Ex7210: E7210: Adiabatic transfer along 2 and 3 sites systems

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The problem:

Consider 2 site system described by the Hamiltonian:

$\mathcal{H} = \frac{\epsilon}{2} \cdot \begin{pmatrix} \sin(\theta) & \cos(\theta) \\ \cos(\theta) & -\sin(\theta) \end{pmatrix}$

The control parameter θ is changed from $-\pi/2$ to $+\pi/2$.
The rate of change is $\dot{\theta}$.
Initially the particle is located in the first site.

(a) Define the "real" adiabatic basis.
(b) Write the Hamiltonian in the Adiabatic basis.
(c) Show in this representation that in the sudden limit the survival probability P is unity.
(d) Find an approximation for P in the adiabatic regime.
(e) Repeat the same items for the 3 site STIRAP Hamiltonian. Here all the sites have zero potential, and the couplings are $\epsilon cos(\theta)$ and $\epsilon sin(\theta)$.

The solution:

(a) The Hamiltonian can be written as:

$$\mathcal{H} = \vec{\Omega} \cdot \vec{S} \tag{1}$$

so that $\vec{\Omega} = \epsilon(\cos(\theta), 0, \sin(\theta))$ and $|\vec{\Omega}| = \epsilon$.
With analogy to spin 1/2, we can obtain the eigenstates by rotating the initial state by an angle α so that

$$\alpha = \arctan\left(\frac{\cos(\theta)}{\sin(\theta)}\right) = \frac{\pi}{2} - \theta \tag{2}$$

thus the energy levels are $E_+ = \epsilon/2$ and $E_- = -\epsilon/2$ adiabatic basis is:

$$|E_+\rangle = \begin{pmatrix} \cos\left(\frac{\pi}{4} - \frac{\theta}{2}\right) \\ \sin\left(\frac{\pi}{4} - \frac{\theta}{2}\right) \end{pmatrix}; \qquad |E_-\rangle \begin{pmatrix} \sin\left(\frac{\pi}{4} - \frac{\theta}{2}\right) \\ -\cos\left(\frac{\pi}{4} - \frac{\theta}{2}\right) \end{pmatrix} \tag{3}$$

(b) The effective Hamiltonian in the adiabatic basis will have an additional term which allows non adiabatic transitions:

$$\mathcal{H}_{eff} = T^\dagger \mathcal{H} T + W \tag{4}$$

Where T is the transformation between the standard and adiabatic basis:

$$T = \begin{pmatrix} |E_+\rangle & |E_-\rangle \end{pmatrix} \tag{5}$$

$\mathcal{H}$ is the original Hamiltonian, and W is the perturbation.
We have only one-parameter driving so that the diagonal elements of W can be gauged out and the off diagonal elements will take the form:

$$W_{nm} = \frac{i\dot{\theta}V_{nm}}{E_n - E_m} \tag{6}$$

Where $V_{nm} = \left(\frac{\partial \mathcal{H}}{\partial \theta}\right)_{nm}$

$$V = \frac{\epsilon}{2} \cdot \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ -\sin(\theta) & -\cos(\theta) \end{pmatrix} \tag{7}$$

The relevant elements of W are the coupling between $E_+ = \epsilon/2$ and $E_- = -\epsilon/2$ which in this particular problem are independent of the parameter θ:

$$W_{E_+,E_-} = -\frac{i\dot{\theta}}{2} \tag{8}$$

Finally the effective Hamiltonian in the adiabatic basis is:

$$\mathcal{H}_{eff} = \begin{pmatrix} \frac{\epsilon}{2} & -\frac{i\dot{\theta}}{2} \\ \frac{i\dot{\theta}}{2} & -\frac{\epsilon}{2} \end{pmatrix} = \left(0, \dot{\theta}, \epsilon\right) \cdot \vec{S} \tag{9}$$

(c) In the sudden approximation we have $\dot{\theta} >> \epsilon$ so we can neglect ϵ in the Hamiltonian. Therefore $\Omega = (0, \dot{\theta}, 0)$.
Initially ($\theta = \pi/2$) the particle was prepared in the first site. In the adiabatic context this translates into being in the lower energy level, thus:

$$|\psi(0)\rangle = |E_-\rangle|_{\theta=-\pi/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{10}$$

$$|\psi(t)\rangle = e^{-i\Phi(t)S_y} |E_-\rangle \tag{11}$$

$$\Phi(t) = \int_o^t \dot{\theta} dt = \int_{-\pi/2}^{\pi/2} d\theta = \pi \tag{12}$$

Thus $|\psi(\theta = \pi/2)\rangle$ is obtained by rotating the initial states by the angle π around the y axis. One can see that:

$$|\psi(\theta = \pi/2)\rangle = |E_+\rangle|_{\theta=\pi/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{13}$$

So the particle remains in the same state in accordance to the sudden approximation.

(d) This particular setup has an exact solution with 2 level dynamics method. Despite this we will use the "interaction picture".
The survival probability is defined as the probability of transitioning from E_- to E_+:

$$P_t(+|-) = \left| \int_0^t \frac{V_{+-}}{E_+ - E_-} \cdot e^{-i(\phi_+ - \phi_-)} \dot{\theta} dt \right|^2 = \left| \int_{-\pi/2}^{\pi/2} -\frac{1}{2} \cdot e^{-i(\frac{\epsilon}{\dot{\theta}})\theta} d\theta \right|^2 = \frac{\pi^2}{4} sinc^2(\frac{\pi\epsilon}{2\dot{\theta}}) \tag{14}$$

Where $\phi_\pm$ defined by:

$$\phi_\pm = \int_0^t E_\pm dt = \int_0^t \frac{\pm\epsilon}{2\dot{\theta}} d\theta = \frac{\pm\epsilon \cdot \theta}{2\dot{\theta}} \tag{15}$$

We can see the in the limit $\dot{\theta} << \epsilon$ the survival probability is:

$$P_t(E_+|E_-) \approx 0 \tag{16}$$

Which means that the particle's energy level remains the same as we would expect for an adiabatic process. Moreover the particle moves from the first site to the second during the process.

(e) The STIRAP Hamiltonian is:

$$\mathcal{H} = \epsilon \cdot \begin{pmatrix} 0 & \cos(\theta) & 0 \\ \cos(\theta) & 0 & \sin(\theta) \\ 0 & \sin(\theta) & 0 \end{pmatrix} \tag{17}$$

The adiabatic basis is:

$$|E_+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos(\theta) \\ 1 \\ \sin(\theta) \end{pmatrix} ; \qquad |E_-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos(\theta) \\ -1 \\ \sin(\theta) \end{pmatrix} ; \qquad |E_0\rangle = \begin{pmatrix} \sin(\theta) \\ 0 \\ -\cos(\theta) \end{pmatrix} \tag{18}$$

The energy levels of this system are also constants and equal to $E_+ = \epsilon$, $E_0 = 0$, $E_- = -\epsilon$.
As in part (b) we will find the effective Hamiltonian:

$$V = \epsilon \cdot \begin{pmatrix} 0 & -\sin(\theta) & 0 \\ -\sin(\theta) & 0 & \cos(\theta) \\ 0 & \cos(\theta) & 0 \end{pmatrix} \tag{19}$$

The couplings are between each of the energy levels:

$$\langle E_+| W |E_0\rangle = -\frac{i\dot{\theta}}{\sqrt{2}} \qquad \langle E_+| W |E_-\rangle = 0 \qquad \langle E_-| W |E_0\rangle = \frac{i\dot{\theta}}{\sqrt{2}} \tag{20}$$

Finally the effective Hamiltonian is:

$$\mathcal{H}_{eff} = \begin{pmatrix} \epsilon & -\frac{i\dot{\theta}}{\sqrt{2}} & 0 \\ \frac{i\dot{\theta}}{\sqrt{2}} & 0 & -\frac{i\dot{\theta}}{\sqrt{2}} \\ 0 & \frac{i\dot{\theta}}{\sqrt{2}} & -\epsilon \end{pmatrix} = \left(0, \dot{\theta}, \epsilon\right) \cdot \vec{S} \tag{21}$$

In the sudden approximation $\dot{\theta} >> \epsilon$ and we can take $\Omega = (0, \dot{\theta}, 0)$ so there is only precession around the y axis.
Initially ($\theta = -\pi/2$) the particle was prepared in the first site. In the adiabatic basis this translates into being with energy level E_0 , thus:

$$|\psi(0)\rangle = |E_0\rangle|_{\theta=-\pi/2} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{22}$$

In the adaiabatic basis the energy states are the same as the polarization states of spin 1 with $|E_0\rangle = |\Updownarrow\rangle$ linear polarization in z direction.

$$|\psi(t)\rangle = e^{-i\Phi(t)S_y} |E_0\rangle = e^{-i\Phi(t)S_y} |\Updownarrow\rangle \tag{23}$$

$$\Phi(t) = \int_o^t \dot{\theta} dt = \int_{-\pi/2}^{\pi/2} d\theta = \pi \tag{24}$$

Thus $|\psi(\theta=\pi/2)\rangle$ is obtained by rotating the initial states by the angle π around the y axis. One can see that:

$$|\psi(\theta=\pi/2)\rangle = |E_0\rangle|_{\theta=\pi/2} = \begin{pmatrix}1\\0\\0\end{pmatrix} \tag{25}$$

A linear polarization state remains unchanged by rotating it by the angle π in the y direction. So the particle remains in the same state in accordance to the sudden approximation.
In order to find the survival probability in the adiabatic regime, we once again used the "interaction picture".
The survival probability is defined as the probability of staying with the same energy E_0.

$$P_t(E_0|E_0) = 1 - P_t(E_+|E_0) - P_t(E_-|E_0) \tag{26}$$

$$P_t(E_+|E_0) = P_t(E_-|E_0) = \left|\int_0^t \frac{V_{\pm 0}}{E_\pm - E_0} \cdot e^{-i(\phi_\pm - \phi_0)}\dot{\theta}dt\right|^2 \tag{27}$$

$$P_t(E_\pm|E_0) = \left|\int_{-\pi/2}^{\pi/2} -e^{\mp i(\frac{\theta\epsilon}{\dot{\theta}})}d\theta\right|^2 = \pi^2\mathrm{sinc}^2(\frac{\pi\epsilon}{2\dot{\theta}}) \tag{28}$$

So the survival probability is:

$$P_t(E_0|E_0) = 1 - 2\pi^2\mathrm{sinc}^2\left(\frac{\pi\epsilon}{2\dot{\theta}}\right) \tag{29}$$

And in the limit $\dot{\theta} << \epsilon$

$$P_t(E_0|E_0) \approx 1 \tag{30}$$

Which means the energy remains the same as expected from an adiabatic process. Note that in this particular case the site associated with E_0 is the same for $\theta = -\pi/2$ as well as for $\theta = \pi/2$. So the survival probability is also unity like in the sudden approximation.