

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

$$|\dot{\psi}'\rangle = \dot{U}_G|\psi\rangle + U_G|\dot{\psi}\rangle \quad (1)$$

$$= \dot{U}_G|\psi\rangle - \frac{i}{\hbar}U_G H|\psi\rangle \quad (2)$$

- (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 $G(t)$.

$$\frac{d}{dt}|\psi'\rangle = \dot{U}_G U_G^\dagger (U_G|\psi\rangle) - \frac{i}{\hbar}U_G H U_G^\dagger (U_G|\psi\rangle) \quad (3)$$

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

Thus we see that

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

- (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

$$H' = U_G H U_G^\dagger \quad (6)$$

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

$$H' = U_G H U_G^\dagger = H U_G U_G^\dagger = H \quad (7)$$

(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

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

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

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

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

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

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

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

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

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

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

$$G^n|2\rangle = (\omega_L t/2)^n|2\rangle \quad (12)$$

and

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

this leads to

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

and similarly we find

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

- (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

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

so that

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

using our results from (a) gives then

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

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

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

- (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

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

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

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

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

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

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

for $\Delta > 0$ we have

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

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

while for $\Delta < 0$ we have

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

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

- (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 $x_0 \rightarrow \infty$, 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 $\Omega(-\infty, 0, 0) \rightarrow 0$. For $\Delta > 0$, the state $|g'(-\infty, 0, 0)\rangle \rightarrow |1\rangle$, 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 if 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 $W = 10^{-3}\text{m}$ and $\Delta = 1\text{GHz}$, 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 $W = 10^{-3}\text{m}$ and $\Delta = 10^9\text{s}^{-1}$, this gives $v_0 \ll 10^6\text{m s}^{-1}$.

With $\frac{1}{2}Mv^2 = k_B T$, we have $T = \frac{Mv^2}{2k_B}$. Taking $M = 10^{-25}\text{kg}$ and $k_B = 10^{-23}\text{J K}^{-1}$, gives a temperature of $T = 10^{10}\text{K}$. 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

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

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,

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

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

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

we can then compute the wave-function at later times

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

so we have

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

and

$$b = i(x-x_0)/\hbar \quad (37)$$

which gives

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

taking the absolute value squared gives

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

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

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