A paradigmatic model for Quantum Devices: Double Quantum Well

We consider an asymmetric double quantum well as depicted in Figure 1(a). We will show that by applying an electric field to this structure, we can control the tunneling effect between the two quantum wells and thus modify the dynamics of the electrons. This effect can be used for various applications such as photodetectors or photovoltaic devices.

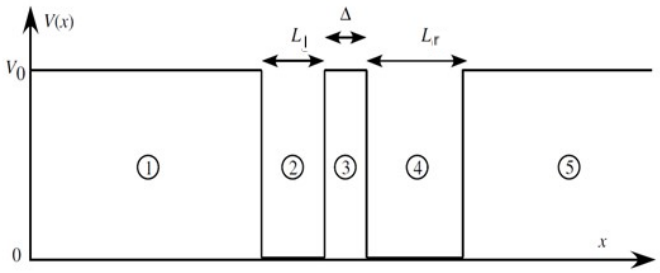

Figure 1: Asymmetric double well depicted here in the absence of an external electric field.

1 Energy level structure

To considerably simplify the calculations, we will assume in the following that V_0 is infinite.

1. Recall from the previous classes (PC4, Exercise 1) the formulas for the eigenenergies in an infinite square well of width L (don't do any calculations...). Deduce from this the eigenenergies in the **asymmetric** double well.

We had computed during PC4, exercise 1 the eigenenergies of the infinite well, which we found to be:

$$E_n = \hbar\omega n^2$$

where $\omega = \frac{\hbar^2\pi^2}{2mL^2}$ where m is the mass of the particle, in this case of an electron, and L is the width of the well.

Using my wisdom and intuition, If I have two uncoupled wells of width L_l and L_r, corresponding to the fundamental well frequencies ω_l and ω_r, I merely sum their two energies:

$$E_{n_l,n_r} = \hbar(\omega_l n_l^2 + \omega_r n_r^2) \qquad n_l, n_r \in \mathbb{N}^+, \text{only one of } n_l \text{ or } n_r \text{ different from zero}$$

Note that this formula is only correct if the two wells do not interact, therefore if they are sufficiently far from each other. In a realistic case, we would find a different energy.

The condition on n_l and n_r comes from the fact that on a single well, the fact that the square integral of the wave-function must be finite (larger than zero) imposes that $n > 0$.

The condition that only one of the two quantum numbers be zero arises from the fact that the two hamiltonians do not commute so they do not share an eigenbasis, therefore we need one wavefunction to be zero in the support of the other one.

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2. Calculate in meV the position of the first 6 energy levels of the system for $m = 6.1 \cdot 10^{-32}$ kg, $L_l = 10$ nm and $L_r = 3L_g/2 = 15$ nm. For each level, specify if the electron is localised in the narrow well (region 2) or the wide well (region 4). Are there any degenerate energy levels? I also remind you the value of $\hbar = 1.055 \cdot 10^{-34}\, Js$ and $1eV = 1.6 \cdot 10^{-19} J$.

I recall that

$$\hbar = 1.05 \cdot 10^{-34}\ Js$$
$$1eV = 1.6 \cdot 10^{-19} J$$

So I obtain $\omega_l = 55.7meV$ and $\omega_r = \left(\frac{2}{3}\right)^2 \omega_l = 24.8meV$. To avoid doing more calculations with numbers, I use the relationship between the two fundamental frequencies to write that

$$E_{n_l,n_r} = \hbar\omega_l \left(n_l^2 + \left(\frac{2}{3}\right)^2 n_r^2 \right) = \hbar\omega_l \frac{9\, n_l^2 + 4\, n_l^2}{9}$$

and the fundamental energies will be

$$\frac{E_{0,1}}{\hbar\omega_l} = \frac{4}{9} \qquad \Rightarrow E_{0,1} = 24.8\, meV$$
$$\frac{E_{1,0}}{\hbar\omega_l} = \frac{9}{9} \qquad \Rightarrow E_{1,0} = 55.7\, meV$$
$$\frac{E_{0,2}}{\hbar\omega_l} = \frac{16}{9} \qquad \Rightarrow E_{0,2} = 99.0\, meV$$
$$\frac{E_{0,3}}{\hbar\omega_l} = \frac{36}{9} \qquad \Rightarrow E_{0,3} = 222.8\, meV$$
$$\frac{E_{2,0}}{\hbar\omega_l} = \frac{36}{9} \qquad \Rightarrow E_{2,0} = 222.8\, meV$$
$$\frac{E_{3,0}}{\hbar\omega_l} = \frac{81}{9} \qquad \Rightarrow E_{3,0} = 501.3\, meV$$

from this we can see that a tuple of degenerate states are $E_{2,0}$ and $E_{0,3}$.

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3. The numerical resolution of the eigenstates and eigenenergies for the double well is indicated in Figure 2 for $V_0 = 1$ eV. Compare the obtained values with the predictions from question 1.3.

The fact that the potential V_0 is finite and not infinite lowers slightly the energy of the

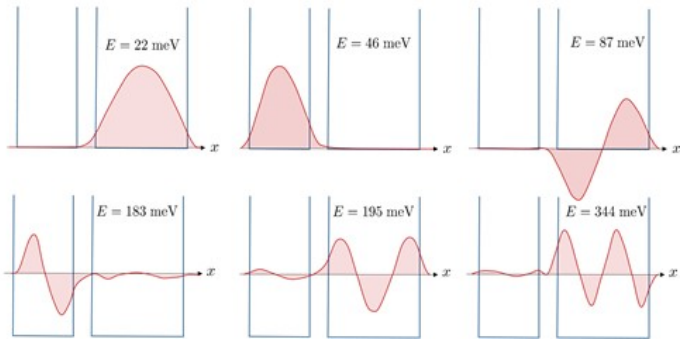

Figure 2: The first 6 eigenstates of the asymmetric double well obtained by numerical simulations.

fundamental mode, for example $\omega_r = 22\,meV$ instead of $24.8\,meV$ found from the analytical calculation. The doubly-degenerate state is no longer degenerate, as the potential barrier lifts the degeneration.

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4. By how much must the energy of the bottom of the left well (region 4) change relative to that of the right well (region 2) so that the fundamental level of the double well is degenerate?

The difference in energy between the two wells is equal to $(1 - 4/9)\hbar\omega_l = 31\,meV$ for the analytical calculation or $46 - 22 = 24\,meV$ in the numerical calculations. If the left well energy is changed by that value, then the ground state will become degenerate.

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5. What is the order of magnitude of the electric field F that needs to be applied along this structure to achieve this relative displacement of the bottoms of the two wells? We will choose for the thickness of the barrier separating the two wells $\Delta = 3$ nm.

As seen in the previous asnwer, we must change the energy of the right well by $24\,meV$.

Recalling that the width of the left and right wells are $L_l = 10\,nm$ and $L_r = 15\,nm$ and that the barrier has thickness $\Delta = 3\,nm$, the distance between the center of the two wells is $3 + 10/2 + 15/2 = 15.5\,nm$, the electric field F that must be applied to obtain such change in energy is given by the change in energy induced by the electric force, given by

$$\Delta E = eFd$$

from which we obtain that

$$F = \frac{\Delta E}{ed} = \frac{24 \cdot 10^{-3}}{15.5 \cdot 10^{-9}} = 1.5 \cdot 10^{6}\,V/m = 15\,kV/cm$$

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2 External Electric Field

In this part, we are interested in the possibility of increasing the tunnel coupling between the two wells by applying an electric field.

We use Dirac's formalism and denote $|\psi_l\rangle$ and $|\psi_r\rangle$ as the states of minimum energy E_l and E_r respectively in the left and right wells when the potential V_0 is infinite. We will limit ourselves to the two-dimensional subspace with the basis $\mathcal{B} = \{|\psi_l\rangle, |\psi_r\rangle\}$ for the Hilbert space $\mathcal{H}$.

1. How are the wavefunctions in $\mathcal{H}$ represented in practice in this space? In other words, what is a commonly used vector-space isomorphic to $\mathcal{H}$?

To achieve a more compact notation, and to be lazy, we might write from now on $|\psi_l\rangle = |l\rangle$ and $|\psi_r\rangle = |r\rangle$. Wavefunctions can be expanded onto this basis as:

$$|\psi\rangle = c_l\,|l\rangle + c_r\,|r\rangle\,,$$

where $c_l, c_r \in \mathbb{C}$. This means that the Hilbert space is isomorphic to $\mathbb{C}^2$ (written as $\mathcal{H} \sim \mathbb{C}^2$, the space of complex vectors with two entries. Consequently, we could also write the wavefunction as

$$|\psi\rangle \sim \begin{bmatrix} c_l \\ c_r \end{bmatrix}$$

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2. How does the condition of square-integrability ($L^2(\cdot)$) translate to this space?

The condition of finite norm implies that $\|v\| < \infty$ where $v \in \mathbb{C}^2$. Which means that

$$|c_l|^2 + |c_r|^2 < \infty$$

which is automatically verified for any complex vector of finite complex coefficients. Luckily for us, $\infty \notin \mathbb{C}$, so we can safely say that:

$$L^2(\mathbb{C}^2) = \mathbb{C}^2$$

For V_0 infinite and in the absence of an electric field, the Hamiltonian is written in the basis $\{|\psi_g\rangle, |\psi_d\rangle\}$:

$$\hat{H}_0 = \begin{pmatrix} E_l & 0 \\ 0 & E_r \end{pmatrix}. \tag{1}$$

The tunnel coupling that appears for a finite value of V_0 is written (with $J > 0$) :

$$\hat{V}_{\text{tun}} = \begin{pmatrix} 0 & -J \\ -J & 0 \end{pmatrix}. \tag{2}$$

3. Determine the eigenenergies of the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}_{\text{tun}}$.

The total Hamiltonian reads

$$H = \begin{pmatrix} E_l & -J \\ -J & E_r \end{pmatrix}.$$

The eigenenergies correspond to the eigenvalues of the Hamiltonian so I can just compute those. To do that, I will search for the roots of the characteristic polynomial of

$$H - \lambda \mathbb{I} = \begin{pmatrix} E_l - \lambda & -J \\ -J & E_r - \lambda \end{pmatrix}.$$

which is

$$\begin{aligned} \|H - \lambda \mathbb{I}\| &= (E_l - \lambda)(E_r - \lambda) - J^2 \\ &= \lambda^2 - \lambda(E_r + E_l) + E_l E_r - J^2 \end{aligned}$$

which is a quadratic form, and has roots at

$$\lambda_\pm = \frac{(E_r + E_l) \pm \sqrt{(E_r + E_l)^2 - 4(E_r E_l - J^2)}}{2}$$

which will correspond to the two eigenenergies of the Hamiltonian. Still, I want to simplify a bit this expression, so I notice that

$$(E_r + E_l)^2 - 4E_r E_l = (E_r - E_l)^2$$

so we obtain

$$\lambda_\pm = \frac{E_r + E_l}{2} \pm \sqrt{\left(\frac{E_r - E_l}{2}\right)^2 + J^2}$$

So if I define the base energy $E_0 \equiv \frac{E_l + E_r}{2}$ and the detuning or energy difference $\Delta \equiv \frac{E_r - E_l}{2}$, we can write the Energy as:

$$\lambda_\pm = E_0 \pm \sqrt{\Delta^2 + J^2},$$

from which you can easily see that the only relevant term is the difference in energy between the two states and the coupling strength.

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4. Give the expansion of these eigenenergies to first order in J when $J \ll |E_l - E_r|$. Can the tunnel effect play a significant role here?

$J \ll |E_l - E_r|$ means also $J \ll \Delta$, in that case I can collect the leading term J in the square root and write

$$\begin{aligned} \lambda_\pm &= E_0 \pm \Delta \sqrt{1 + \left(\frac{J}{\Delta}\right)^2} \\ &= E_0 \pm \Delta \left[1 + \left(\frac{J}{\sqrt{2}\Delta}\right)^2 + \mathcal{O}\left(\frac{J^4}{\Delta^4}\right)\right] \end{aligned}$$

where in the second line I have used the Taylor expansion of the square root. Therefore, the expression correct to first order in J is

$$\lambda_\pm = E_0 \pm \Delta + \mathcal{O}\left(\frac{J^2}{\Delta^2}\right),$$

which suggests that when the tunnel coupling is small wrt the difference in energy of the two wells, it has little effect on the eigenenergies and therefore on the structure of the stationary states.

We can go to a few orders beyond to see what is the effect of the tunnel coupling, finding that:

$$\lambda_\pm = E_0 \pm \left(\Delta + \frac{J^2}{2\Delta}\right) + \mathcal{O}\left(\frac{J^4}{\Delta^4}\right),$$

, meaning that at order 2 in the tunnel coupling J the tunnel coupling further increases the gap between the first two eigenstates.

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5. We now apply an electric field F which displaces the positions of the levels $|\psi_g\rangle$ and $|\psi_d\rangle$ differently. We model this field by the coupling:

$$\hat{V}_{\text{elec.}} = \begin{pmatrix} a_g F & 0 \\ 0 & a_d F \end{pmatrix}, \tag{3}$$

where a_g and a_d are distances depending on the characteristics of the quantum well ($a_g \neq a_d$). Determine the new energy levels of the system and plot qualitatively their variation as a function of F in the case $a_g < a_d < 0$.

- Remember that the coupling term will appear in the Hamiltonian as a term $H = H_0 + eV_{elec}$

Notice that with the definitions we used in the previous answer we can rewrite the Hamiltonian using $E_0 \equiv \frac{E_l+E_r}{2}$ and $\Delta \equiv \frac{E_r-E_l}{2}$ such that:

$$\begin{aligned} H &= \begin{pmatrix} E_l & -J \\ -J & E_r \end{pmatrix} \\ &= \begin{pmatrix} \frac{E_l+E_r}{2} + \frac{E_l-E_r}{2} & -J \\ -J & \frac{E_l+E_r}{2} - \frac{E_l-E_r}{2} \end{pmatrix} \\ &= E_0 \hat{\mathbb{I}} + \begin{pmatrix} \Delta & -J \\ -J & -\Delta \end{pmatrix}, \end{aligned}$$

And as we know, the constant shift in energy given by E_l will not affect the eigenstate structure of the Hamiltonian but simply shift the eigenvalues by E_l, so we can largely ignore it in the following calculations. The physical interpretation in this case is that the physics of the system is determined by the asymmetry of the potential between the left and right wells.

Likewise, we can give the same treatment to $\hat{V}_{\text{elec.}}$, defining

$$\epsilon_F = e\frac{a_g + a_d}{2} \qquad \delta_F = e\frac{a_g - a_d}{2}$$

we can easily prove that

$$e\hat{V}_{\text{elec.}} = \begin{pmatrix} ea_g F & 0 \\ 0 & ea_d F \end{pmatrix} = F\epsilon_F \hat{\mathbb{I}} + F \begin{pmatrix} \delta_F & 0 \\ 0 & -\delta_F \end{pmatrix}, \tag{4}$$

This means that for the eigenenergies we don't need to repeat the calculations, instead, taking the solution from the previous point, we substitute

$$E_0 \to E_0 + \epsilon_F F \qquad \Delta \to \Delta + \delta_F F,$$

obtaining for the two eigenenergies

$$\lambda_\pm = E_0 + \epsilon_F F \pm \sqrt{J^2 + (\Delta + \delta_F F)^2}$$

and the minimal gap is achieved when $(\Delta + \delta_F F)^2 = 0$ meaning when

$$F = -\frac{\Delta}{\delta_F} = -\frac{E_l - E_r}{e(a_g - a_d)}$$

So if we are careful enough to set the electric potential to exactly this value we can get the minimum gap which will be $2J$.

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6. What are the eigenstates of $\hat{H}$ when the gap between the two energy levels is minimal?

The eigenstates $|+\rangle$ and $|-\rangle$ should respect the eigenvalue equations for their respective eigenvalues

$$\hat{H}|+\rangle = E_+ |+\rangle$$
$$\hat{H}|-\rangle = E_+ |-\rangle$$

Considering the minimum-gap condition $F = -\frac{\Delta}{\delta_F}$, we have that the Hamiltonian reads:

$$\hat{H} = \left(E_0 - \Delta\frac{\epsilon_F}{\delta_F}\right)\hat{\mathbb{I}} + \begin{pmatrix} 0 & -J \\ -J & 0 \end{pmatrix}$$

and I will define for ease of notation $\tilde{E}_0 \equiv E_0 - \frac{\Delta}{\delta_F}$. The eigenvalues equation for $|\pm\rangle$ will be:

$$\left[\left(E_0 - \Delta\frac{\epsilon_F}{\delta_F}\right)\hat{\mathbb{I}} + \begin{pmatrix} 0 & -J \\ -J & 0 \end{pmatrix}\right] \begin{pmatrix} c_l^\pm \\ c_r^\pm \end{pmatrix} = E_\pm \begin{pmatrix} c_l^\pm \\ c_r^\pm \end{pmatrix}$$

and as $E_\pm = (E_0 - \Delta\frac{\epsilon_F}{\delta_F}) \pm J$ we get

$$\begin{pmatrix} 0 & -J \\ -J & 0 \end{pmatrix} \begin{pmatrix} c_l^\pm \\ c_r^\pm \end{pmatrix} = \pm J \begin{pmatrix} c_l^\pm \\ c_r^\pm \end{pmatrix}$$

which yields for the eigenstate of energy $E_+ = J$ the eigenvalue

$$\begin{pmatrix} c_l^+ \\ c_r^+ \end{pmatrix} = \begin{pmatrix} -c_r^+ \\ c_r^+ \end{pmatrix}$$

and therefore, to keep the normalisation condition $(c_l^+)^2 + (c_r^+)^2 = 1$ we get

$$\begin{pmatrix} c_l^+ \\ c_r^+ \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

while similarly it is possible to show that the other state with a lower energy is

$$\begin{pmatrix} c_l^- \\ c_r^- \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Do notice that the lowest-energy state is E_- which is symmetric under the action of the parity operator, while the excited state is anti-symmetric.

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7. An experimental measurement of the two lowest levels of an asymmetric double quantum well is shown in Figure 2.a. Comment on this and extract the value of the tunneling coefficient J.

This is the expected curve. The minimal distance is at around $F \approx 35kV/cm$, which corresponds to about $14meV$, meaning that $J \approx 7meV$.

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3 Coherent Oscillations

With a suitably chosen laser pulse, we can prepare the electrons in the left well at a given time $t = 0$.

In the basis of $\{|\psi_l\rangle, |\psi_r\rangle\}$ this means that the state is $|\psi(t=0)\rangle = |l\rangle$, or

$$\begin{pmatrix} c_l(t=0) \\ c_r(t=0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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1. Calculate $|\psi(t)\rangle$ in the basis $\{|\psi_l\rangle, |\psi_r\rangle\}$.

In the previous step we have diagonalised the Hamiltonian, and you should hopefully remember that it is rather easy to write the time-evolved state in the basis that diagonalises the Hamiltonian. We therefore rewrite the state $\psi(t=0)$ in this basis. The diagonalising basis is given by

$$|+\rangle = \frac{1}{\sqrt{2}}(|l\rangle + |r\rangle) \qquad |-\rangle = \frac{1}{\sqrt{2}}(|l\rangle - |r\rangle)$$

therefore the state $|\psi(t=0)\rangle = |l\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$, with coefficients $c_+(0) = c_-(0) = 1/\sqrt{2}$
With that in mind, and recalling the formula for the time-evolved state in the diagonal basis

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|l\rangle = \sum_{i=\{\pm\}} e^{-iE_it/\hbar}c_i(0)|i\rangle$$

and substituting $E_\pm = E_0 \pm J$, we have that the time-evolved state will be

$$\begin{aligned}|\psi(t)\rangle &= \frac{1}{\sqrt{2}}\left(e^{-iE_+t/\hbar}|+\rangle + e^{-iE_-t/\hbar}|-\rangle\right)\\ &= \frac{1}{\sqrt{2}}\left(e^{-i(E_0+J)t/\hbar}|+\rangle + e^{-i(E_0-J)t/\hbar}|-\rangle\right)\\ &= \frac{e^{iE_0t/\hbar}}{\sqrt{2}}\left(e^{-iJt/\hbar}|+\rangle + e^{iJt/\hbar}|-\rangle\right)\end{aligned}$$

and notice that the global phase I extracted in front of the state can be neglected as it cannot be measured. Therefore, the only parameter affecting the dynamics at that point is the coupling J between the two wells.

Note that we can also rewrite the wavefunction in the original basis obtaining

$$\begin{aligned}|\psi(t)\rangle &= \frac{e^{iE_0t/\hbar}}{\sqrt{2}}\left(e^{-iJt/\hbar}|+\rangle + e^{iJt/\hbar}|-\rangle\right)\\ &= \frac{e^{iE_0t/\hbar}}{\sqrt{2}}\left(e^{-iJt/\hbar}\frac{|l\rangle+|r\rangle}{\sqrt{2}} + e^{iJt/\hbar}\frac{|l\rangle-|r\rangle}{\sqrt{2}}\right)\\ &= e^{iE_0t/\hbar}\left(\frac{e^{-iJt/\hbar}+e^{iJt/\hbar}}{2}|l\rangle + \frac{e^{-iJt/\hbar}-e^{iJt/\hbar}}{2}|r\rangle\right)\\ &= e^{iE_0t/\hbar}\left(\cos(Jt/\hbar)|l\rangle + i\sin(Jt/\hbar)|r\rangle\right)\end{aligned}$$

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2. When the electrons oscillate between the two quantum wells, the device behaves like an antenna and an electromagnetic field is radiated at the corresponding frequency. What value of F maximizes the amplitude of this radiated electromagnetic field? One could be interested in the oscillating part of the average value of the dipole operator $\hat{d}$, which has $|\psi_r\rangle$ and $|\psi_l\rangle$ as eigenstates with eigenvalues $+d_0$ and $-d_0$. (Answer this question with a simple reasoning, not by doing extensive calculations)

Doing calculations we would need to diagonalize the Hamiltonian for arbitrary F, which is somewhat a long calculation. Instead, we can argue the following: if the dipole operator has as eigenstates $|l\rangle$ and $|r\rangle$ with eigenvalues $\pm d_0$, the largest oscillations of the dipole is obtained by oscillating between those two states. If I was oscillating between two states that are a linear combination of l and r I would have a smaller electric dipole and therefore smaller oscillations.

This imposes that the oscillations must pass through the two eigenstates of the dipole operator, and the Hamiltonian evolution will pass through those states only if they are eigenvalues of the Hamiltonian, meaning that this only happens when F is as has been computed before (Resonance).

Alternatively, The dipole operator is therefore

$$\hat{d} = \begin{pmatrix} d_0 & 0 \\ 0 & -d_0 \end{pmatrix}$$

in the basis of left and right. the expectation value is then

$$d(t) = \langle\psi(t)|\hat{d}|\psi(t)\rangle = d_0|\langle l|\psi(t)\rangle|^2 - d_0|\langle r|\psi(t)\rangle|^2$$

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3. Under these conditions, calculate the probability $p_r(t)$ of finding the particle in the right well at time t. Discuss.

The probability to find the particle at time t in the right well is equal to

$$\begin{aligned} p_r(t) &= |\langle r|\psi(t)\rangle|^2 \\ &= \left|\frac{e^{iE_0 t/\hbar}}{\sqrt{2}}\left(e^{-iJt/\hbar}\langle r|+\rangle + e^{iJt/\hbar}\langle r|-\rangle\right)\right|^2 \end{aligned}$$

and reminding that $|\pm\rangle = \frac{1}{\sqrt{2}}(|l\rangle \pm |r\rangle)$ then we obtain that

$$\langle r|\pm\rangle = \frac{1}{\sqrt{2}}(\langle r|l\rangle \pm \langle r|r\rangle) = \pm\frac{1}{\sqrt{2}}$$

and therefore

$$\begin{aligned} p_r(t) &= \left|\frac{1}{2}\left(e^{-iJt/\hbar} - e^{iJt/\hbar}\right)\right|^2 \\ &= \left|\sin\left(\frac{J}{\hbar}t\right)\right|^2 \\ &= \frac{1}{2}\left[1 - \cos\left(2\frac{J}{\hbar}t\right)\right] \end{aligned}$$

this signifies that the probability starts at $t = 0$ being 0, consistent with the initial condition, and then it oscillates with frequency $J/\hbar$, meaning that the electron is moving from the left well to the right well.

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4. An experimental result showing the radiated electromagnetic field as a function of time is presented in Figure 2.b. The electric field F has been adjusted to maximize the amplitude of the radiated field. Deduce the value of the tunneling coefficient J in this second experiment from these data.

In the experimental data we can count 8 oscillations in about $5\,ps$, so this gives a value of... $3.1meV$

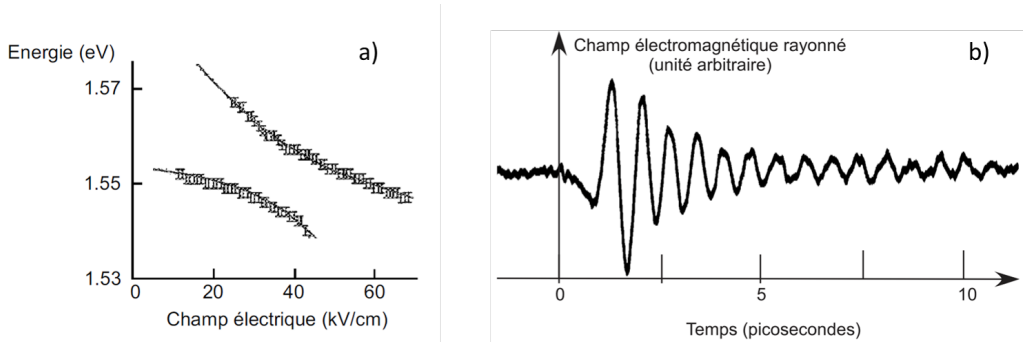

Figure 3: Two experimental results: a) Energies of the two lowest levels of an asymmetric double quantum well measured as a function of the applied electric field (J.E. Golub et al., Appl.Phys.Lett. **53,** 2584 (1988)). The vertical energy scale is defined up to an additive constant that is irrelevant to this problem. b) Radiated electromagnetic field, after preparation at $t = 0$ of the electrons in the left quantum well. (H.G. Roskos et al., Phys. Rev. Lett. 68, 2216 (1992)).