1. (Quantum Mechanics)

Consider two particles of masses $m_{1,2}$ in a one-dimensional harmonic oscillator potential $V = \frac{1}{2}m_1\omega_1^2 x_1^2 + \frac{1}{2}m_2\omega_2^2 x_2^2$. In the far past, the x_1-oscillator is in the ground state while the x_2-oscillator is in its first excited state. They then experience a perturbation $\Delta V(x_1, x_2, t) = \lambda(x_1 - x_2)^2 e^{-\frac{1}{2}\alpha^2 t^2}$. Compute, to lowest nontrivial order in λ, the probability that in the far future the x_1-oscillator is in the first excited state while the x_2-oscillator is in its ground state.

Solution: *Solution by Jonah Hyman (jthyman@g.ucla.edu)*

This problem combines the quantum harmonic oscillator with time-dependent perturbation theory. Both are extremely common comp topics. A short review of each follows.

Quantum harmonic oscillator:

The Hamiltonian for a harmonic oscillator centered at the origin, with mass m and natural frequency ω, is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{1}$$

We can rescale p and x into the dimensionless coordinates P and X, which simplifies the Hamiltonian considerably:

$$H = \frac{1}{2}\hbar\omega(P^2 + X^2) \quad \text{with } P \equiv \frac{p}{(m\omega\hbar)^{1/2}} \text{ and } X \equiv \left(\frac{m\omega}{\hbar}\right)^{1/2} x \tag{2}$$

From these dimensionless coordinates, we can write the raising and lowering operators:

$$\text{Lowering operator:} \quad a \equiv \frac{X + iP}{\sqrt{2}} \tag{3}$$

$$\text{Raising operator:} \quad a^\dagger \equiv \frac{X - iP}{\sqrt{2}} \tag{4}$$

We can then derive the canonical quantization relations of the raising and lowering operators, and we can rewrite the Hamiltonian in terms of them:

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \quad \text{with } [a, a^\dagger] = 1 \tag{5}$$

We may also write X and P in terms of a and $a^\dagger$:

$$X = \frac{a + a^\dagger}{\sqrt{2}} \quad \text{and} \quad P = \frac{a - a^\dagger}{\sqrt{2}i} \tag{6}$$

There is a ladder of energy eigenstates $\{|n\rangle\}_{n=0}^{\infty}$, where

$$H|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle \tag{7}$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle \tag{8}$$

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{9}$$

Time-dependent perturbation theory:

The key to deriving the formulas for time-dependent perturbation theory is to work in the interaction picture. For an unperturbed, time-independent Hamiltonian H_0 added to a time-dependent perturbation $V(t)$,

$$H(t) = H_0 + V(t) \tag{10}$$

we write the interaction picture by folding the time-evolution of each state under H_0 into the quantum operators. If $\mathcal{O}_S$ is an operator in the (typical) Schrödinger picture, the equivalent operator $\mathcal{O}_I$ in the interaction picture is defined by

$$\mathcal{O}_I(t) \equiv e^{iH_0 t/\hbar}\,\mathcal{O}_S\,e^{-iH_0 t/\hbar} \tag{11}$$

To make sure that the expectation value $\langle\psi|\mathcal{O}|\psi\rangle$ is the same in both pictures, we must change the state $|\psi\rangle$ accordingly. If $|\psi_S(t)\rangle$ is a time-evolved ket in the Schrödinger picture, the equivalent ket $|\psi_I(t)\rangle$ in the interaction picture is defined by

$$|\psi_I(t)\rangle \equiv e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle \tag{12}$$

Kets in the interaction picture obey the Schrödinger equation for the perturbation Hamiltonian $V_I(t)$ in the interaction picture:

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = V_I(t)\,|\psi_I(t)\rangle \tag{13}$$

We can integrate this equation (applying the initial condition for the state ψ at a reference time t_0) to get

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,V_I(t')\,|\psi_I(t')\rangle \tag{14}$$

To lowest order in perturbation theory, $|\psi_I(t')\rangle \approx |\psi_I(t_0)\rangle$, so this equation becomes

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,V_I(t')\,|\psi_I(t_0)\rangle \quad \text{to lowest order} \tag{15}$$

Now suppose that at $t = t_0$, the system is in an eigenstate $|n\rangle$ of H_0, and we are interested in the transition amplitude to another eigenstate $|m\rangle$. We can then take the inner product of (15) with $\langle m|$:

$$\begin{aligned}\langle m|\psi_I(t)\rangle &= \langle m|n\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ \langle m|V_I(t')|n\rangle \\ &= \delta_{mn} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,e^{i(E_m-E_n)t'/\hbar}\,\langle m|V_S(t')|n\rangle \quad \text{to lowest order}\end{aligned} \tag{16}$$

In the second line, we have applied the definition of an operator in the interaction picture (11). Since $\langle m|\psi_I(t)\rangle = e^{-iE_m t/\hbar}\,\langle m|\psi_S(t)\rangle$ by (12), this is what we need to calculate transition probabilities.

With all this in mind, here is how you solve the problem. The unperturbed Hamiltonian is a sum of two harmonic oscillator Hamiltonians

$$H_0 = \frac{p_1^2}{2m_1} + \frac{1}{2}m_1\omega_1^2 x_1^2 + \frac{p_2^2}{2m_2} + \frac{1}{2}m_2\omega_2^2 x_2^2 \tag{17}$$

Let $|n_1, n_2\rangle$ be the eigenstate associated with the n_1 eigenstate of the first oscillator and the n_2 eigenstate of the second oscillator. The problem tells us that "in the far past, the x_1-oscillator is in the ground state while the x_2-oscillator is in its first excited state." This means that $|\psi(-\infty)\rangle = |0, 1\rangle$.

We are interested in "the probability that in the far future the x_1-oscillator is in the first excited state while the x_2-oscillator is in its ground state." This means that we want to find $\langle 1, 0|\psi(+\infty)\rangle$.

(We are being slightly vague about whether we are in the Schrödinger picture or the interaction picture. We also haven't mentioned when the two pictures are set to coincide. The reason for this is because the difference between $\langle 1, 0|\psi_S(t)\rangle$ and $\langle 1, 0|\psi_I(t)\rangle$ is some phase factor $e^{-iE_{(1,0)}(t-t_0)/\hbar}$, and such factors don't change transition probabilities.)

Equation (16) tells us how to start:

For all time-dependent perturbation theory problems, start by calculating the matrix elements of the perturbation Hamiltonian between initial and final states.

In this case, that means we need to calculate $\langle 1, 0|\Delta V|0, 1\rangle$, where ΔV is the perturbation Hamiltonian

$$\Delta V(x_1, x_2, t) \equiv f(t)(x_1 - x_2)^2 \quad \text{for } f(t) \equiv \lambda e^{-\frac{1}{2}\alpha^2 t^2} \tag{18}$$

Notice that we are pulling out all non-operator constants, even the time-dependent ones, in order to focus on the operators that contribute to the matrix element. The next step is to expand ΔV in its terms, bearing in mind that the operators x_1 and x_2 commute with one another:

$$\Delta V(x_1, x_2, t) = f(t)\left(x_1^2 + x_2^2 - 2x_1x_2\right) \tag{19}$$

The next step is to write x_1 and x_2 in terms of raising and lowering operators. But before doing this, note the following time-saving fact (which comes from (6)):

For a harmonic oscillator, the operators x and p either raise an energy eigenstate exactly once or lower an energy eigenstate exactly once.

In other words, x_1 moves us exactly one step (up or down) on the x_1-oscillator ladder of eigenstates, and x_2 moves us exactly one step on the x_2-oscillator ladder. We want to know the transition probability between $|0,1\rangle$ and $|1,0\rangle$, so we want to know about processes that move us one step up the x_1-ladder and one step down the x_2-ladder.

The first two terms in (19) cannot move us one step on both ladders: x_1^2 either moves us 2 steps up the x_1-ladder, moves us 2 steps down the x_1-ladder, or moves us nowhere. The same logic applies to x_2^2 and the x_2-ladder. So for the purposes of calculating $\langle 1,0|\Delta V|0,1\rangle$, we can ignore these terms and examine only the third term in (19):

$$\langle 1,0|\Delta V|0,1\rangle = -2f(t)\,\langle 1,0|x_1x_2|0,1\rangle \tag{20}$$

Now we can use (1) and (6) to write this equation in terms of raising and lowering operators for each oscillator:

$$\begin{aligned}
\langle 1,0|\Delta V|0,1\rangle &= -2f(t)\left(\frac{\hbar}{m_1\omega_1}\right)^{1/2}\left(\frac{\hbar}{m_2\omega_2}\right)^{1/2}\langle 1,0|X_1X_2|0,1\rangle \\
&= -2f(t)\left(\frac{\hbar}{m_1\omega_1}\right)^{1/2}\left(\frac{\hbar}{m_2\omega_2}\right)^{1/2}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\langle 1,0|(a_1+a_1^\dagger)(a_2+a_2^\dagger)|0,1\rangle \\
&= -f(t)\frac{\hbar}{(m_1\omega_1m_2\omega_2)^{1/2}}\langle 1,0|\Big(a_1a_2 + a_1^\dagger a_2^\dagger + a_1a_2^\dagger + a_1^\dagger a_2\Big)|0,1\rangle
\end{aligned} \tag{21}$$

Again, we are only interested in processes that moves us one step up the x_1-ladder and one step down the x_2-ladder. Only the last term in the matrix element ($a_1^\dagger a_2$) does this, so we can ignore the other three:

$$\langle 1,0|\Delta V|0,1\rangle = -f(t)\frac{\hbar}{(m_1\omega_1m_2\omega_2)^{1/2}}\langle 1,0|a_1^\dagger a_2|0,1\rangle \tag{22}$$

By application of (8) and (9), we get that

$$\langle 1,0|a_1^\dagger a_2|0,1\rangle = \sqrt{1}\sqrt{1}\,\langle 1,0|1,0\rangle = 1 \tag{23}$$

so

$$\boxed{\langle 1,0|\Delta V|0,1\rangle = -f(t)\frac{\hbar}{(m_1\omega_1m_2\omega_2)^{1/2}} = -\lambda e^{-\frac{1}{2}\alpha^2t^2}\frac{\hbar}{(m_1\omega_1m_2\omega_2)^{1/2}}} \tag{24}$$

With this knowledge, we are ready to apply the first-order time-dependent perturbation theory formula (16).

$$\begin{aligned}
\langle 1,0|\psi_I(+\infty)\rangle &= \delta_{(1,0),(0,1)} - \frac{i}{\hbar}\int_{-\infty}^{+\infty} dt'\, e^{i(E_{(1,0)}-E_{(0,1)})t'/\hbar}\,\langle 1,0|\Delta V(t')|0,1\rangle \quad \text{to lowest order} \\
&= i\lambda\frac{1}{(m_1\omega_1m_2\omega_2)^{1/2}}\int_{-\infty}^{\infty} dt'\, e^{i(E_{(1,0)}-E_{(0,1)})t'/\hbar}e^{-\frac{1}{2}\alpha^2(t')^2}
\end{aligned} \tag{25}$$

In the second line, we used (24) to simplify $\langle 1,0|\Delta V(t')|0,1\rangle$. Here, we have the energy of an eigenstate (n_1, n_2) as the sum of the energies of each of the oscillators:

$$E_{(n_1,n_2)} = \hbar\omega_1\left(n_1 + \frac{1}{2}\right) + \hbar\omega_2\left(n_2 + \frac{1}{2}\right) \tag{26}$$

so

$$E_{(1,0)} - E_{(0,1)} = \left(\frac{3}{2}\hbar\omega_1 + \frac{1}{2}\hbar\omega_2\right) - \left(\frac{1}{2}\hbar\omega_1 + \frac{3}{2}\hbar\omega_2\right) = \hbar(\omega_1 - \omega_2) \tag{27}$$

We may simplify equation (25) with this information:

$$\langle 1,0|\psi_I(+\infty)\rangle = i\lambda\frac{1}{(m_1\omega_1 m_2\omega_2)^{1/2}}\int_{-\infty}^{\infty} dt'\, \exp\left(-\frac{1}{2}\alpha^2(t')^2 + i\omega_{12}t'\right) \quad \text{for} \quad \omega_{12} \equiv \omega_1 - \omega_2 \tag{28}$$

All that remains is to take the Gaussian integral. The starting point is completing the square in the exponential:

$$\begin{aligned}
-\frac{1}{2}\alpha^2(t')^2 + i\omega_{12}t' &= -\frac{1}{2}\alpha^2\left((t')^2 + 2\left(\frac{i\omega_{12}}{\alpha^2}\right)t'\right) \\
&= -\frac{1}{2}\alpha^2\left(\left(t' + \frac{i\omega_{12}}{\alpha^2}\right)^2 + \frac{\omega_{12}^2}{\alpha^4}\right) \\
&= -\frac{1}{2}\alpha^2\left(t' + \frac{i\omega_{12}}{\alpha^2}\right)^2 - \frac{\omega_{12}^2}{2\alpha^2}
\end{aligned} \tag{29}$$

Then, the integral in (28) simplifies to

$$\int_{-\infty}^{\infty} dt'\, \exp\left(-\frac{1}{2}\alpha^2(t')^2 + i\omega_{12}t'\right) = \exp\left(-\frac{\omega_{12}^2}{2\alpha^2}\right)\int_{-\infty}^{\infty} dt'\, \exp\left(-\frac{1}{2}\alpha^2\left(t' + \frac{i\omega_{12}}{\alpha^2}\right)^2\right)$$

Making the change of variables $u \equiv \left(\frac{1}{2}\alpha^2\right)^{1/2}\left(t' + \frac{i\omega_{12}}{\alpha^2}\right)$, we get that

$$\int_{-\infty}^{\infty} dt'\, \exp\left(-\frac{1}{2}\alpha^2(t')^2 + i\omega_{12}t'\right) = \exp\left(-\frac{\omega_{12}^2}{2\alpha^2}\right)\left(\frac{2}{\alpha^2}\right)^{1/2}\int_{-\infty}^{\infty} du\, e^{-u^2}$$

Using the known Gaussian integral $\int_{-\infty}^{\infty} du\, e^{-u^2} = \pi^{1/2}$, this gives us

$$\int_{-\infty}^{\infty} dt'\, \exp\left(-\frac{1}{2}\alpha^2(t')^2 + i\omega_{12}t'\right) = \frac{(2\pi)^{1/2}}{\alpha}\exp\left(-\frac{\omega_{12}^2}{2\alpha^2}\right) \tag{30}$$

Plugging into (28), we get that

$$\langle 1,0|\psi_I(+\infty)\rangle = i\lambda\frac{1}{\alpha}\left(\frac{2\pi}{m_1\omega_1 m_2\omega_2}\right)^{1/2}\exp\left(-\frac{\omega_{12}^2}{2\alpha^2}\right) \tag{31}$$

This is the transition *amplitude*; to get the transition *probability*, we must take the square root of its absolute value:

$$P_{(0,1)\to(1,0)} = |\langle 1,0|\psi_I(+\infty)\rangle|^2 = \frac{\lambda^2}{\alpha^2}\frac{2\pi}{m_1\omega_1 m_2\omega_2}\exp\left(-\frac{\omega_{12}^2}{\alpha^2}\right)$$

Recalling that $\omega_{12} \equiv \omega_1 - \omega_2$, we can write our final answer

$$\boxed{P_{(0,1)\to(1,0)} = \frac{\lambda^2}{\alpha^2}\frac{2\pi}{m_1\omega_1 m_2\omega_2}\exp\left(-\frac{(\omega_1 - \omega_2)^2}{\alpha^2}\right)} \tag{32}$$