1. **Double Quantum Wells**

This problem relates to some aspects of an optics experiment performed on a double quantum well structure. In the frequency range of interest, we can neglect all the excited states of the isolated quantum wells and restrict to one electronic level in each of the two quantum wells. We denote by $|1\rangle$ and $|2\rangle$ the above electron energy eigenstates in the isolated wells, with energy eigenvalues $E_1 \neq E_2$ respectively. Since an electron can tunnel between the two wells, the above states are not eigenstates of the double–well system. However, we assume that they form a basis $\{|1\rangle, |2\rangle\}$ that we then use to write down the matrix representing the Hamiltonian of the double–well system, whose off–diagonal matrix elements are proportional to the tunneling strength. The experiment measured the absorption spectrum of the above nanostructure for different values of an applied electric field F. To first approximation, this external field only changes the values of E_1 and E_2. For $F = 0, E_2 > E_1$. As F increases,$|E_2 - E_1|$ first decreases. For $F = F_R$, we have that $E_1 = E_2$, and for $F > F_R$ we have $E_2 < E_1$. The absorption spectrum as a function of photon energy ω can be calculated from the following equation:

$$\alpha(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} \langle 1|e^{-iHt/\hbar}|1\rangle \, dt$$

where $|1\rangle$ is the above single-well state. Using the above equation, calculate the absorption spectrum $\alpha(\omega)$ as a function of ω for $F = F_R$. Find the frequencies ω of the absorption spectrum peaks.

Solution.

a.) We begin this solution by first looking at the equation for our absorption spectra. First, we notice that we have an $e^{i\omega t}$ factor, which is the term which defines the function of the spectra as absorption energy. Next, we notice that we have the Hamiltonian of the full system, H, acting on the isolated well $|1\rangle$. This means that the absorption spectrum of this system is governed by the interaction of the coupled Hamiltonian and the isolated well $|1\rangle$. So far this hasn't helped us calculate anything, but it is important to make these distinctions to ensure we are understanding not only the problem but the physical process that is occurring.

First, we are told some information regarding the Hamiltonian of the full system, particularly the fact that we can form a basis with $\{|1\rangle, |2\rangle\}$, what the energy eigenvalues in the isolated wells are, and what the off diagonal components are. Using this, we can write the matrix representation of the coupled Hamiltonian as

$$H = \begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle \end{pmatrix} = \begin{pmatrix} E_1 & -\tau \\ -\tau^{\star} & E_2 \end{pmatrix}$$

Note, there could also be a phase component to accompany the off-diagonal component τ, but we have set the phase to zero to simplify this. Having the matrix written out as so, we can continue with our investigation. First, we note the problem tells us to only calculate the absorption spectra when $F = F_R$, which simplifies this greatly, as $E_1 = E_2 = E$ so we rewrite our Hamiltonian as

$$H = \begin{pmatrix} E & -\tau \\ -\tau^\star & E \end{pmatrix}$$

which we can directly solve for the eigenvalues using the characteristic equation, resulting in eigenvalues of

$$\lambda = E \pm |\tau|$$

where the absolute value signifies we are only taking the real portion of the tunneling coefficient. We can then solve for the eigenvectors, resulting in

$$\begin{aligned} \lambda = E - |\tau| :\ |-\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \\ \lambda = E + |\tau| :\ |+\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{aligned}$$

With this, we now know how the coupled Hamiltonian acts on our energy eigenkets $|+\rangle, |-\rangle$, but not on $|1\rangle$. We can approach this next part in a few ways, but if we write these energy eigenkets in terms of

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

we will then be able to expand in the energy basis with no issues. Using that approach, we write

$$\begin{aligned} |-\rangle &= \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \\ |+\rangle &= \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) \end{aligned}$$

Then, writing $|1\rangle$ in terms of the energy basis we have

$$|1\rangle = |+\rangle \langle +|1\rangle + |-\rangle \langle -|1\rangle$$

and then introducing our time evolution operator for the coupled system, we have

$$e^{-iHt/\hbar} |1\rangle = e^{-iHt/\hbar} |+\rangle \langle +|1\rangle + e^{-iHt/\hbar} |-\rangle \langle -|1\rangle$$

which with our already known energy eigenvalues for these energy eigenkets we then have

$$\begin{aligned} e^{-iHt/\hbar} |1\rangle &= e^{-i(E+|\tau|)t/\hbar} |+\rangle \langle +|1\rangle + e^{-i(E-|\tau|)t/\hbar} |-\rangle \langle -|1\rangle \\ &= e^{-iEt/\hbar} \left[e^{-i|\tau|t/\hbar} |+\rangle \langle +|1\rangle + e^{i|\tau|t/\hbar} |-\rangle \langle -|1\rangle \right] \end{aligned}$$

Now we plug in our energy eigenkets written in terms of $|1\rangle, |2\rangle$, which simply introduces a factor of $1/\sqrt{2}$ and simplify and we have

$$e^{-iHt/\hbar}|1\rangle = \frac{e^{-iEt/\hbar}}{\sqrt{2}}\left[e^{-i|\tau|t/\hbar}|+\rangle + e^{i|\tau|t/\hbar}|-\rangle\right]$$

We now return back to the full form of what we are trying to calculate,

$$\langle 1|e^{-iHt/\hbar}|1\rangle = \frac{e^{-iEt/\hbar}}{\sqrt{2}}\left[e^{-i|\tau|t/\hbar}\langle 1|+\rangle + e^{i|\tau|t/\hbar}\langle 1|-\rangle\right]$$

recognize the inner products are simply going to give us another factor of $1/\sqrt{2}$, and we then have

$$\langle 1|e^{-iHt/\hbar}|1\rangle = \frac{e^{-iEt/\hbar}}{2}\left[e^{-i|\tau|t/\hbar} + e^{i|\tau|t/\hbar}\right]$$

we should see quickly that we can simplify this with a cosine, to our expression now simply being

$$\langle 1|e^{-iHt/\hbar}|1\rangle = e^{-iEt/\hbar}\cos\left(\frac{|\tau|t}{\hbar}\right)$$

This representation doesn't help us with the integral though, so lets leave it in the second to last form, plug it back into the integral for our absorption spectra, and conbine the exponentials.

$$\begin{aligned}\alpha(\omega) &= \int_{-\infty}^{\infty} e^{i\omega t}\frac{e^{-iEt/\hbar}}{2}\left[e^{-i|\tau|t/\hbar} + e^{i|\tau|t/\hbar}\right]dt \\ &= \frac{1}{2}\int_{-\infty}^{\infty} e^{i(\omega - E/\hbar - |\tau|/\hbar)t}dt + \frac{1}{2}\int_{-\infty}^{\infty} e^{i(\omega - E/\hbar + |\tau|/\hbar)t}dt\end{aligned}$$

These can be simplified to delta function representations, giving us

$$\alpha(\omega) = \pi\left[\delta(\omega - \frac{E}{\hbar} - \frac{|\tau|}{\hbar}) + \delta(\omega - \frac{E}{\hbar} + \frac{|\tau|}{\hbar})\right]$$

which means that our absorption spectrum will have two peaks of equal height located at

$$\omega = \frac{E \pm |\tau|}{\hbar}$$

which means the peaks correspond to the eigenvalues of the Hamiltonian. ■