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 $|\psi'(t)⟩ = U_G|\psi(t)⟩$, where $|\psi(t)⟩$ is the original state-vector, and $|\psi'(t)⟩$ 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 $|\psi'(t)⟩$.

(a) Begin by differentiating both sides of the equation $|\psi'(t)⟩ = U_G|\psi(t)⟩$ with respect to time. Use Schrödinger’s equation to eliminate $\frac{d}{dt}|\psi(t)⟩$.

(Tip: keep in mind that in general $[H(t), G(t)] \neq 0$)

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

$$= \dot{U}_G|\psi⟩ - \frac{i}{\hbar}U_GH|\psi⟩ \quad (2)$$

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

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

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 $G(t)$.

$$\frac{d}{dt}|\psi'⟩ = \dot{U}_GU_G^\dagger (U_G|\psi⟩) - \frac{i}{\hbar}U_GHU_G^\dagger (U_G|\psi⟩) \quad (3)$$

$$= -\frac{i}{\hbar} \left[ U_GHU_G^\dagger + i\hbar \dot{U}_GU_G^\dagger \right]|\psi'⟩ \quad (4)$$

Thus we see that

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

(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

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

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

$$H' = U_GHU_G^\dagger = HU_GU_G^\dagger = H \quad (7)$$
(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

\[
|\psi'\rangle = -\frac{i}{\hbar} H'|\psi'\rangle
\]

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

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

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

\[
|\psi(t)\rangle = \sum_n U_G^\dagger |\omega_n\rangle e^{-i\omega_n t} \langle \omega'_n |U_G|\psi(0)\rangle
\]
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 \( \omega_a \) 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 \( \omega_L \) 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 \( E_0(x, y) = E_0 \exp\left(-\frac{x^2 + y^2}{W^2}\right) \), where \( W \) is the transverse dimension of the beam.

(a) Consider a Unitary transformation generated by the Hermitian operator \( G = \frac{\omega_L t}{2} (|2\rangle \langle 2| - |1\rangle \langle 1|) \). 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

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

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

\[ G^n|2\rangle = (\omega_L t/2)^n|2\rangle \] (12)

and

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

this leads to

\[ |1'\rangle = U_G(t)|1\rangle = \left[I + iG - \frac{i}{2}G^2 - \frac{1}{6}G^3 + \ldots\right]|1\rangle \]

\[ = I + i\left(-\omega_L t/2\right) - \frac{i}{2}\left(-\omega_L t/2\right)^2 - \frac{1}{6}\left(-\omega_L t/2\right)^3 + \ldots\]|1\rangle \]

\[ = e^{-i\omega_L t/2}|1\rangle \] (14)

and similarly we find

\[ |2'\rangle = e^{i\omega_L t/2}|2\rangle \] (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
\[ G = \frac{\omega}{2} (|2\rangle \langle 2| - |1\rangle \langle 1|) t. \]
What are the matrix elements of $H'$ in the \{\[1\rangle, |2\rangle\} basis?

First we compute
\[ \dot{U}_G = i \frac{\omega}{2} (|2\rangle \langle 2| - |1\rangle \langle 1|) U_G \]
so that
\[ H' = U_G \left[ \frac{\hbar \omega}{2} (|2\rangle \langle 2| - |1\rangle \langle 1|) - dE_0(y,x) \cos(k_L z) \cos(\omega_L t) (|1\rangle \langle 2| + |2\rangle \langle 1|) \right] U_G^\dagger \]
\[ + \ - \frac{\hbar \omega}{2} (|2\rangle \langle 2| - |1\rangle \langle 1|) \]
using our results from (a) gives then
\[ H' = \frac{\hbar (\omega - \omega_L)}{2} |2\rangle \langle 2| - \frac{\hbar (\omega - \omega_L)}{2} |1\rangle \langle 1| - dE_0(x,y) \cos(k_L z) \cos(\omega_L t) (e^{-i\omega_L t} |1\rangle \langle 2| + e^{i\omega_L t} |2\rangle \langle 1|) \]
in the \{\[1\rangle, |2\rangle\} basis, this has the matrix form:
\[ H' = \begin{pmatrix}
\frac{\hbar (\omega - \omega_L)}{2} & -dE_0(x,y) \cos(k_L z) e^{-i\omega_L t} \\
-dE_0(x,y) \cos(k_L z) e^{-i\omega_L t} & -\frac{\hbar (\omega - \omega_L)}{2}
\end{pmatrix} \]
(c) Make the rotating wave approximation (RWA) by henceforth neglecting the oscillating terms in $H'(t)$. How should we then define $\Delta$ and $\Omega = \Omega(x, y, z)$ in order to map $H'$ onto the Rabi model?

Dropping the rotating terms gives
\[ H' = \begin{pmatrix}
\frac{\hbar (\omega - \omega_L)}{2} & -\frac{1}{2} dE_0(x,y) \cos(k_L z) \\
-\frac{1}{2} dE_0(x,y) \cos(k_L z) & -\frac{\hbar (\omega - \omega_L)}{2}
\end{pmatrix} \]
with the definitions $\Delta = \omega - \omega_L$ and $\hbar \Omega(x,y,z) = -dE_0(x,y) \cos(k_L z)$, this becomes
\[ H' = \frac{\hbar}{2} \begin{pmatrix}
\Delta & \Omega(x,y,z) \\
\Omega(x,y,z) & -\Delta
\end{pmatrix} \]
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 $\omega_g'$ and $\omega_e'$. 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

$$\omega_g'(x, y, z) = -\frac{1}{2}\sqrt{\Delta^2 + \Omega^2(x, y, z)}$$  \hspace{1cm} (22)$$
$$\omega_e'(x, y, z) = \frac{1}{2}\sqrt{\Delta^2 + \Omega^2(x, y, z)}$$  \hspace{1cm} (23)$$

for $\Delta > 0$ we have

$$|g'(x, y, z)\rangle = \frac{(\Delta + \sqrt{\Delta^2 + \Omega^2(x, y, z)})|1\rangle - \Omega(x, y, z)|2\rangle}{\sqrt{(\Delta + \sqrt{\Delta^2 + \Omega^2(x, y, z)})^2 + \Omega^2(x, y, z)}}$$  \hspace{1cm} (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)}}$$  \hspace{1cm} (25)$$

while for $\Delta < 0$ we have

$$|g'(x, y, z)\rangle = \frac{-\Omega(x, y, z)|1\rangle + (|\Delta| + \sqrt{|\Delta|^2 + \Omega^2(x, y, z)})|2\rangle}{\sqrt{(|\Delta| + \sqrt{|\Delta|^2 + \Omega^2(x, y, z)})^2 + \Omega^2(x, y, z)}}$$  \hspace{1cm} (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)}}$$  \hspace{1cm} (27)$$

(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 $|e'\rangle$. 

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(f) What is the minimum possible gap frequency $\omega_{gap}(x, y, z) := \omega'_g(x, y, z) - \omega'_e(x, y, z)$ that the atom would encounter it were to continue traveling along its initial trajectory? Expand $\omega_{gap}$ 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 $\Delta$ 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 $10^{-25}\text{kg}$, 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 $\Omega$ becomes non-zero, the gap is always greater than $\hbar|\Delta|$. We have

$$\omega_{gap}(x, y, z) = \sqrt{\Delta^2 + \Omega^2(x, y, z)}$$

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

$$= |\Delta|\left(1 + \frac{\Omega^2(x, y, z)}{2\Delta^2} + \ldots\right)$$

$$\approx |\Delta| + \frac{\Omega^2(x, y, z)}{2|\Delta|} \quad (28)$$

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 $v_0T \sim W$, 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 $v_0 \ll 10^6\text{m/s}$.

With $\frac{1}{2}Mv^2 = k_BT$, we have $T = \frac{Mv^2}{2k_B}$. Taking $M = 10^{-25}\text{kg}$ and $k_B = 10^{-23}\text{J/K}$, 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 $\Delta$, and attracted by the laser field for positive $\Delta$ (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

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

This gives for $\Delta > 0$

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

while for $\Delta < 0$ this gives

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

\[
\langle x|[P, F(X)]|\psi \rangle = \langle x|PF(X)|\psi \rangle - \langle x|F(X)P|\psi \rangle
\]

\[
= -i\hbar \frac{d}{dx} \langle x|F(X)|\psi \rangle - F(x) \langle x|P|\psi \rangle
\]

\[
= -i\hbar \frac{d}{dx} F(x)\psi(x) + i\hbar F(x) \frac{d}{dx} \psi(x)
\]

\[
= -i\hbar F(x) \frac{d}{dx} \psi(x) - i\hbar \psi(x) \frac{d}{dx} F(x) + i\hbar F(x) \frac{d}{dx} \psi(x)
\]

\[
= -i\hbar \psi(x) F'(x)
\]

\[
= -i\hbar \langle x|F'(X)|\psi \rangle
\]

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

\[
[P, F(X)] = -i\hbar F'(X)
\]
4. For a free-particle, we have

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

For an initial Gaussian wavepacket,

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

use the formula

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

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

\[
\langle p | \psi(0) \rangle = \int dx \langle p | x \rangle \langle x | \psi(0) \rangle \\
= \left[ \frac{\pi \sigma_0^2}{2} \right]^{-1/4} \int_{-\infty}^{\infty} dx \ e^{-\frac{(x-x_0)^2}{2\sigma_0^2}} e^{-i px/\hbar} \\
= \left[ \frac{\pi \sigma_0^2}{2} \right]^{-1/4} \int_{-\infty}^{\infty} dx \ e^{-\frac{x^2}{2\sigma_0^2}} e^{-i p(x-x_0)/\hbar} \\
= \left[ \frac{\pi \sigma_0^2}{2} \right]^{-1/4} \frac{\sqrt{\pi}}{\sqrt{2\pi \sigma_0^2}} e^{\frac{p^2 \sigma_0^2}{2\hbar^2}} e^{-i px_0/\hbar} \\
= \frac{\sqrt{\sigma_0}}{\sqrt{2\pi \sqrt{\pi}}} e^{\frac{p^2 \sigma_0^2}{2\hbar^2}} e^{-i px_0/\hbar} \\
\]  

(34)

we can then compute the wave-function at later times

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

(35)

so we have

\[
a = \frac{\sigma_0^2}{2\hbar^2} + \frac{t}{2m\hbar} \\
\]  

(36)

and

\[
b = i(x - x_0)/\hbar \\
\]  

(37)

which gives

\[
\langle x | \psi(t) \rangle = \frac{1}{\sqrt{\pi}} \frac{e^{-\frac{(x-x_0)^2}{2\sigma_0^2}}}{\sqrt{\sigma_0 + \frac{\hbar t}{m \sigma_0}}} \\
\]  

(38)
taking the absolute value squared gives

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

(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

\[ \sigma(t) = \sigma_0 \sqrt{1 + \left(\frac{\hbar t}{m\sigma_0^2}\right)} \]  

(40)