Ex:854 - Decay from 3 sites

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The problem:

An annexation particle (energy E_0), can decay to a band of stats ($E_f < E < E_\infty$).
The density of state is uniform and equal to ν.
The hopping amplitude per unit time, to all one of the states in the band, is σ.

(1) Calculate the Enrgy corection, as a result of the association to the band.
(2) Calculate the decay factor.

Let's asume that there are 3 sites, that all of them associated to the same band of states.
The hopping amplitude of the particle from site to site is c.
(3) Write down the complex effective hemiltonian of the system as 3x3 matrix.

Lets asume that in time $t = 0$ a patricle has been put in one of the sites.
(4) Calculate the probability to find the particle at the **same** site after a while t.
(5) Calculate the probability to find the particle at **a diffente** site after a while t.
(6) What would be the answer to the last two questions, for $t = \infty$?

The solution:

(1) The hemiltonian looks like: $H = \begin{pmatrix} E_0 & \sigma & \cdots & \sigma \\ \sigma & E_f & 0 & 0 \\ \vdots & 0 & \ddots & \\ \sigma & 0 & & E_\infty \end{pmatrix}$

$$\sum^p = \sum_k \langle 0|V|k\rangle\langle k|G_0|k\rangle\langle k|V|0\rangle = \sum_k \frac{|V_k|^2}{E-E_k+i0} = \underbrace{\sum_k \frac{|V_k|^2}{E-E_k}}_{\delta E} - i\pi \sum_k \delta\left(E - E_k\right)$$

$\Rightarrow$ The energy shift is: $\delta E = \sum_k \frac{|V_k|^2}{E-E_k}$.

(2) The decay constant is : $\Gamma_0 = 2\pi \sum_{k=k_f}^{k_\infty} \sigma^2 \delta\left(E_0 - E_k\right) = 2\pi\sigma^2\nu$

(3) $H = \begin{pmatrix} H^P & V^{PQ} \\ V^{QP} & H^Q \end{pmatrix}$

$$H_{eff} = H_0^p + \sum^p = \begin{pmatrix} E_0 & c & c \\ c & E_0 & c \\ c & c & E_0 \end{pmatrix} + \sum_k^{k_\infty} \frac{|V_k|^2}{E-E_k} \cdot \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} - i\pi\sigma^2\nu \cdot \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

$$\Rightarrow Im[H_{eff}] = -i\pi\sigma^2\nu \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

(4) I would like to diagonalize the Hemiltonian in order to know how ψ evolves with time.
The Hemiltonian is composed of 2 parts, a real and an imaginary. Both of them has the same form

for the non-diagonalized part. Let's call this form as $\tilde{H}$.

So, that $\tilde{H} = const \cdot \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$.

Therefore, all we have to do is to diagonalize the matrix $\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$.

This matrix can be written with the help of the Transmition opperator D.

$$\tilde{H} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} = (D + D^{\dagger}) = (\exp^{-i\hat{p}} + \exp^{i\hat{p}}) = 2\cos(\hat{p}).$$

Therefore, the eigenstates that diagonalize it, are the momentum states $|K\rangle$.

$\tilde{H}\,|K\rangle = 2\cos(\hat{p})|K\rangle = 2\cos(k)|K\rangle$. where $k_n = \frac{2\pi}{3}n$, $n = -1, 0, 1$

The momentum states which are defined as $|K_n\rangle = \sum_n \frac{1}{\sqrt{N}} \exp^{ik_n x}|x\rangle$, are:

$$|K_0\rangle = \frac{1}{\sqrt{3}}\left[|-1\rangle + |0\rangle + |1\rangle\right]$$
$$|K_1\rangle = \frac{1}{\sqrt{3}}\left[\exp^{-i\frac{2\pi}{3}}|-1\rangle + |0\rangle + \exp^{i\frac{2\pi}{3}}|1\rangle\right]$$
$$|K_{-1}\rangle = \frac{1}{\sqrt{3}}\left[\exp^{i\frac{2\pi}{3}}|-1\rangle + |0\rangle + \exp^{-i\frac{2\pi}{3}}|1\rangle\right]$$

Eigenstates$\|K\rangle$	Eigenvalue
$\|K_0\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$	2
$\|K_1\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} \exp^{-i\frac{2\pi}{3}} \\ 1 \\ \exp^{i\frac{2\pi}{3}} \end{pmatrix}$	-1
$\|K_{-1}\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} \exp^{i\frac{2\pi}{3}} \\ 1 \\ \exp^{-i\frac{2\pi}{3}} \end{pmatrix}$	-1

Thus: in the basis $(|K_0\rangle, |K_1\rangle, |K_{-1}\rangle)$, the hemiltonian looks like:

$$H_{eff} = (E + \delta E) \cdot \hat{I} + (c + \delta E)\begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} - i\pi\sigma^2\nu \begin{pmatrix} 3 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} =$$

$$= \begin{pmatrix} E_0 + 3\delta E + 2c & & \\ & E_0 - c & \\ & & E_0 - c \end{pmatrix} - i\pi\sigma^2\nu \begin{pmatrix} 3 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix};$$

Let's assume that the particle has been put in site number $|-1\rangle$ at $t = 0$.

so: $|\psi(0)\rangle = |-1\rangle$

& using $|\, i\rangle = \sum_K |K\rangle\langle K|\, i\rangle$ (where i represents the site number: -1,0,1) we get:

$$|-1\rangle = |\psi(0)\rangle = \frac{1}{\sqrt{3}}\left[|K_0\rangle + \exp^{-i\frac{2\pi}{3}}|K_1\rangle + \exp^{i\frac{2\pi}{3}}|K_{-1}\rangle\right]$$

where $|\psi(t)\rangle = \exp^{-iH_{eff}t}|\psi_{(t=0)}\rangle$, so:

$$\psi(t) = \frac{1}{\sqrt{3}}\left[\exp^{-i(E_0+3\delta E+2c)t}\cdot\exp^{-3\pi\sigma^2\nu t}|K_0\rangle + \exp^{-i\frac{2\pi}{3}}\cdot\exp^{-i(E_0-c)t}|K_1\rangle + \exp^{i\frac{2\pi}{3}}\cdot\exp^{-i(E_0-c)t}|K_{-1}\rangle\right]$$

$$\rightarrow \psi(t) = \frac{1}{\sqrt{3}}\exp^{-i(E_0-c)t}\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}|K_0\rangle + \exp^{-i\frac{2\pi}{3}}|K_1\rangle + \exp^{i\frac{2\pi}{3}}|K_{-1}\rangle\right]$$

And the probability to find the particle at the same site $|-1\rangle$after time t is:

$$P(t)_{|-1\rangle} = |\langle\psi_{\langle -1|}(0)|\,\psi(t)\rangle|^2 = \frac{1}{9}|\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}+1+1\right]|^2 = \frac{1}{9}|\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}+2\right]|^2$$

(5) Now, we'll calculate the probabilities to find the particle at sites $|1\rangle$ & $|0\rangle$, after a while t.

Using $|\, i\rangle = \sum_K |K\rangle\langle K|\, i\rangle$ we get:

$$|1\rangle = \frac{1}{\sqrt{3}}\left[|K_0\rangle + \exp^{i\frac{2\pi}{3}}|K_1\rangle + \exp^{-i\frac{2\pi}{3}}|K_{-1}\rangle\right]$$

$$|0\rangle = \frac{1}{\sqrt{3}}\left[|K_0\rangle + |K_1\rangle + |K_{-1}\rangle\right]$$

Therefore, the probability to find the particle at site $|1\rangle$ after time t is:

$$P(t)_{|\,1\rangle} = |\langle 1\,|\psi(t)\rangle|^2 = \frac{1}{9}|\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}+\exp^{-i\frac{4\pi}{3}}+\exp^{i\frac{4\pi}{3}}\right]|^2$$

$$= \frac{1}{9}|\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}+2\cos(\tfrac{4\pi}{3})\right]|^2 = \frac{1}{9}|\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}-1\right]|^2$$

& the probability to find the particle at site $|0\rangle$ after time t is:

$$P(t)_{|\,0\rangle} = |\langle 0\,|\psi(t)\rangle|^2 = \frac{1}{9}|\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}+\exp^{-i\frac{2\pi}{3}}+\exp^{i\frac{2\pi}{3}}\right]|^2$$

$$= \frac{1}{9}|\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}+2\cos(\tfrac{2\pi}{3})\right]|^2 = \frac{1}{9}|\left[\exp^{-3i(\delta E+c)t}\cdot\exp^{-\frac{3\Gamma}{2}t}-1\right]|^2$$

(6) For $t\rightarrow\infty$we get:

The probability to find the particle at the same site for $t\rightarrow\infty$ is:
$P(t\rightarrow\infty)_{|-1\rangle} = \frac{4}{9}$.

The probabilities to find the particle at the different site when $t\rightarrow\infty$ are:
$P(t\rightarrow\infty)_{|\,1\rangle} = \frac{1}{9}$.

$P(t\rightarrow\infty)_{|\,0\rangle} = \frac{1}{9}$.

$\Rightarrow$ The total probability to find the particle in the sites after $t\rightarrow\infty$, is $P_{total} = \sum_i P_{|\,i\rangle} = \frac{2}{3}$.
$P_{total} < 1$, an answer that we would expect to get, becase part of the particle has decayed.

Note:

It's irrelevant which site you have assumed the particle has been put in, (In question 4). You should get the same results (for the probability to be at the same and at different sites, after a while), like the above results, whether you have assumed that the particle has been put at site $|-1\rangle$, or at a different one.