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 $[H(t), G(t)] \neq 0$)

   (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 $G(t)$.

   (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 $[H, G] = 0$?

   (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?

   (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 $|\psi'(0)\rangle$.

   (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 $|\psi(0)\rangle$.

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 $|2'\rangle := U_G(t)|2\rangle$.

(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?

(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?

(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 $\{|1\rangle, |2\rangle\}$.

(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 $\Delta < 0$?

(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?

(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).

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 $F'(x) = \frac{dF(x)}{dx}$.

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.