E8550: Decay to Continuum using Fermi Golden Rule or P+Q Formalism

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The problem:

The purpose of this problem is to find the probability $P(t)$ to find the particle at site 0 after time t for the following scenarios.

(I) A particle is placed in a site 0 and is coupled to an infinite wire (continuum). The hopping amplitude per unit time between site 0 and the continuum is c_0 and c between the continuum states.

(II) A particle is placed in a site 0 and is coupled to a circular wire (continuum). The hopping amplitude per unit time between site 0 and the continuum is c_0 and c between the continuum states.

(III) A particle is placed in a site 0 and is coupled to all of the sites in a circular wire (continuum). The hopping amplitude per unit time between site 0 and the continuum is c_0 and c between the continuum states.

(IV) A particle is placed in an arbitrary site and is coupled to all of the sites in a grid (continuum). The hopping amplitude per unit time between sites in the continuum is c_0.

Use the following guidance:

(1) Write the Hamiltonian in the position basis.
(2) Find the eigenstates of the Hamiltonian.
(3) Write the Hamiltonian without the perturbation in a diagonalized form.
(4) Write the perturbation using the same basis.
(5) Use P+Q or FGR to deduce the survival amplitude.

The solution:

Case (I)

(1) The Hamiltonian in the position basis is -

$$H=\begin{pmatrix} E_0 & c_0 & 0 & 0 & 0 & 0 & . & . & . \\ c_0 & E_1 & c & 0 & 0 & 0 & & & \\ 0 & c & E_1 & c & 0 & 0 & & & \\ 0 & 0 & c & E_1 & c & 0 & & & \\ 0 & 0 & 0 & c & E_1 & c & & & \\ 0 & 0 & 0 & 0 & c & E_1 & & & \\ . & & & & & & . & & \\ . & & & & & & & . & \\ . & & & & & & & & . \end{pmatrix}=\begin{pmatrix} E_0 & 0 & 0 & 0 & 0 & 0 & . & . & . \\ 0 & E_1 & c & 0 & 0 & 0 & & & \\ 0 & c & E_1 & c & 0 & 0 & & & \\ 0 & 0 & c & E_1 & c & 0 & & & \\ 0 & 0 & 0 & c & E_1 & c & & & \\ 0 & 0 & 0 & 0 & c & E_1 & & & \\ . & & & & & & . & & \\ . & & & & & & & . & \\ . & & & & & & & & . \end{pmatrix}+\begin{pmatrix} 0 & c_0 & 0 & 0 & 0 & 0 & . & . & . \\ c_0 & 0 & 0 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & & & \\ . & & & & & & . & & \\ . & & & & & & & . & \\ . & & & & & & & & . \end{pmatrix}$$

(2) The eigenstates of the Hamiltonian are $|k>=\sqrt{\frac{2}{L}}\sum sink_n x|x>$ since zero boundary conditions apply at the beginning of the lead. Because zero boundary conditions apply at the end of the lead (length L). $k_n=\frac{\pi}{Na}n=\frac{\pi}{L}n$. This is because $Na=L$, The number of sites $N\to\infty$ and the distance between the sites a is constant, a fact which is consistant with $L\to\infty$.

(3) The diagonalized Hamiltonian is-

$$\tilde{H_0}=\begin{pmatrix} E_0 & 0 & 0 & 0 & . & . \\ 0 & E_{k_1} & 0 & 0 & & \\ 0 & 0 & E_{k_2} & 0 & & \\ 0 & 0 & 0 & E_{k_3} & & \\ . & & & & . & \\ . & & & & & . \end{pmatrix}$$

The original Hamiltonain can be written as a superposition of $\hat{H}_0, \hat{D}, \hat{D}^{\dagger}$ and $\hat{A}$.

Where $\hat{A}=\begin{pmatrix} 0 & 0 & 0 & . & . & -1 \\ 0 & 0 & 0 & & & \\ 0 & 0 & 0 & & & \\ . & & & . & & \\ . & & & & . & \\ -1 & & & & & . \end{pmatrix}$

Noticing that because of zero boudary conditions at the edges the first and last elements in the eigenstates are zero $\hat{A}|k_n>=0$. Therefore we can omit $\hat{A}$ from the Hamiltonian and write it as $\hat{H}=\hat{H}_0+c\hat{D}+c\hat{D}^{\dagger}$ leading to eigenvalues in the form $E_{k_n}=2c\cos k_n a+E_1, k_n=\frac{\pi}{L}n$

(4) Using the same basis to diagonalize the perturbation gives-

$<0|H|k_n>=\sum_x<0|H|x><x|k_n>=<0|H|x=1><1|k_n>=c_0\sqrt{\frac{2}{N}}\sin(k_n a)$, or in matrix form:

$$\tilde{H}_1=c_0\sqrt{\frac{2}{N}}\begin{pmatrix} 0 & \sin k_1 a & \sin k_2 a & \sin k_3 a & . & . \\ \sin k_1 a & 0 & 0 & 0 & & \\ \sin k_2 a & 0 & 0 & 0 & & \\ \sin k_3 a & 0 & 0 & 0 & & \\ . & & & & . & \\ . & & & & & . \end{pmatrix}$$

(5) The probability to find the particle at site 0 after time t is given by the Fourier transform of the resolvent: $P=|FT[<\psi|G(\omega)|\psi>]|^2=|FT[<\psi|G^P(\omega)|\psi>]|^2$. Now, G^P is given by-

$G^P=\frac{1}{z-(H_0^P+\sum^P)}$

Where the self energy $\sum^P=\sum_k\frac{|V_k|^2}{E-E_k}-i\pi\sum_k|V_k|^2\delta(E-E_k)\equiv\delta E_0-i\frac{\Gamma_0}{2}$

In our problem, $\delta E_0 = \sum_k \frac{c_0^2 \frac{2}{N} \sin^2 k_n a}{E-(2c\cos k_n a+E_1)}$ and $\Gamma_0 = 2\pi c_0^2 \frac{2}{N} \sum_k \sin^2 k_n a \delta(E - E_k)$. Substituting this into the resolvent:

$$G^P = \frac{1}{z-(H_0^P+\sum_k \frac{c_0^2 \frac{2}{N} \sin^2 k_n a}{E-(2c\cos k_n a+E_1)} - i\pi c_0^2 \frac{2}{N} \sum_k \sin^2 k_n a \delta(E-E_k))}$$

Again, the Fourier transform of the above expression gives the survival probability.

Case (II)

(1) The Hamiltonian in the position basis is -

$$H = \begin{pmatrix} E_0 & c_0 & 0 & 0 & 0 & . & . & . & 0 \\ c_0 & E_1 & c & 0 & 0 & & & & c \\ 0 & c & E_1 & c & 0 & & & & 0 \\ 0 & 0 & c & E_1 & c & & & & 0 \\ 0 & 0 & 0 & c & E_1 & & & & 0 \\ . & & & & & . & & & . \\ . & & & & & & . & & . \\ . & & & & & & & . & . \\ 0 & c & 0 & 0 & 0 & . & . & . & 0 \end{pmatrix} = \begin{pmatrix} E_0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ 0 & E_1 & c & 0 & 0 & & & & c \\ 0 & c & E_1 & c & 0 & & & & 0 \\ 0 & 0 & c & E_1 & c & & & & 0 \\ 0 & 0 & 0 & c & E_1 & & & & 0 \\ . & & & & & . & & & . \\ . & & & & & & . & & . \\ . & & & & & & & . & . \\ 0 & c & 0 & 0 & 0 & . & . & . & 0 \end{pmatrix} + \begin{pmatrix} 0 & c_0 & 0 & 0 & 0 & 0 & . & . & . \\ c_0 & 0 & 0 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & & & \\ . & & & & & & . & & \\ . & & & & & & & . & \\ . & & & & & & & & . \end{pmatrix}$$

(2) The eigenstates of the Hamiltonian are $|k>=\sqrt{\frac{1}{N}}\sum e^{ik_n x}|x>$ since periodical boundary conditions apply. $k_n = \frac{2\pi}{Na}n = \frac{\pi}{L}n$. This is because $Na = L$, although the number of sites $N \to \infty$, the distance between the sites $a \to 0$ keeping L, the perimeter of the loop, constant.

(3) The diagonalized Hamiltonian is-

$$\tilde{H_0} = \begin{pmatrix} E_0 & 0 & 0 & 0 & . & . \\ 0 & E_{k_1} & 0 & 0 & & \\ 0 & 0 & E_{k_2} & 0 & & \\ 0 & 0 & 0 & E_{k_3} & & \\ . & & & & . & \\ . & & & & & . \end{pmatrix}$$

The original Hamiltonain can be written as a superposition of $\hat{H}_0, \hat{D}$ and $\hat{D}^\dagger$.

Noticing that we can write the hamiltonian as $\hat{H} = \hat{H}_0 + c\hat{D} + c\hat{D}^\dagger$ leading to eigenvalues in the form $E_k = 2c\cos k_n a + E_1$.

(4) Using the same basis to diagonalize the perturbation gives-

$$\tilde{H}_1 = \begin{pmatrix} 0 & \frac{1}{\sqrt{N-1}}c_0 & \frac{1}{\sqrt{N-1}}c_0 & \frac{1}{\sqrt{N-1}}c_0 & . & . \\ \frac{1}{\sqrt{N-1}}c_0 & 0 & 0 & 0 & & \\ \frac{1}{\sqrt{N-1}}c_0 & 0 & 0 & 0 & & \\ \frac{1}{\sqrt{N-1}}c_0 & 0 & 0 & 0 & & \\ . & & & & . & \\ . & & & & & . \end{pmatrix}$$

(5) The probability to find the particle at site 0 after time t is given by the FGR as $e^{-\Gamma t}$, where Γ is-

$\Gamma_{ij} = 2\pi \sum_k |V_k|^2 \delta(E - E_k) = 2\pi\rho(E)|V|^2 = \frac{2\pi c_0^2}{N-1}\rho(E)$

The energy density $\rho(E) \propto N$ and therefore for sufficiently large N's the dependency on N is taken out of the equation.

Γ is the same decay constant as can be recieved from the $P + Q$ formalism. The FGR is a survival probability approximation of the resolvent theory for $E \propto E_0$.

*If one chooses to diagonalize the Hamiltonian using a real basis comprised of sin or cos instead of the complex exp basis we chose here, it can be noticed that the perturbation couples only half of the energies (the symmetric part including E_0).

Case (III)

(1) The Hamiltonian in the position basis is -

$$H = \begin{pmatrix} E_0 & c_0 & c_0 & c_0 & c_0 & \cdots & c_0 \\ c_0 & E_1 & c & 0 & 0 & & c \\ c_0 & c & E_1 & c & 0 & & 0 \\ c_0 & 0 & c & E_1 & c & & 0 \\ c_0 & 0 & 0 & c & E_1 & & 0 \\ \vdots & & & & & \ddots & \vdots \\ c_0 & c & 0 & 0 & 0 & \cdots & 0 \end{pmatrix} = \begin{pmatrix} E_0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & E_1 & c & 0 & 0 & & c \\ 0 & c & E_1 & c & 0 & & 0 \\ 0 & 0 & c & E_1 & c & & 0 \\ 0 & 0 & 0 & c & E_1 & & 0 \\ \vdots & & & & & \ddots & \vdots \\ 0 & c & 0 & 0 & 0 & \cdots & 0 \end{pmatrix} + \begin{pmatrix} 0 & c_0 & c_0 & c_0 & c_0 & \cdots & c_0 \\ c_0 & 0 & 0 & 0 & 0 & & 0 \\ c_0 & 0 & 0 & 0 & 0 & & 0 \\ c_0 & 0 & 0 & 0 & 0 & & 0 \\ c_0 & 0 & 0 & 0 & 0 & & 0 \\ \vdots & & & & & \ddots & \vdots \\ c_0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

(2) The eigenstates of the Hamiltonian are $|k>=\sqrt{\frac{1}{N}}\sum e^{ik_n x}|x>$ since periodical boundary conditions apply. $k_n = \frac{2\pi}{Na}n = \frac{\pi}{L}n$. This is because $Na = L$, although the number of sites $N \rightarrow \infty$, the distance between the sites $a \rightarrow 0$ keeping L, the perimeter of the loop, constant.

(3) The diagonalized Hamiltonian is-

$$\tilde{H_0} = \begin{pmatrix} E_0 & 0 & 0 & 0 & \cdot & \cdot \\ 0 & E_{k_1} & 0 & 0 & & \\ 0 & 0 & E_{k_2} & 0 & & \\ 0 & 0 & 0 & E_{k_3} & & \\ \cdot & & & & \cdot & \\ \cdot & & & & & \cdot \end{pmatrix}$$

The original Hamiltonain can be written as a superposition of $\hat{H}_0, \hat{D}$ and $\hat{D}^{\dagger}$.

Noticing that we can write the hamiltonian as $\hat{H} = \hat{H}_0 + c\hat{D} + c\hat{D}^{\dagger}$ leading to eigenvalues in the form $E_k = 2c\cos k_n a + E_1$.

(4) Using the same basis to diagonalize the perturbation gives-

$$\tilde{H_1} = \begin{pmatrix} 0 & \sqrt{N-1}c_0 & 0 & 0 & \cdot & \cdot \\ \sqrt{N-1}c_0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ \cdot & & & & \cdot & \\ \cdot & & & & & \cdot \end{pmatrix}$$

(5) The probability to find the particle at site 0 after time t is given by the $P+Q$ formalism as the Fourier transform of the resolvent: $P = |FT[<\psi|G(\omega)|\psi>]|^2 = |FT[<\psi|G^P(\omega)|\psi>]|^2$. Now, G^P is given by-

$$G^P = \frac{1}{z-(H_0^P + \sum^P)}$$

Where the self energy $\sum^P = \sum_k \frac{|V_k|^2}{E-E_k} - i\pi\sum_k |V_k|^2\delta(E-E_k) \equiv \delta E_0 - i\frac{\Gamma_0}{2}$

In our problem, $\delta E_0 = \frac{c_0^2(N-1)}{E-(2c\cos k_1 a + E_1)}$ and $\Gamma_0 = 2\pi c_0^2(N-1)\delta(E-E_1)$. Substituting this into the resolvent:

$$G^P = \frac{1}{z-(H_0^P + \frac{c_0^2(N-1)}{E-(2c\cos k_1 a+E_1)} - i\pi c_0^2(N-1)\delta(E-E_1)}$$

Again, the Fourier transform of the above expression gives the survival probability.

*One may notice that the coupling is only to one energy level.

Case (IV)

(1) The Hamiltonian in the position basis is -

$$H = \begin{pmatrix} E_1 & c_0 & c_0 & c_0 & c_0 & . & . & . & c_0 \\ c_0 & E_1 & c_0 & c_0 & c_0 & & & & c_0 \\ c_0 & c_0 & E_1 & c_0 & c_0 & & & & c_0 \\ c_0 & c_0 & c_0 & E_1 & c_0 & & & & c_0 \\ c_0 & c_0 & c_0 & c_0 & E_1 & & & & . \\ . & & & & & . & & & . \\ . & & & & & & . & & . \\ . & & & & & & & . & c_0 \\ c_0 & c_0 & c_0 & c_0 & . & . & . & c_0 & E_1 \end{pmatrix} = \begin{pmatrix} E_1 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ 0 & E_1 & 0 & 0 & 0 & & & & 0 \\ 0 & 0 & E_1 & 0 & 0 & & & & 0 \\ 0 & 0 & 0 & E_1 & 0 & & & & 0 \\ 0 & 0 & 0 & 0 & E_1 & & & & . \\ . & & & & & . & & & . \\ . & & & & & & . & & . \\ . & & & & & & & . & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & E_1 \end{pmatrix} + \begin{pmatrix} 0 & c_0 & c_0 & c_0 & c_0 & . & . & . & c_0 \\ c_0 & 0 & c_0 & c_0 & c_0 & & & & c_0 \\ c_0 & c_0 & 0 & c_0 & c_0 & & & & c_0 \\ c_0 & c_0 & c_0 & 0 & c_0 & & & & c_0 \\ c_0 & c_0 & c_0 & c_0 & 0 & & & & . \\ . & & & & & . & & & . \\ . & & & & & & . & & . \\ . & & & & & & & . & c_0 \\ c_0 & c_0 & c_0 & c_0 & . & . & . & c_0 & 0 \end{pmatrix}$$

(2) The original Hamiltonian is already diagonalized, hence we shall try and find a basis which diagonalizes the perturbation. This basis is the momentum basis: $|k >= \sqrt{\frac{1}{N}} \sum e^{ik_n x}|x >$, where $k_n = \frac{2\pi}{\sqrt{N}} n$.

(3) The diagonalized Hamiltonian is given by:

$\langle k|(c_0 \sum_x \sum_{x'} |x\rangle\langle x'|)|k'\rangle = c_0 \sum_x \langle k|x\rangle \sum_{x'} \langle k'|x'\rangle = c_0 \sum_x \frac{e^{ikx}}{\sqrt{N}} \sum_{x'} \frac{e^{ik'x'}}{\sqrt{N}} = c_0 \frac{1}{\sqrt{N}} N\delta_{k,0} \frac{1}{\sqrt{N}} N\delta_{k',0} = -Nc_0\delta_{k,0}\delta_{k',0}$

In matrix form the Hamiltonian is:

$$\tilde{H_0} = \begin{pmatrix} E_{k_0} & 0 & 0 & 0 & . & . \\ 0 & E_{k_1} & 0 & 0 & & \\ 0 & 0 & E_{k_2} & 0 & & \\ 0 & 0 & 0 & E_{k_3} & & \\ . & & & & . & \\ . & & & & & . \end{pmatrix}$$

Where $E_{k_0} = Nc_0 + E_1$ and $E_{k_{n>0}} = -c_0 + E_1$.

(5) This is an exact solution, hence the survival probability is given by

$P(t) = | < x = 0|e^{-iHt}|x = 0 > |^2 = | \sum\limits_k < x = 0|e^{-iHt}|k >< k|x = 0 >| = | \sum\limits_k e^{-iE_{k_n}t}| < x = 0||k > |^2|^2 =$
$|\frac{1}{N} \sum\limits_n e^{-iE_{k_n}t}|e^{2ik_n \cdot x_0}|^2|^2 = |\frac{1}{N} \sum\limits_n e^{-iE_{k_n}t}|^2$
$= |\frac{1}{N}(e^{-iE_{k_0}t} + Ne^{-iE_{k_1}t}|^2$