7212

E7212: Adiabatic Transfer Along Chain (2019A)

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The problem:

In this problem we assume a chain with 5 states x=1,2,3,4,5 with jump frequencies between adjacent states are (a,b,a,b) where a=Csin(θ), b=Ccos(θ).
The potential energy in all states is 0, beside the 2^{nd} state which is V.
There is no possibility to jump between states 1 and 5 directly (non-cyclic).
The system starts with one particle in the first state and then the value of θ starts to change "slowly" from the value of $\theta = 0$ to the value $\theta = \frac{\pi}{2}$

(1) For V=0, write the matrix R that represents a gauge action so $R^{-1}\mathcal{H}R = -\mathcal{H}$
Therefore, the Hemiltonian has an eigenstate with the eigenvalue of 0.

(2) For V=0 write in the standard base the adiabatic state that is implied by the initial condition.
Where will the particle be at the end of the adiabatic process? does the answer depend on the value of the potential barrier V?

(3) For V=0 write the energies for $\theta = 0$ and $\theta = \frac{\pi}{4}$.
Hint: notice that for the 2^{nd} case, the problem is the same as a potential well in length of L=6.

(4) Repeat section 3 for $V \gg C$
In this case, the leading order answer will be enough. This section demands a diagonalizing of a 3X3 matrix in order to set the energies. The correctness of the numerical coefficient in the result is important.

(5) Draw a schematic graph of the energies as a function of θ for V=0.
Draw a schematic graph of the energies as a function of V for $\theta = 0$.
Make sure that the graph will be clear.

(6) What is the adiabatic condition on $\dot{\theta}$?
solve for the cases V=0 and the case $V \gg C$
You can ignore numerical factors.

Hint: without solving sections 1 and 2, you can still successfully handle with the other sections.

The solution:

The Hamiltonian describing the system is:

$$\mathcal{H} \mapsto \begin{pmatrix} 0 & Csin(\theta) & 0 & 0 & 0 \\ Csin(\theta) & V & Ccos(\theta) & 0 & 0 \\ 0 & Ccos(\theta) & 0 & Csin(\theta) & 0 \\ 0 & 0 & Csin(\theta) & 0 & Ccos(\theta) \\ 0 & 0 & 0 & Ccos(\theta) & 0 \end{pmatrix}$$

(1) For V=0 we are looking for a matrix R that will:
multiply (by -1) the 2^{nd} and 4^{th} rows, when multiplying from the left side (the inverse), and also multiply (by -1) the 2^{nd} and 4^{th} columns, when multiplying from the right side.
We will choose the following R:

$$R \mapsto \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Note that $R = R^{-1}$ and $R^{-1}\mathcal{H}R = -\mathcal{H}$ as requested.
Therefore, $\mathcal{H}$ and $-\mathcal{H}$ has the same eigenvalues, so for each eigenvalue E of $\mathcal{H}$, there is a complete eigenvalue -E. Since there are odd number of eigenvalues, at least one of them must be 0.

(2) In adiabatic processes the particles remain with the same initial energy.
For V=0, and the initial condition ($\Psi = |1\rangle$ and $\theta = 0$) we get:

$$\mathcal{H} \cdot \Psi = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & C & 0 & 0 \\ 0 & C & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & C \\ 0 & 0 & 0 & C & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 0 \cdot \Psi$$

Therefore, the state $|1\rangle$ in time t=0 is an eigenstate of $\mathcal{H}$ with the eigenvalue of E=0.
In order to find the adiabatic state we must demand that the energy remains 0:

$$\mathcal{H}\Psi = \begin{pmatrix} 0 & Csin(\theta) & 0 & 0 & 0 \\ Csin(\theta) & 0 & Ccos(\theta) & 0 & 0 \\ 0 & Ccos(\theta) & 0 & Csin(\theta) & 0 \\ 0 & 0 & Csin(\theta) & 0 & Ccos(\theta) \\ 0 & 0 & 0 & Ccos(\theta) & 0 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

We get 5 equations that must be true for each value of θ
i. b$\cdot \sin(\theta)$=0
ii. a$\cdot \sin(\theta)$+c$\cdot \cos(\theta)$=0
iii. b$\cdot \cos(\theta)$+d$\cdot \sin(\theta)$=0
iv. c$\cdot \sin(\theta)$+e$\cdot \cos(\theta)$=0
v. d$\cdot \cos(\theta)$=0
With the choose of a=1 (for non-normalized state) we get:

$$|\Psi(\theta)\rangle \mapsto \begin{pmatrix} 1 \\ 0 \\ -tg(\theta) \\ 0 \\ tg^2(\theta) \end{pmatrix}$$

Note that the state $|2\rangle$ is always 0, so the partical has 0 probability to get there. The answer for $\Psi(\theta)$ stays the same for any value of V.

At the end of the process $\theta = \frac{\pi}{2}$:

$$\mathcal{H} \mapsto \begin{pmatrix} 0 & C & 0 & 0 & 0 \\ C & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & C & 0 \\ 0 & 0 & C & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

For V=0 the $\mathcal{H}(\theta = \frac{\pi}{2})$ is symetric to $\mathcal{H}(\theta = 0)$, so it is easy to see that state $|5\rangle$ has the eigenenergy of 0. Therefore, at the end of the adiabatic process, the particle is at state $|5\rangle$.
From another point of view, when we normalized $\Psi(\theta)$ and take the limit $\theta \longrightarrow \frac{\pi}{2}$ we get that $\Psi(\theta) = |5\rangle$.
The value of V has no effect here since the particle dose not get there during the process.

(3) For V=0 and $\theta = 0$ we get:

$$\mathcal{H} \mapsto \left(\begin{array}{c|cc|cc} 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & C & 0 & 0 \\ 0 & C & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & C \\ 0 & 0 & 0 & C & 0 \end{array}\right)$$

We can diagonalize each 2X2 block separately according to the symmetric and a-symmetric eigenvectors:

$$|+\rangle \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, |-\rangle \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

And then we get the full eigenvectors base:

$$|1\rangle \mapsto \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |2\rangle \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, |3\rangle \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |4\rangle \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}, |5\rangle \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

With the eigenvalues: $E_1 = 0$, $E_2 = -C$, $E_3 = C$, $E_4 = -C$, $E_5 = C$

For V=0 and $\theta = \frac{\pi}{4}$ we get:

$$\mathcal{H} \mapsto \frac{C}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

By diagonalizing the matrix we get:

$$|1\rangle \mapsto \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 1 \end{pmatrix}, |2\rangle \mapsto \frac{1}{3} \begin{pmatrix} 1 \\ \sqrt{3} \\ 2 \\ \sqrt{3} \\ 1 \end{pmatrix}, |3\rangle \mapsto \frac{1}{3} \begin{pmatrix} 1 \\ -\sqrt{3} \\ 2 \\ -\sqrt{3} \\ 1 \end{pmatrix}, |4\rangle \mapsto \frac{1}{2} \begin{pmatrix} -1 \\ -1 \\ 0 \\ 1 \\ 1 \end{pmatrix}, |5\rangle \mapsto \frac{1}{2} \begin{pmatrix} -1 \\ 1 \\ 0 \\ -1 \\ 1 \end{pmatrix}$$

With the eigenvalues:
$E_1 = 0$, $E_2 = \sqrt{\frac{3}{2}}C$, $E_3 = -\sqrt{\frac{3}{2}}C$, $E_4 = \sqrt{\frac{1}{2}}C$, $E_5 = -\sqrt{\frac{1}{2}}C$

Another option to solve this question is to notice that we are looking on a discrete version of a potential well with L=6. The 5 values of each vector represent 5 samples of the continues state with equal length between each 2 samples.
Reminder: the eiganstates of a potential well between in the range [-L/2,L/2] are $sin(\frac{2\pi n}{L}x)$ and $cos(\frac{2\pi(n+\frac{1}{2})}{L}x)$.
Therefore, the non-normalized eigenstate will be the samples of those wave functions in the points x= 2,1,0,-1,-2. For each continues wave function we sampled the function and got:

$$cos(\frac{\pi}{6}x) \mapsto \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \\ 1 \\ \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, cos(\frac{3\pi}{6}x) \mapsto \begin{pmatrix} -1 \\ 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, cos(\frac{5\pi}{6}x) \mapsto \begin{pmatrix} \frac{1}{2} \\ \frac{-\sqrt{3}}{2} \\ 1 \\ \frac{-\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, sin(\frac{2\pi}{6}x) \mapsto \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} \\ 0 \\ \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} \end{pmatrix}, sin(\frac{4\pi}{6}x) \mapsto \begin{pmatrix} \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} \\ 0 \\ \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}$$

Note: for higher orders of n, we will get the same answers as we got, since there are no more that 5 orthogonal states in a 5^{th} order matrix.
As you can see, each state from the potential well states, has a matching state from the normalized eigenstates. So, they have the same eigenvalues.
Note: it is possible to solve it also for x in range [0,L] and use only sin() functions.

(4) For $V \gg C$ and $\theta = 0$:

$$\mathcal{H} \mapsto \left(\begin{array}{c|cc|cc} 0 & 0 & 0 & 0 & 0 \\ \hline 0 & V & C & 0 & 0 \\ 0 & C & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & C \\ 0 & 0 & 0 & C & 0 \end{array}\right)$$

Let us observe each block separately:
The lower block can be diagonalize with the standard $|+\rangle$, $|-\rangle$ states:

$$base: \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \Longrightarrow \mathcal{H} \mapsto \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & V & C & 0 & 0 \\ 0 & C & 0 & 0 & 0 \\ 0 & 0 & 0 & C & 0 \\ 0 & 0 & 0 & 0 & -C \end{pmatrix}$$

The upper block, state $|1\rangle$ is not coupled with any other state.
For the middle block, we get the eigenvalues using perturbation theory:
$E_1 = 0$
$E_2 = V^{[0]} + 0^{[1]} + \frac{C^2}{V-0}^{[2]} \approx V$
$E_3 = 0^{[0]} + 0^{[1]} + \frac{C^2}{0-V}^{[2]} \approx \frac{-C^2}{V}$
$E_4 = C$
$E_5 = -C$

For $V \gg C$ and $\theta = \frac{\pi}{4}$:

$$\mathcal{H} \mapsto \begin{pmatrix} 0 & \frac{C}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{C}{\sqrt{2}} & V & \frac{C}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{C}{\sqrt{2}} & 0 & \frac{C}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{C}{\sqrt{2}} & 0 & \frac{C}{\sqrt{2}} \\ 0 & 0 & 0 & \frac{C}{\sqrt{2}} & 0 \end{pmatrix}$$

The first step is to choose the base where the matrix $\begin{pmatrix} 0 & \frac{C}{\sqrt{2}} & 0 \\ \frac{C}{\sqrt{2}} & 0 & \frac{C}{\sqrt{2}} \\ 0 & \frac{C}{\sqrt{2}} & 0 \end{pmatrix}$ will be diagonolized.

We can see that this matrix is equal to C·S$_x$. We are familiar with the basis $|\Uparrow\rangle$,$|\Updownarrow\rangle$,$|\Downarrow\rangle$ where S_z is diagonal, and we can rotate these vectors by 90^o around y axis to get the basis where S_x would be diagonal:

$$|3\rangle=\mathrm{U}(\tfrac{\pi}{2}\ n_y)|\Uparrow\rangle = \tfrac{1}{2}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$$

$$|4\rangle=\mathrm{U}(\tfrac{\pi}{2}\ n_y)|\Updownarrow\rangle = \tfrac{1}{2}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \tfrac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$

$$|5\rangle=\mathrm{U}(\tfrac{\pi}{2}\ n_y)|\Downarrow\rangle = \tfrac{1}{2}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

By working with the following basis, we get:

$$\mathcal{H}\mapsto \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix}^T \begin{pmatrix} 0 & \frac{C}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{C}{\sqrt{2}} & V & \frac{C}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{C}{\sqrt{2}} & 0 & \frac{C}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{C}{\sqrt{2}} & 0 & \frac{C}{\sqrt{2}} \\ 0 & 0 & 0 & \frac{C}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix}$$

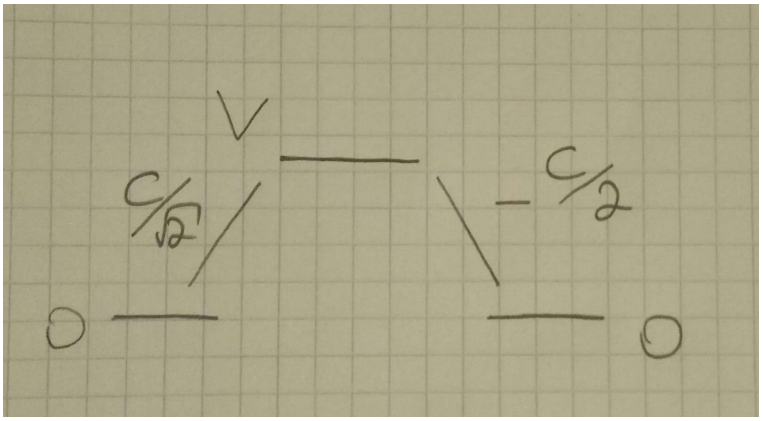
$$= \begin{pmatrix} 0 & \frac{C}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{C}{\sqrt{2}} & V & \frac{C}{2\sqrt{2}} & \frac{-C}{2} & \frac{C}{2\sqrt{2}} \\ 0 & \frac{C}{2\sqrt{2}} & C & 0 & 0 \\ 0 & \frac{-C}{2} & 0 & 0 & 0 \\ 0 & \frac{C}{2\sqrt{2}} & 0 & 0 & -C \end{pmatrix}$$

Now, since we are only looking for the leading order, we can clearly see that 3 energies will be V, C, -C (C and -C are coupled only with V so the next correction will be proportional to $\frac{C^2}{V-C}$ and much smaller than C). For the other 2 energies, we can observe only the relevant parts of the matrix:

$$\begin{pmatrix} 0 & \frac{C}{\sqrt{2}} & 0 \\ \frac{C}{\sqrt{2}} & V & -\frac{C}{2} \\ 0 & -\frac{C}{2} & 0 \end{pmatrix}$$

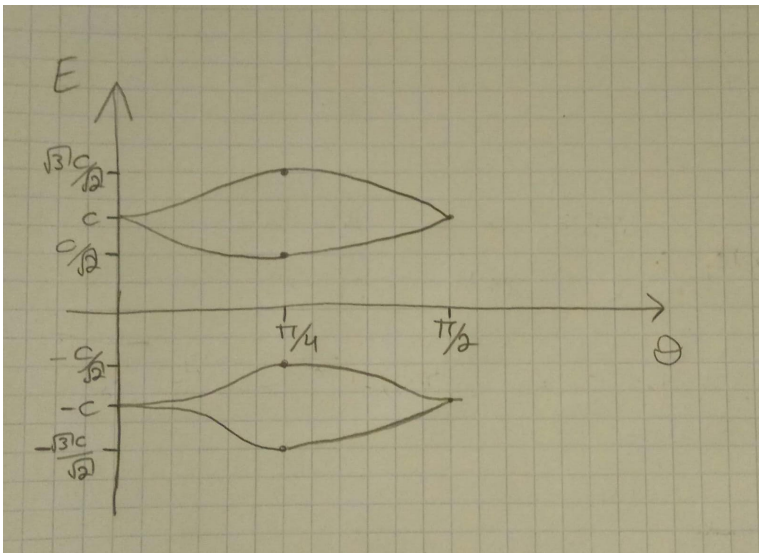
The 3^{rd} and the 5^{th} rows and columns are not interesting since they are not related to the energies we are looking for.

We must notice that using perturbation theory will not be accurate enough because we have degenerated energies:



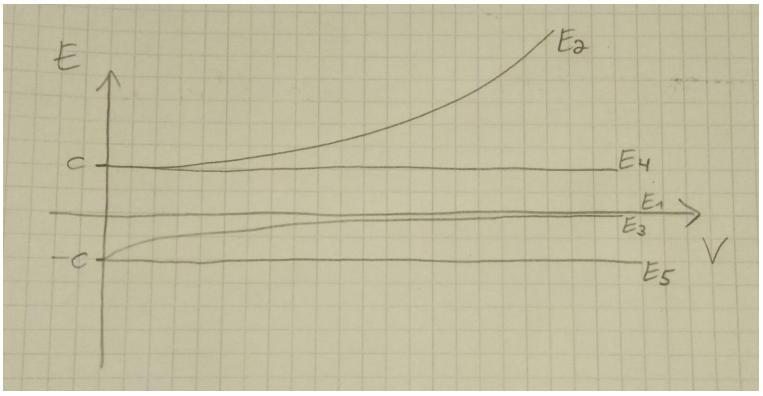
Even though the two degenerated states are not directly coupled, they are indirectly coupled through a third state with energy V.
There are various ways to solve the problem such as choosing a different basis or considering the contribution of the indirect hopping (the latter is out of the scope of this course). We will follow the guidance in the question and diagonalize the 3X3 matrix to get:
E_1=0
E_2=$\frac{V}{2}+\frac{V}{2}\sqrt{1+3\frac{C^2}{V^2}}\approx V$
E_3=$\frac{V}{2}-\frac{V}{2}\sqrt{1+3\frac{C^2}{V^2}}\approx -\frac{3}{4}\frac{C^2}{V}$
Finall answer: E $= V, C, -C, -\frac{3}{4}\frac{C^2}{V}, 0$

(5) E(θ) for V=0:
We saw that for $\theta = 0$ and $\theta = \frac{\pi}{2}$ we get a symmetric Hemiltonian, and thus the same energies.
In fact the Hemiltonian is symmetric around $\mathcal{H}(\theta = \frac{\pi}{4})$ and there is no degeneracy, so one can infer:



for $\theta = 0$ and E(V):

The exact solution for the eigenvalues can be achieved by diagonalizing $\begin{pmatrix} V & C \\ C & 0 \end{pmatrix}$ and we get: $E_1 = 0$, $E_2 = \frac{V}{2} + \sqrt{\frac{V^2}{4} + C^2}$, $E_3 = \frac{V}{2} - \sqrt{\frac{V^2}{4} + C^2}$, $E_4 = C$, $E_5 = -C$



(6) The adiabatic condition as learned in class is:

$$\dot{\theta} \ll \frac{\Delta^2}{V_{nm}}$$

Where Δ is the minimal distance between any 2 energy levels and V_{nm} is the corresponding matrix element.

For V=0:

The energy difference $\Delta \sim$ C so:

$$\dot{\theta} \ll \frac{C^2}{C} = C$$

For V$\gg C$:

We saw that after losing the degeneracy we get $\Delta \sim \frac{C^2}{V}$ for any value of θ. In order to find V_{nm} we can remember that $V_{nm} = (\frac{d\mathcal{H}}{d\theta})_{nm}$. So, we can observe $\mathcal{H}(\theta = \frac{\pi}{4})$ in the base that diagonalized $\mathcal{H}(\theta = 0)$ (or choose any other 2 times) and that will be an approximation for V_{nm}.

Finally, we get $V_{nm} \sim \frac{C^2}{V}$, and:

$$\dot{\theta} \ll \frac{C^2}{V}$$