assume that the eigenstates of $H'(t)$ are the energy eigenstates of the system?
No, it would not be a safe assumption, because H' is not just a unitary transformation on H, due to the addition of the $\dot{U}_G$ term. Thus H' and H' will likely not have the same spectrum.

(e) Let us assume that the original Hamiltonian is explicitly time-dependent, but that $G(t)$ is chosen so that H' is time-independent. Write an expression for $|\psi'(t)\rangle$ in terms of the eigenvalues and eigenstates of H', and the initial state $|\psi'(0)\rangle$.
We start from

$$|\dot{\psi}'\rangle = -\frac{i}{\hbar} H' |\psi'\rangle \tag{8}$$

since H' is time-independent, this has the solution

$$|\psi'(t)\rangle = e^{-iH't/\hbar}|\psi'(0)\rangle = \sum_n |\omega'_n\rangle e^{-i\omega'_n t}\langle \omega'_n|\psi'(0)\rangle \tag{9}$$

where $H'|\omega'_n\rangle = \hbar\omega'_n|\omega'_n\rangle$

(f) Use the relationship between $|\psi(t)\rangle$ and $|\psi'(t)\rangle$, to convert your result from 1e, into an expression for $|\psi(t)\rangle$ in terms of the initial state $|\psi(0)\rangle$.
Since $|\psi'\rangle = U_G|\psi\rangle$ it follows that $|\psi\rangle = U_G^{-1}|\psi'\rangle = U_G^\dagger|\psi'\rangle$. Thus we have

$$|\psi(t)\rangle = \sum_n U_G^\dagger |\omega_n\rangle e^{-i\omega'_n t}\langle \omega'_n|U_G|\psi(0)\rangle \tag{10}$$

2. The Hamiltonian for an atom in the field of a standing-wave laser field is given in the two-level approximation by

$$H = \frac{\hbar\omega_a}{2}\left(|2\rangle\langle 2| - |1\rangle\langle 1|\right) - dE_0(y,x)\cos(k_L z)\cos(\omega_L t)\left(|1\rangle\langle 2| + |2\rangle\langle 1|\right)$$

where ω_a is the two-level transition frequency, d is the dipole moment of the transition, $E_0(x,y)\cos(k_L z)$ is the amplitude of the electric field of the laser beam at the location of the atom, k_L is the wave-vector of the laser beam, and ω_L is the frequency of the laser beam. Here x, y, z refer to the location of that atom's center of mass, whose motion we will treat classically. Thus you can just view x, y, z as parameters. Lasers typically have gaussian transverse profiles, so that $E_0(x,y) = E_0 \exp(-(x^2+y^2)/W^2)$, where W is the transverse dimension of the beam.

(a) Consider a Unitary transformation generated by the Hermitian operator $G = \frac{\omega_L}{2}(|2\rangle\langle 2| - |1\rangle\langle 1|)t$. Use the Taylor series for the exponential to compute the transformed states $|1'\rangle := U_G(t)|1\rangle$ and $|2'\rangle := U_G(t)|2\rangle$.

We have

$$e^{iG(t)} = I + iG - \frac{i}{2}G^2 - \frac{1}{6}G^3 + \ldots \tag{11}$$

with $G = \frac{\omega_L t}{2}\left(|2\rangle\langle 2| - |1\rangle\langle 1|\right)$, we see that

$$G^n|2\rangle = (\omega_L t/2)^n|2\rangle \tag{12}$$

and

$$G^n|1\rangle = (-\omega_L t/2)^n|1\rangle \tag{13}$$

this leads to

$$\begin{aligned} |1'\rangle &= U_G(t)|1\rangle \\ &= \left[I + iG - \frac{i}{2}G^2 - \frac{1}{6}G^3 + \ldots\right]|1\rangle \\ &= \left[I + i(-\omega_L t/2) - \frac{i}{2}(-\omega_L t/2)^2 - \frac{1}{6}(-\omega_L t/2)^3 + \ldots\right]|1\rangle \\ &= e^{-i\omega_L t/2}|1\rangle \end{aligned} \tag{14}$$

and similarly we find

$$|2'\rangle = e^{i\omega_L t/2}|2\rangle \tag{15}$$

(b) Use your results from 1b and part 2a to compute the effective Hamiltonian, $H'(t)$, for what we will call the 'rotating frame' (i.e. rotating in Hilbert space) defined by the generator $G = \frac{\omega_L}{2}(|2\rangle\langle 2| - |1\rangle\langle 1|)t$. What are the matrix elements of H' in the $\{|1\rangle, |2\rangle\}$ basis?

First we compute

$$\dot{U}_G = i\frac{\omega_L}{2}\left(|2\rangle\langle 2| - |1\rangle\langle 1|\right)U_G \tag{16}$$

so that

$$\begin{aligned} H' &= U_G\left[\frac{\hbar\omega_a}{2}\left(|2\rangle\langle 2| - |1\rangle\langle 1|\right) - dE_0(y,x)\cos(k_L z)\cos(\omega_L t)\left(|1\rangle\langle 2| + |2\rangle\langle 1|\right)\right]U_G^\dagger \\ &+ -\hbar\frac{\omega_L}{2}\left(|2\rangle\langle 2| - |1\rangle\langle 1|\right) \end{aligned} \tag{17}$$

using our results from (a) gives then

$$H' = \hbar\frac{\omega_a - \omega_L}{2}|2\rangle\langle 2| - \hbar\frac{\omega_a - \omega_L}{2}|1\rangle\langle 1| - dE_0(x,y)\cos(k_L z)\cos(\omega_L t)\left(e^{-i\omega_L t}|1\rangle\langle 2| + e^{i\omega_L t}|2\rangle\langle 1|\right) \tag{18}$$

in the $\{|1\rangle, |2\rangle\}$ basis, this has the matrix form:

$$H' = \begin{pmatrix} \frac{\hbar(\omega_a - \omega_L)}{2} & -dE_0(x,y)\cos(k_L z)e^{-i\omega_L t} \\ -dE_0(x,y)\cos(k_L z)\cos(\omega_L t)e^{-i\omega_L t} & -\frac{\hbar(\omega_a - \omega_L)}{2} \end{pmatrix} \tag{19}$$

(c) Make the rotating wave approximation (RWA) by henceforth neglecting the oscillating terms in $H'(t)$. How should we then define Δ and $\Omega = \Omega(x,y,z)$ in order to map H' onto the Rabi model?

Dropping the rotating terms gives

$$H' = \begin{pmatrix} \frac{\hbar(\omega_a - \omega_L)}{2} & -\frac{1}{2}dE_0(x,y)\cos(k_L z) \\ -\frac{1}{2}dE_0(x,y)\cos(k_L z) & -\frac{\hbar(\omega_a - \omega_L)}{2} \end{pmatrix} \tag{20}$$

with the definitions $\Delta = \omega_a - \omega_L$ and $\hbar\Omega(x,y,z) = -dE_0(x,y)\cos(k_L z)$, this becomes

$$H' = \frac{\hbar}{2}\begin{pmatrix} \Delta & \Omega(x,y,z) \\ \Omega(x,y,z) & -\Delta \end{pmatrix} \tag{21}$$

which therefore maps the problem onto the Rabi Model.

(d) The matrix elements of H' depend on the atom's position $\vec{r} = (x, y, z)$, hence we can say $H' = H'(x, y, z)$. We can therefore refer to the eigenstates of $H'(x, y, z)$ as $|g'(x, y, z)\rangle$ and $|e'(x, y, z)\rangle$, and the eigenvalues as ω'_g and ω'_e. Use your results from problem 4.1 to write expressions for $\omega'_g(x, y, z)$, $\omega'_e(x, y, z)$, and expand $|g'(x, y, z)\rangle$ and $|e'(x, y, z)\rangle$ onto the basis $\{|1\rangle, |2\rangle\}$.

We have

$$\omega'_g(x,y,z) = -\frac{1}{2}\sqrt{\Delta^2 + \Omega^2(x,y,z)} \tag{22}$$

$$\omega'_e(x,y,z) = \frac{1}{2}\sqrt{\Delta^2 + \Omega^2(x,y,z)} \tag{23}$$

for $\Delta > 0$ we have

$$|g'(x,y,z)\rangle = \frac{(\Delta + \sqrt{\Delta^2 + \Omega^2(x,y,z)})|1\rangle - \Omega(x,y,z)|2\rangle}{\sqrt{(\Delta + \sqrt{\Delta^2 + \Omega^2(x,y,z)})^2 + \Omega^2(x,y,z)}} \tag{24}$$

$$|e'(x,y,z)\rangle = \frac{\Omega(x,y,z)|1\rangle + (\Delta + \sqrt{\Delta^2 + \Omega^2(x,y,z)})|2\rangle}{\sqrt{(\Delta + \sqrt{\Delta^2 + \Omega^2(x,y,z)})^2 + \Omega^2(x,y,z)}} \tag{25}$$

while for $\Delta < 0$ we have

$$|g'(x,y,z)\rangle = \frac{-\Omega(x,y,z)|1\rangle + (|\Delta| + \sqrt{\Delta^2 + \Omega^2(x,y,z)})|2\rangle}{\sqrt{(|\Delta| + \sqrt{\Delta^2 + \Omega^2(x,y,z)})^2 + \Omega^2(x,y,z)}} \tag{26}$$

$$|e'(x,y,z)\rangle = \frac{(|\Delta| + \sqrt{\Delta^2 + \Omega^2(x,y,z)})|1\rangle + \Omega(x,y,z)||2\rangle}{\sqrt{(|\Delta| + \sqrt{\Delta^2 + \Omega^2(x,y,z)})^2 + \Omega^2(x,y,z)}} \tag{27}$$

(e) Assume that the atom starts out at coordinates $\vec{r}_0 = (-x_0, 0, 0)$, where $|x_0| \gg W$ (i.e. outside of the beam region). Take as the initial velocity of the atom $\vec{v}_0 = (v_0, 0, 0)$, and as the initial internal state, $|1\rangle$. Show that in the limit $x_0 \to \infty$, this state corresponds to the state $|g'(-x_0, 0, 0)\rangle$ for $\Delta > 0$. What state does it correspond to for $\Delta < 0$?

We have $\Delta \neq 0$ but $\Omega(-\infty, 0, 0) \to 0$. For $\Delta > 0$, the state $|g'(-\infty, 0, 0)\rangle \to |1\rangle$, so the atom is initially in state $|g'\rangle$.
For negative detuning, $\Delta < 0$, the state $|e'(-\infty, 0, 0)\rangle = |1\rangle$, so in this case, the atom would be initially in state $|e'\rangle$.

(f) What is the minimum possible gap frequency $\omega_{gap}(x,y,z) := \omega'_e(x,y,z) - \omega'_g(x,y,z)$ that the atom would encounter it were to continue traveling along its initial trajectory? Expand ω_{gap} in powers of $\Omega(x,y,z)/\Delta$, and keep only the leading term. Then, use this to derive the condition on the initial velocity, v_0, for the atom to adiabatically follow $|g'(x,y,z)\rangle$ or $|e'(x,y,z)\rangle$ as it continues along its trajectory, again assuming uniform motion. (Hint: the answer should depend on v_0, W, and Δ only). To put in some real numbers, take $W = 10^{-3}$m and $\Delta = 1$GHz, and compute the velocity at which adiabatic following breaks down. Assuming an atomic mass of 10^{-25}kg, at what temperature would adiabatic following break down?

The minimum gap energy is $\hbar|\Delta|$, which occurs at the beginning of its motion. As it moves into the region where Ω becomes non-zero, the gap is always greater than $\hbar|\Delta|$.
We have

$$\begin{aligned}\omega_{gap}(x,y,z) &= \sqrt{\Delta^2 + \Omega^2(x,y,z)} \\ &= |\Delta|\sqrt{1 + \frac{\Omega^2(x,y,z)}{\Delta^2}} \\ &= |\Delta|\left(1 + \frac{\Omega^2(x,y,z)}{2\Delta^2} + \dots\right) \\ &\approx |\Delta| + \frac{\Omega^2(x,y,z)}{2|\Delta|}\end{aligned} \tag{28}$$

The adiabaticity condition is $T \gg \hbar/\min(E_{gap})$ which gives $T \gg 1/|\Delta|$.
The length scale over which the field changes is W, so we must have $v_0 T \sim W$, which gives $v_0 \sim W/T$ so that adiabaticity requires $v_0 \ll W|\Delta|$.
For $W = 10^{-3}$m and $\Delta = 10^9\text{s}^{-1}$, this gives $v_0 \ll 10^6\,\text{m}\,\text{s}^{-1}$.
With $\frac{1}{2}Mv^2 = k_B T$, we have $T = \frac{Mv^2}{2k_B}$. Taking $M = 10^{-25}$kg and $k_B = 10^{-23}\text{J}\,\text{K}^{-1}$, gives a temperature of $T = 10^{10}$K. The point being that atoms will never move this fast outside of a particle accelerator.

(g) Compute the mean internal energy of an atom in state $|g'(x,y,z)\rangle$, defined as $\langle g'(x,y,z)|H|g'(x,y,z)\rangle$, and time-average any oscillating terms. Based on this result, give a reasonable argument as to why the atom should be repelled by the laser field for negative Δ, and attracted by the laser field for positive Δ (Hint: Potential Energy is defined as any energy which depends on position).

Following the problem as worded, we find that after time-averaging, we have

$$\langle g'|H|g'\rangle = \frac{\hbar\omega_a}{2}\left[\langle g'|2\rangle\langle 2|g'\rangle - \langle g'|1\rangle\langle 1|g'\rangle\right] \tag{29}$$

This gives for $\Delta > 0$

$$\langle g'|H|g'\rangle = 1 + \frac{2\Omega^2(\vec{r})}{2\Delta^2 + 2\Omega^2(\vec{r}) + 2|\Delta|\sqrt{\Delta^2 + \Omega^2(\vec{r})}} \tag{30}$$

while for $\Delta < 0$ this gives

$$\langle g'|H|g'\rangle = -1 - \frac{2\Omega^2(\vec{r})}{2\Delta^2 + 2\Omega^2(\vec{r}) + 2|\Delta|\sqrt{\Delta^2 + \Omega^2(\vec{r})}} \tag{31}$$

3. Use the fact that $\langle x|P|\psi\rangle = -i\hbar \frac{d}{dx}\langle x|\psi\rangle$ for any x and any state $|\psi\rangle$, to show that

$$[P, F(X)] = -i\hbar F'(X)$$

where $F(x)$ is an arbitrary function, and $F'(x) = \frac{dF(x)}{dx}$.

We start by evaluating $\langle x|\,[P, F(X)]\,|\psi\rangle$, which gives

$$\begin{aligned}
\langle x|\,[P, F(X)]\,|\psi\rangle &= \langle x|PF(X)|\psi\rangle - \langle x|F(X)P|\psi\rangle \\
&= -i\hbar\frac{d}{dx}\langle x|F(X)|\psi\rangle - F(x)\langle x|P|\psi\rangle \\
&= -i\hbar\frac{d}{dx}F(x)\psi(x) + i\hbar F(x)\frac{d}{dx}\psi(x) \\
&= -i\hbar F(x)\frac{d}{dx}\psi(x) - i\hbar\psi(x)\frac{d}{dx}F(x) + i\hbar F(x)\frac{d}{dx}\psi(x) \\
&= -i\hbar\psi(x)F'(x) \\
&= -i\hbar\langle x|F'(X)|\psi\rangle
\end{aligned} \tag{32}$$

Since this is true for any x and any $|\psi\rangle$, it follows that

$$[P, F(X)] = -i\hbar F'(X) \tag{33}$$

4. For a free-particle, we have

$$\langle x|\psi(t)\rangle = \int dp\, \langle x|p\rangle e^{-i\frac{p^2}{2m\hbar}t}\langle p|\psi(0)\rangle.$$

For an initial Gaussian wavepacket,

$$\langle x|\psi(0)\rangle = \left[\pi\sigma_0^2\right]^{-1/4} e^{-\frac{(x-x_0)^2}{2\sigma_0^2}},$$

use the formula

$$\int_{-\infty}^{\infty} dy\, e^{-ay^2+by} = \int_{-\infty}^{\infty} dy\, e^{-a\left(y-2\frac{b}{2a}+\frac{b^2}{4a^2}\right)+\frac{b^2}{4a}} = e^{\frac{b^2}{4a}}\int_{-\infty}^{\infty} dy\, e^{-a\left(y-\frac{b}{2a}\right)^2} = e^{\frac{b^2}{4a}}\int_{-\infty}^{\infty} du\, e^{-au^2} = \sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}}$$

to first compute $\langle p|\psi(0)\rangle$. Then use the same formula to do the final p-integration and obtain an analytic expression for $\langle x|\psi(t)\rangle$.

Lastly, compute $|\langle x|\psi(t)\rangle|^2$, and show that the probability distribution remains a gaussian, whose center moves as a classical free-particle with initial position, x_0, and initial momentum p_0. Give an expression for the width of this gaussian as a function of time.

Compute first $\langle p|\psi(0)\rangle$

$$\begin{aligned}
\langle p|\psi(0)\rangle &= \int dx\, \langle p|x\rangle\langle x|\psi(0)\rangle \\
&= \frac{\left[\pi\sigma_0^2\right]^{-1/4}}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, e^{-\frac{(x-x_0)^2}{2\sigma_0^2}-ipx/\hbar} \\
&= \frac{\left[\pi\sigma_0^2\right]^{-1/4}}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2\sigma_0^2}-ip(x+x_0)/\hbar} \\
&= \frac{\left[\pi\sigma_0^2\right]^{-1/4}}{\sqrt{2\pi\hbar}} e^{-ipx_0/\hbar}\sqrt{2\pi\sigma_0^2}e^{-\frac{p^2\sigma_0^2}{2\hbar^2}} \\
&= \frac{\sqrt{\sigma_0}}{\sqrt{\hbar}\sqrt[4]{\pi}} e^{-\frac{p^2\sigma_0^2}{2\hbar^2}} e^{-ipx_0/\hbar}
\end{aligned} \tag{34}$$

we can then compute the wave-function at later times

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2\pi\hbar}}\frac{\sqrt{\sigma_0}}{\sqrt{\hbar}\sqrt[4]{\pi}}\int_{-\infty}^{\infty} dp\, e^{ip(x-x_0)/\hbar}e^{-i\frac{p^2}{2m\hbar}t}e^{-\frac{p^2\sigma_0^2}{2\hbar^2}} \tag{35}$$

so we have

$$a = \frac{\sigma_0^2}{2\hbar^2} + i\frac{t}{2m\hbar} \tag{36}$$

and

$$b = i(x-x_0)/\hbar \tag{37}$$

which gives

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt[4]{\pi}\sqrt{\sigma_0 + i\frac{\hbar t}{m\sigma_0}}} e^{-\frac{(x-x_0)^2}{2\sigma_0^2\left(1+i\frac{\hbar t}{m\sigma_0^2}\right)}} \tag{38}$$

taking the absolute value squared gives

$$|\langle x|\psi(t)\rangle|^2 = \frac{1}{\sqrt{\pi}\sigma_0\sqrt{1+\frac{\hbar^2 t^2}{m^2\sigma_0^4}}} e^{\frac{(x-x_0)^2}{\sigma_0^2\left(1+\frac{\hbar^2 t^2}{m^2\sigma_0^4}\right)}} \tag{39}$$

The center is at rest, which is correct for a free particle with $p_0 = 0$. The width as a function of time is

$$\sigma(t) = \sigma_0\sqrt{1+\left(\frac{\hbar t}{m\sigma_0^2}\right)} \tag{40}$$