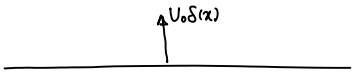
Session 13 _ chapter 9, 10.1

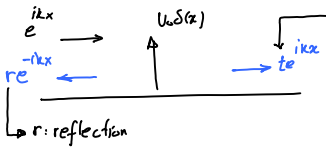
Note Title 11/6/2008

Example calculate transmission probability function for a nanowire with a point defect inside. Model the point defect with the potential:

$U(x) = U_0\delta(x)$.



Solution 1 direct analytical solution of the Schrödinger equation



t: Transmission amplitude

$\rightarrow T = |t|^2$ transmission probability

Schrödinger Equ in effective mass:

$$\left[E_c - \frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]\psi(x) = E\psi(x)$$

$A \neq 0 \rightarrow U(x) = 0 \rightarrow \psi(x) = e^{\pm ikx}$ and $E = E_c + \hbar^2k^2/2m$

Since e^{ikx} and e^{-ikx} both satisfy the schrödinger equation which is linear, any linear combination of them also is a solution.

This is 2nd order differential equation and we need two boundary conditions. one is on ψ and the other on $\frac{d\psi}{dx}$ at $x=0$.

we need to check ψ at $x=0$ now. ψ is alway continous $\rightarrow$ $e^{ikx} + re^{-ikx} = te^{ikx}$ at $x=0 \rightarrow 1+r=t$ (I)

To check for $\frac{d\psi}{dx}$ we need to work further. Since there is a delta function in the equation, we need to integrate it out:

$$E_c\psi(x) - \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U_0\delta(x)\psi(x) = E\psi(x) \rightarrow \int_{0^-}^{0^+} E_c\psi(x)dx - \frac{\hbar^2}{2m}\int_{0^-}^{0^+}\frac{d^2}{dx^2}\psi(x)dx + U_0\int_{0^-}^{0^+}\delta(x)\psi(x)dx = E\int_{0^-}^{0^+}E(x)dx$$

$\int_{0^-}^{0^+} E_c\psi(x)dx = 0$; $\int_{0^-}^{0^+}\frac{d^2}{dx^2}\psi(x)dx = \frac{d\psi}{dx}\Big|_{0^+} - \frac{d\psi}{dx}\Big|_{0^-}$; $U_0\int_{0^-}^{0^+}\delta(x)\psi(x)dx = \psi(0)$; $\int_{0^-}^{0^+}E(x)dx = 0$

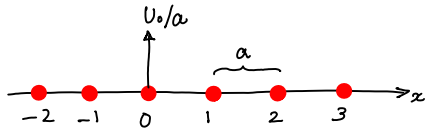
$$\rightarrow \underbrace{\frac{d\psi}{dx}\Big|_{x=0^+}}_{ikt} - \underbrace{\frac{d\psi}{dx}\Big|_{x=0^-}}_{ik-irk} = \frac{2mU_0}{\hbar^2}\underbrace{\psi(0)}_{t} \rightarrow ik(t-1+r) = \frac{2mU_0t}{\hbar^2} \rightarrow r = 1 - t - i\frac{2mU_0t}{\hbar^2k}$$ Substitute in (I) $\rightarrow$

$$t - 1 = 1 - t - \frac{i2mU_0t}{\hbar^2k} \rightarrow t\left(1 + \frac{imU_0}{\hbar^2k}\right) = 1 \rightarrow t = \frac{\hbar^2k}{\hbar^2k + imU_0} = \frac{\hbar(\hbar k/m)}{\hbar(\hbar k/m) + iU_0} = \frac{\hbar v}{\hbar v + iU_0}$$

(v: velocity)

$$T = |t|^2 = \frac{\hbar^2v^2}{\hbar^2v^2 + U_0^2}$$ note that $v = \frac{\hbar k}{m} = v(E)$

Solution 2: Discrete lattice approach



Now we have instead of $\psi(x) \rightarrow$ $\begin{bmatrix}\vdots\\ \psi_{-2}\\ \psi_{-1}\\ \psi_0\\ \psi_1\\ \psi_2\\ \vdots\end{bmatrix}$

Note that $U_0\delta(x)$ has become $\frac{U_0}{a}$ because $\int_{0^-}^{0^+}\delta(x)dx = \int_{\text{unit cell}}\frac{1}{a}dx = 1$

At point $x=0$, we can write: $\left(E_c - \frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U_0\delta(x)\right)\psi(x) = E\psi(x) \rightarrow E_c\psi(0) + \frac{U_0}{a}\psi(0) - \underbrace{\frac{\hbar^2}{2ma^2}}_{t_0}(\psi_{-1} + \psi_1 - 2\psi_0) = E\psi_0$

$\rightarrow \left(E_c + 2t_0 + \frac{U_0}{a}\right)\psi_0 - t_0\psi_{-1} - t_0\psi_1 = E\psi_0$

At $x=0^+$: $\psi_{+1} = te^{ika}$ and $\psi_0 = t \rightarrow \psi_{+1} = \psi_0e^{ika}$

At $x=0^-$: $\psi_{-1} = e^{-ika} + re^{ika}$ and $\psi_0 = 1+r \rightarrow \psi_{-1} = e^{-ika} + (\psi_0 - 1)e^{ika}$

Substitute ψ_{+1} and $\psi_{-1} \Rightarrow$

$$\left(E_c+2t_0+\frac{U_0}{a}-t_0e^{ika}-t_0e^{ika}\right)\psi_0-t_0\left(e^{-ika}-e^{ika}\right)=E\psi_0 \quad \text{group the terms} \rightarrow$$

$$\left(E-E_c-2t_0-\frac{U_0}{a}+\underbrace{t_0e^{ika}}_{-t_0e^{-ika}}+\underbrace{t_0e^{ika}}_{-t_0e^{-ika}}\right)\psi_0=-\underbrace{t_0\left(e^{ika}-e^{-ika}\right)}_{i2t_0\sin ka=i\hbar v/a}$$

$-t_0e^{-ika}$ → $i\hbar v/a$; $+t_0e^{ika}$ → $2t_0\cos ka$

Note: For 1D lattice $E=E_c+2t_0(1-\cos ka)$ → $v=\frac{1}{\hbar}\frac{\partial E}{\partial k}$ → $\hbar v=2at_0\sin ka$ (velocity)

$$\left(\cancel{E}-\cancel{E_c}-2t_0(1-\cancel{\cos ka})-\frac{U_0}{a}+\frac{i\hbar v}{a}\right)\psi_0=\frac{i\hbar v}{a} \rightarrow \psi_0=\frac{i\hbar v}{i\hbar v-U_0} \quad \text{but } \psi_0=t \rightarrow T=|t|^2=\frac{\hbar^2v^2}{\hbar^2v^2+U_0^2}$$ Same as before.

Solution 3: Green's function approach

$T(E)=\text{Trace}\left(\Gamma_1 G \Gamma_2 G^\dagger\right)$ $\quad \Gamma_1=i(\Sigma_1-\Sigma_1^\dagger)=i(-t_0e^{ika}+t_0e^{-ika})=it_0(-2i\sin ka)=2t_0\sin ka=\frac{\hbar v}{a}$

Similarly $\Gamma_2=2t_0\sin ka=\frac{\hbar v}{a}$ (Note that for 1D lattice we had $\Sigma=-t_0e^{ika}$)

$$G=(EI-H-\Sigma_1-\Sigma_2)^{-1} \quad ; \quad H=E_c+2t_0+\frac{U_0}{a} \rightarrow$$

$$G=\left(E-E_c-2t_0+2t_0e^{ika}-\frac{U_0}{a}\right)^{-1}=\Big(\overbrace{\cancel{E_c}+\cancel{2t_0}\underbrace{-2t_0\cos ka}_{-t_0e^{ika}-t_0e^{-ika}}}^{E}-\cancel{E_c}-\cancel{2t_0}+2t_0e^{ika}-\frac{U_0}{a}\Big)^{-1}$$

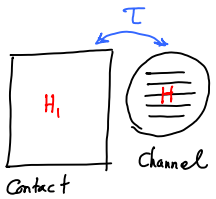
$$=\left(\underbrace{2it_0\sin ka}_{i\hbar v/a}-\frac{U_0}{a}\right)^{-1}=\frac{a}{i\hbar v-U_0}$$

$$\rightarrow T(E)=\left(\frac{\hbar v}{a}\right)\left(\frac{a}{i\hbar v-U_0}\right)\left(\frac{\hbar v}{a}\right)\left(\frac{a}{i\hbar v+U_0}\right)=\frac{\hbar^2v^2}{\hbar^2v^2+U_0^2}$$ which is same as before.

The power the Green's functran approach is that one can apply it similarly to any complex problem without going into detail of its physics. The disadvantage is that we can calculate everything without really understanding anything!

Non-equilibrium Density Matrix

We want to show $[\rho]=\int\frac{dE}{2\pi}G^n(E)$. For simplicity I consider one contact. But you can generalize to two or more contacts.



Start from Schrödinger equation in Matrix form in real space:

$$E\psi=H\psi$$

$$E\begin{Bmatrix}\psi\\ \hline \phi\end{Bmatrix}=\left[\begin{array}{c|c} H & \tau_1 \\ \hline \tau_1^\dagger & H_1+i0^+\end{array}\right]$$

Note: $\psi=\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{Bmatrix}$ in channel and $\phi=\begin{Bmatrix}\phi_1\\ \phi_2\\ \vdots\end{Bmatrix}$ in contact. H, τ, and H_1 are also a matrix each.

If we consider the contact before connecting to the channel, we have: $(EI-H_1+i0^+)\phi_1=0$.

After the connection ϕ_1 changes and say becomes ϕ_1+X. So we have,

$$E\begin{Bmatrix}\psi\\ \hline \phi_1+X\end{Bmatrix}=\begin{bmatrix} H & \tau_1 \\ \tau_1^\dagger & H_1-i0^+\end{bmatrix}\begin{Bmatrix}\psi\\ \phi_1+X\end{Bmatrix} \rightarrow \begin{cases} E\psi=H\psi+\tau_1\phi_1+\tau_1X & (I)\\ \cancel{E\phi_1}+EX=\tau_1^\dagger\psi+(H_1-\cancel{i0^+})\phi_1+(H_1-i0^+)X \rightarrow X\end{cases}$$

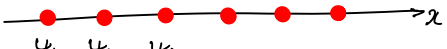
$$(EI+i0^+-H_1)X=\tau_1^\dagger\psi \rightarrow X=\underbrace{(EI+i0^+-H_1)^{-1}}_{G_1}\tau_1^\dagger\psi=G_1\tau_1^\dagger\psi \quad \text{Substitute in } (I) \Rightarrow$$

$$E\psi = H\psi + \tau_1\phi_1 + \underbrace{\tau_1 G_1 \tau_1^+}_{\Sigma_1}\psi \Rightarrow (EI - H - \Sigma_1)\psi = \tau_1\phi_1$$

Note: For two contacts we would have: $(EI - H - \Sigma_1 - \Sigma_2)\psi = \tau_1\phi_1 + \tau_2\phi_2$ Let's continue with one contact:

$$\rightarrow \psi = \underbrace{(EI - H - \Sigma_1)^{-1}}_{G} \underbrace{\tau_1\phi_1}_{S_1} = G S_1$$ Having ψ, now we want to find the electron density.

Note that ψ is a vector with elements for each lattice point in real space. Since there are many states available in contact, let's call them ϕ_α, by coupling each of these ϕ_α's induce a state in channel. So we would have many ψ_α vectors that each vector corresponds to a separate state. So to count the net electron density we should sum over α: $\sum_\alpha |\psi_\alpha|^2$



$\psi_{\alpha 1}$ $\psi_{\alpha 2}$ $\psi_{\alpha 3}$ ...

$|\psi_{\alpha 1}|^2$ $|\psi_{\alpha 2}|^2$ $|\psi_{\alpha 3}|^2$ ... $\Rightarrow$ electron density $\propto \sum_\alpha \left(|\psi_{\alpha 1}|^2 + |\psi_{\alpha 2}|^2 + |\psi_{\alpha 3}|^2 + \cdots \right) = \sum_\alpha \underbrace{[\psi_{1\alpha}^* \ \psi_{2\alpha}^* \cdots]}_{\psi_\alpha^+} \underbrace{\begin{bmatrix} \psi_{1\alpha} \\ \psi_{2\alpha} \\ \vdots \end{bmatrix}}_{\psi_\alpha} = \sum_\alpha \psi_\alpha^+ \psi_\alpha$

We could also say $\psi_\alpha \psi_\alpha^+ = \sum_\alpha \begin{bmatrix} \psi_{\alpha 1} \\ \psi_{\alpha 2} \\ \vdots \end{bmatrix} [\psi_{\alpha 1}^* \ \psi_{\alpha 2}^* \cdots] = \sum_\alpha \begin{bmatrix} |\psi_{\alpha 1}|^2 & \psi_{\alpha 1}\psi_{\alpha 2}^* & \cdots \\ \psi_{\alpha 1}^*\psi_{\alpha 2} & |\psi_{\alpha 2}|^2 & \\ \vdots & & \ddots \end{bmatrix} \rightarrow$ density $\propto \sum_\alpha$ Trace $(\psi_\alpha \psi_\alpha^+)$

note that $\psi_\alpha^+\psi_\alpha$ is a number, but $\psi_\alpha\psi_\alpha^+$ is a matrix. So if you use $\psi_\alpha \psi_\alpha^+$, you must take a trace.

We derived $\psi_\alpha = G\tau_1\phi_\alpha \rightarrow$ electron density $= \sum_\alpha f_1(\varepsilon_\alpha)\psi_\alpha\psi_\alpha^+ = \sum_\alpha f_1(\varepsilon_\alpha) G\tau_1\phi_\alpha\phi_\alpha^+\tau_1^+ G^+$

If we use delta function property that $\sum_\alpha f_1(\varepsilon_\alpha) = \int dE\, f_1(E) \sum_\alpha \delta(E - \varepsilon_\alpha) \Rightarrow$

density matrix $\rho = \int dE\, f_1(E)\, G\tau_1 \underbrace{\sum_\alpha \phi_\alpha \phi_\alpha^+ \delta(E-\varepsilon_\alpha)}_{\text{spectral function } \frac{A_1}{2\pi}} \tau_1^+ G^+$ (I use small a to distinguish with A_1)

$$= \int \frac{dE}{2\pi} f_1(E) \underbrace{G \overbrace{\tau_1 a_1 \tau_1^+}^{\Gamma_1} G^+}_{A_1 = G\Gamma_1 G^+}$$

note: $\Gamma_1 = i(\Sigma_1 - \Sigma_1^+) = i(\tau_1 G_1 \tau_1^+ - \tau_1 G_1^+ \tau_1^+) = i\tau_1 (G_1 - G_1^+)\tau_1^+ = \tau_1 a_1 \tau_1^+$

$G_n = f_1 A_1$ ⟶ for two contact we would have: $G_n = A_1 f_1 + A_2 f_2$

$$\rightarrow \quad [\rho] = \int \frac{dE}{2\pi} G^n$$ ⟶ G_n is matrix version of $n(E)$

Current: inflow/outflow

We would like to derive the matrix equations for the current. we again consider only one contact for simplicity, and start with Schrodinger equ:

$$E\begin{bmatrix} \psi \\ \phi \end{bmatrix} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R \end{bmatrix} \begin{bmatrix} \psi \\ \phi \end{bmatrix}$$ If the contact wavefunction before connection is ϕ_R, we assume after it is connected to the channel it changes to: $\phi = \phi_R + X \rightarrow$

$$E\begin{bmatrix} \psi \\ \phi_R + X \end{bmatrix} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R - i\eta \end{bmatrix} \begin{bmatrix} \psi \\ \phi_R + X \end{bmatrix} \rightarrow \begin{cases} E\psi = H\psi + \tau\phi_R + \tau X \rightarrow E\psi = H\psi + \overbrace{\tau\phi_R}^{S} + \overbrace{\tau G_R \tau^+}^{\Sigma}\psi & (I) \\ E\phi_R + EX = \tau^+\psi + (H_R - i\eta)\phi_R + (H_R - i\eta)X \rightarrow X = G_R\tau^+\psi \end{cases}$$

$\eta \triangleq 0^+ I$

$(I) \rightarrow \quad E\psi = (H+\Sigma)\psi + S \rightarrow \psi = (EI - H - \Sigma)^{-1} S = GS$

current is the rate at which the probability is changing inside the device: $\frac{d}{dt}\psi^\dagger\psi$

$$i\hbar \frac{\partial}{\partial t}\begin{bmatrix}\psi \\ \phi\end{bmatrix} = \begin{bmatrix} H & \tau \\ \tau^\dagger & H_R - i\eta \end{bmatrix}\begin{bmatrix}\psi \\ \phi\end{bmatrix}$$

$$\frac{d}{dt}(\psi^\dagger\psi) = \frac{d\psi^\dagger}{dt}\psi + \psi^\dagger\frac{d\psi}{dt}$$

from schrodinger equ: $i\hbar\frac{d\psi}{dt} = H\psi + \tau\phi \rightarrow -i\hbar\frac{\partial\psi^\dagger}{\partial t} = \psi^\dagger H + \phi^\dagger\tau^\dagger$

$\downarrow \psi^\dagger_x$ $\qquad$ $\downarrow x\psi$

① $i\hbar\,\psi^\dagger\frac{d\psi}{dt} = \psi^\dagger H\psi + \psi^\dagger\tau\phi$ $\qquad$ ② $-i\hbar\frac{d\psi^\dagger}{dt}\psi = \psi^\dagger H\psi + \phi^\dagger\tau^\dagger\psi$

① − ② $\rightarrow$ $i\hbar\left(\psi^\dagger\frac{d\psi}{dt} + \frac{d\psi^\dagger}{dt}\psi\right) = \psi^\dagger\tau\phi - \phi^\dagger\tau^\dagger\psi \rightarrow \frac{d}{dt}(\psi\psi^\dagger) = \frac{\psi^\dagger\tau\phi - \phi^\dagger\tau^\dagger\psi}{i\hbar}$

For current we have: $I = \text{Trace}\left(\frac{\psi^\dagger\tau\phi - \phi^\dagger\tau^\dagger\psi}{i\hbar}\right)$

$\phi = \phi_R + \chi \rightarrow I = \underbrace{\text{Trace}\left(\frac{\psi^\dagger\tau\phi_R - \phi_R^\dagger\tau^\dagger\psi}{i\hbar}\right)}_{I_{in}:\ \text{inflow to the channel}} + \underbrace{\text{Trace}\left(\frac{\psi^\dagger\tau\chi - \chi^\dagger\tau^\dagger\psi}{i\hbar}\right)}_{-I_{out}:\ \text{outflow from channel to contact}}$

$S^\dagger G^\dagger$ $\quad$ S $\quad$ $S^\dagger$ $\quad$ GS

$$I_{in} = \text{Trace}\left[\frac{\psi^\dagger\tau\phi_R - \phi_R^\dagger\tau^\dagger\psi}{i\hbar}\right] = \text{Trace}\left[\frac{S^\dagger G^\dagger S - S^\dagger G S}{i\hbar}\right] = \text{Trace}\left[\frac{S^\dagger(G^\dagger - G)S}{i\hbar}\right] = \text{Trace}\left[\frac{S^\dagger A S}{\hbar}\right] = \text{Trace}\left(\frac{ASS^\dagger}{\hbar}\right)$$

This is for one state. We should also consider summing over all occupied states: $S = \tau\phi_R$

$$I_{in} = \sum_\alpha f(\varepsilon_\alpha - \mu)\,\text{Trace}\left(\frac{AS_\alpha^\dagger S_\alpha}{\hbar}\right) = \frac{1}{\hbar}\int dE\, f(\varepsilon_\alpha - \mu)\,\text{Trace}\left(\sum S_\alpha S_\alpha^\dagger \delta(E-\varepsilon_\alpha)\, A\right)$$

$$\sum \tau\phi_{R\alpha}\phi_{R\alpha}^\dagger\tau^\dagger\delta(E-\varepsilon_\alpha)$$

$$\tau\underbrace{\sum_\alpha \phi_{R\alpha}\phi_{R\alpha}^\dagger\delta(E-\varepsilon_\alpha)}_{a/2\pi}\tau^\dagger$$

$$\Gamma = \tau a \tau^\dagger/2\pi$$

$$\rightarrow I_{in} = \frac{1}{\hbar}\int\frac{dE}{2\pi} f_1(E)\,\text{Trace}(\Gamma A_1)$$

$\alpha = G_R\tau^\dagger\psi$

Similarly for the outflow, we have: $I_{out} = -\text{Trace}\left(\frac{\psi^\dagger\tau\chi - \chi^\dagger\tau^\dagger\psi}{i\hbar}\right) = \frac{-1}{i\hbar}\text{Trace}\left(\psi^\dagger\tau G_R\tau^\dagger\psi - \psi^\dagger\tau G_R^\dagger\tau^\dagger\psi\right)$

$$= \frac{-1}{i\hbar}\text{Trace}\left(\overbrace{\tau G_R\tau^\dagger}^{\Sigma}\psi\psi^\dagger - \overbrace{\tau G_R^\dagger\tau^\dagger}^{\Sigma^\dagger}\psi\psi^\dagger\right) = \frac{1}{\hbar}\text{Trace}\left\{\overbrace{i(\Sigma - \Sigma^\dagger)}^{\Gamma}\psi\psi^\dagger\right\}$$

Now Sum over α:

$\psi_\alpha = G\tau_i\phi_\alpha$

$$I_{out} = \frac{1}{\hbar}\sum_\alpha f(\varepsilon_\alpha - \mu)\,\text{Trace}(\Gamma\psi\psi^\dagger) = \frac{1}{\hbar}\int dE\, f_1(E)\,\text{Trace}\left(\Gamma\sum_\alpha \psi_\alpha\psi_\alpha^\dagger\delta(E-\varepsilon_\alpha)\right)$$

$$= \frac{1}{h}\int dE\ \mathrm{Trace}\Big(\Gamma f_1(E)\ \Gamma\ G\ \underbrace{\tau_1\ \overbrace{\textstyle\sum_\alpha \Phi_\alpha \Phi_\alpha^\dagger \delta(E-\varepsilon_\alpha)}^{\alpha/2\pi}\ \tau_1^\dagger}_{\Gamma_1/2\pi}\ G^\dagger\Big)$$

$$= \frac{1}{h}\int \frac{dE}{2\pi}\ \mathrm{Trace}\Big(\Gamma \underbrace{A}_{G^n} f_1\Big) \rightarrow I_{out} = \frac{1}{h}\int \frac{dE}{2\pi}\ \mathrm{Trace}\,(\Gamma G^n)$$

$A_{1/2\pi}$

A big picture of what we have been doing in this course:

1) We derived expressions for electron density and current for a one-level device.

2) We spent the rest of the course to figure out the Hamiltonian and self-energy matrices. Having these matrices, we became able to derive the matrix version of electron density inside the device and current through it. How?

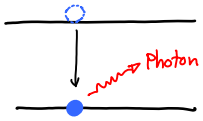
3) We started with Schrodinger equ- for the whole system. We partitioned it into two equations for channel and contact. We eliminated the contact and focused on the channel.

Note: If H and Σ could be diagonalized simultaneously, we wouldn't need to go through all this and derive matrix versions of the one level device or we could work with diagonalized matrices like scalars. However this is not possible as H and Σ cannot be both diagonalized simultaneously.

Chap. 10: Non- Coherent Transport

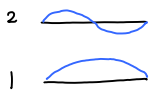
We will now focus on interaction of electrons with the surrounding media, specifically with photons and phonons. Let's first look at the electron- photon interaction.

We have heard that when an electron make a transition from a state to a lower energy level, it emits light.



But why the electron emits photon?

Can we explain this with Schrödinger equation? Let's consider only a two level system for the electron. Then the Hamiltonian is a 2x2 matrix in eigenstate space. Namely:



$$ih\frac{d}{dt}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} = \overbrace{\begin{bmatrix}\varepsilon_1 & 0\\ 0 & \varepsilon_2\end{bmatrix}}^{H}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$$

This system evolves in time as: $\begin{cases}\psi_1(t)=\psi_1(0)e^{-i\frac{\varepsilon_1}{h}t}\\ \psi_2(t)=\psi_2(0)e^{-i\frac{\varepsilon_2}{h}t}\end{cases} \rightarrow \begin{cases}P_1(t)=P_1(0)\\ P_2(t)=P_2(0)\end{cases}$

So the probability of the electron is staying in each energy level does not change, which means no transition! What did we do wrong?! well, we should check our Hamiltonian. In fact the way we wrote the Hamiltonian, there is no connection between the two states. We need off-diagonal terms in the matrix:

$$ih\frac{d}{dt}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} = \overbrace{\begin{bmatrix}\varepsilon_1 & U_{12}\\ U_{21} & \varepsilon_2\end{bmatrix}}^{H}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$$

Now the question is that if $U_{12}=U_{21}^*$, in other word, is H hermitian?

To answer this consider the system at zero kelvin. The electron still makes transition from level 2 to 1, hence $U_{12}\neq 0$. But it cannot make transition from 1 to 2, hence $U_{21}=0$. In fact as we will see $|U_{12}|>|U_{21}|$ at all temperatures. we can show this fact by considering

the Fermi distribution of electrons:

Rate at which electrons go from level 2 to 1, $S_{2\to1}$, is proportional to the product of the Fermi functions:

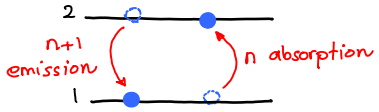
$S_{2\to1} = K_{2\to1} f_2 (1-f_1)$ where $K_{2\to1}$ is a constant.

$S_{1\to2} = K_{1\to2} f_1 (1-f_2)$

At equilibrium $S_{2\to1} = S_{1\to2} \Rightarrow \frac{K_{2\to1}}{K_{1\to2}} = \frac{f_1(1-f_2)}{f_2(1-f_1)} = \frac{1/f_2 - 1}{1/f_1 - 1}$

Since $f = \frac{1}{1+e^{(\varepsilon-\zeta)/k_BT}} \Rightarrow \frac{K_{2\to1}}{K_{1\to2}} = \frac{e^{\frac{\varepsilon_2-\zeta}{k_BT}}}{e^{\frac{\varepsilon_1-\zeta}{k_BT}}} = e^{\frac{\varepsilon_2-\varepsilon_1}{k_BT}} > 1$

In early 20th century Einstein argued that if the number of photons present is n, then the number of downward transitions is proportional to (n+1) and the number upward transition to n:



Downward $\propto n+1$: $K_{2\to1} = K(n+1)$

Upward $\propto n$: $K_{1\to2} = Kn$

where n is given by Bose–Einstein distribution: $n = \frac{1}{e^{\hbar\omega/k_BT} - 1}$

So based on Einstein argument, we have $\frac{K_{2\to1}}{K_{1\to2}} = \frac{K(n+1)}{Kn} = 1 + \frac{1}{n} = 1 + e^{\hbar\omega/k_BT} - 1 = e^{\hbar\omega/k_BT} = e^{(\varepsilon_2-\varepsilon_1)/k_BT}$

showing that Bose–Einstein factor demonstrates same proportionality as the Fermi functions of levels 1 and 2.

We would like to be able to explain photon emission and absorption more accurately namely in many particle view point.

Many-particle viewpoint

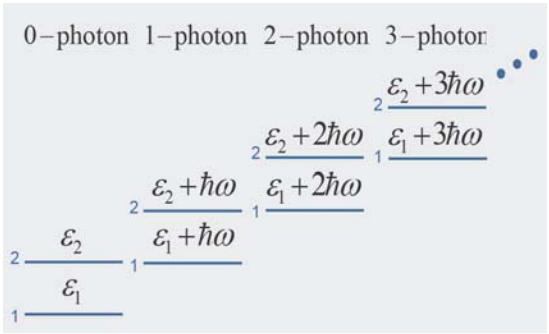
An electron interacting with several photons can be viewed as one big many-particle system with a single wave-function:

$\Psi = \psi \otimes \phi$

ψ: electron wavefunction; ϕ: photon wavefunction

→ This system has an infinite number of electron–photon states.

The first four possible states are shown here:



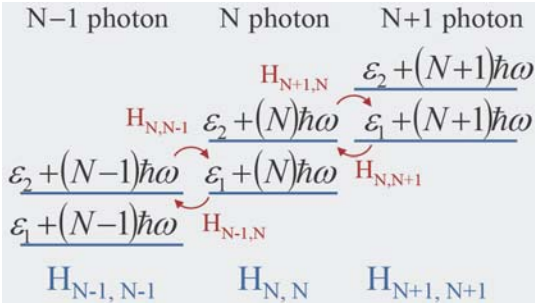
We can write in general the Schrödinger equation including both electrons and photons:

$$i\hbar \frac{d}{dt} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} H_{00} & H_{01} & 0 \\ H_{10} & H_{11} & H_{12} \\ & H_{21} & H_{22} \\ 0 & & \ddots \end{bmatrix} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \vdots \end{bmatrix}$$

In general, there is coupling between adjacent levels:

$H_{N+1,N}, H_{N,N+1}, H_{N,N-1}, H_{N-1,N}$

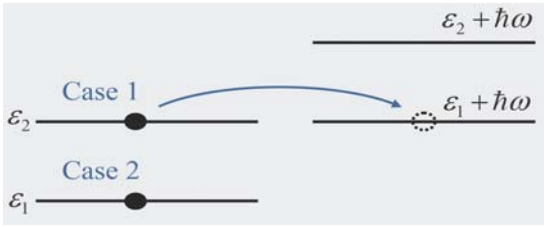
we can find the basis functions (wavefunctions) of the electron-photon Hilbert space by solving this equation.



To check the mechanism, let consider again putting an electron in a state at T=0 K:

Case 1: Electron is initially in level ε_2.

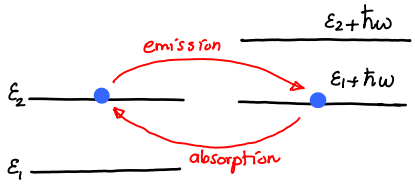
Since the level ε_1 with 1-photon, $\varepsilon_1+\hbar\omega$, is the degenerate adjacent level to ε_2, due to electron-photon coupling the electron wants to make transition to state $\varepsilon_1+\hbar\omega$. So the whole process of emission becomes a transfer between two degenerate states.



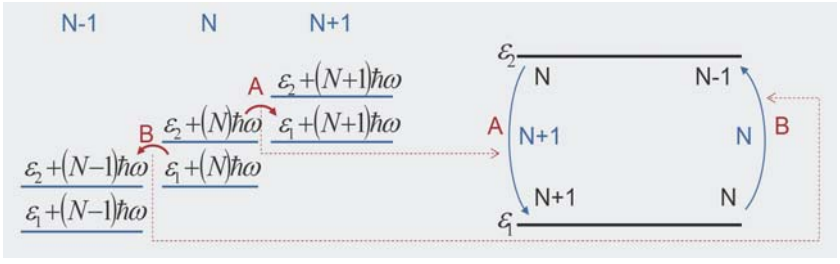
Case 2: Electron is initially in level ε_1. In this case there is no degenerate state (or lower electronic state) for the electron to go to. Hence the electron doesn't move from ε_1 and at T=0 it stays there forever, as expected.

Why don't we see continous emission and absorption cycle?

Base on our above schrödinge equation, the electron would have the choice to iterate back and forth between the two ε_2 and $\varepsilon_1+\hbar\omega$ states. In other word, continous emission and absorption cycle. But in the real world our photon is released when electron is at state $\varepsilon_1+\hbar\omega$ and is dissipated. So the system is reduced and the degenerate state is diminished. The result is that the electron-photon multiparticle falls down from $\varepsilon_1+\hbar\omega$ to ε_1. In this sense, the adjacent level act much like a contact which the photon escapes into; like dissipation of an electron into an infinite reservoir. Again the recurrence (cycle) should be numerically limitted by $i0^+$.



We can relate our general multiparticle picture of the N-photon subspace to the conventional single particle picture as show below:



A and B show equivalent level coupling in bothe representation.

In zero kelvin everything happens in the 0-photon subspace. At higher temperatures transitions happen in some positive integer n-photon subspace found by the Bose-Einstein factor.

Device Equivalent model:

We can relate the above formalism to our original device picture. In this model, the device is the current N-photon subspace and the adjacent N-1 and N+1 subspaces are treated as contacts with their own self-energy and coupling:

The device coupling to N+1 and N-1 photon subspaces can be described by self-energy matrices as usual.