Density of States, Quantum Wells and Wires

Review of Quantum Mechanics

Schrodinger Equation

$$H\Psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)$$

$H = \dfrac{P^2}{2m} + V(\vec{r},t)$ Hamiltonian = Kinetic + Potential Energy

$\Psi(\vec{r},t)$ Wavefunction

$\left|\Psi(\vec{r},t)\right|^2 = \Psi(\vec{r},t)\cdot\Psi(\vec{r},t)^*$ Probability of finding particle at $\vec{r}$

$\vec{P} = -i\hbar\nabla$ Momentum operator

$\left\langle \vec{P} \right\rangle = -i\hbar\int\Psi(\vec{r},t)^*\nabla\Psi(\vec{r},t)d\vec{r}$ Average Momentum

$\left\langle \vec{r} \right\rangle = \int\Psi(\vec{r},t)^*\vec{r}\Psi(\vec{r},t)d\vec{r}$ Average Position

Electron Plane Wave

$$\Psi(\vec{r},t) = e^{i\vec{k}\cdot\vec{r}-i\omega t}$$

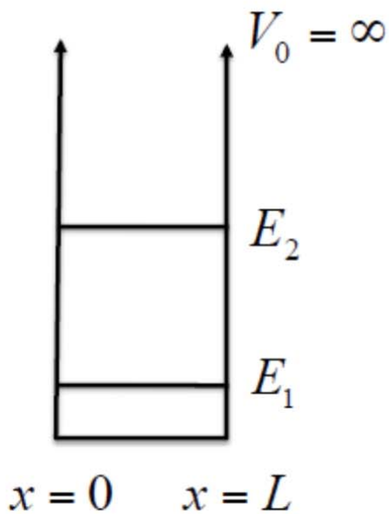
$$\text{LHS:} \quad H\Psi(\vec{r},t) = \frac{\hbar^2 k^2}{2m}\Psi(\vec{r},t) + V(\vec{r},t)\Psi(\vec{r},t)$$

$$P = \hbar k$$

$$\text{RHS:} \quad i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \hbar\omega\Psi(\vec{r},t)$$

$$\Rightarrow \frac{\hbar^2 k^2}{2m} + V(\vec{r},t) = \hbar\omega$$

Example: Infinite Potential Well



Time Independent Potential

$$V(z) = \begin{cases} 0 & \text{for } 0 < z < L \\ \infty & \text{for } z < 0 \text{ or } z > L \end{cases}$$

$$\Psi(z,t) = \phi(z) e^{-i\omega t}$$

Solve Eigenvalue $E = \hbar\omega$ in

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\phi(z) + V(z)\phi(z) = E\phi(z)$$

For $0 < z < L$, $\quad \dfrac{d^2}{dz^2}\phi(z) + \dfrac{2mE}{\hbar^2}\phi(z) = 0$

$$\phi(z) = \begin{cases} \sin(kz) \\ \cos(kz) \end{cases}$$

B.C. $\quad \phi(z = 0) = \phi(z = L) = 0$

$$\phi_n(z) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} z\right)$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

Typical Examples

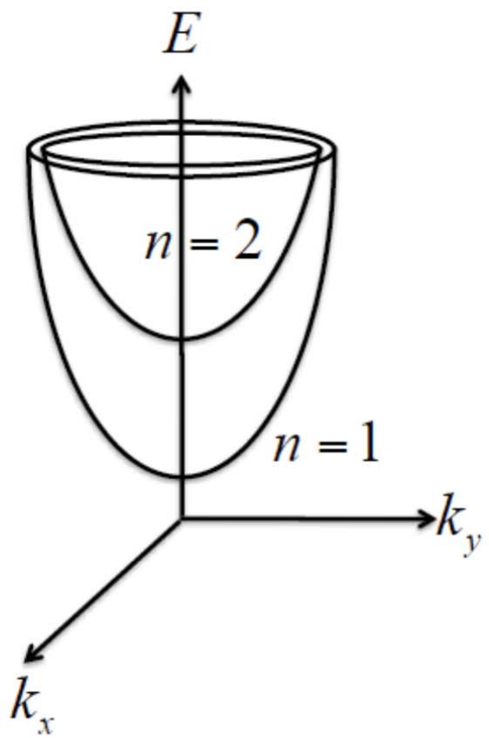
In GaAs, $m_e^* = 0.067m_0$

For a 10-nm-wide potential well $(L = 10nm)$

$E_1 = 56$ meV

$E_2 = 4E_1 = 224$ meV

Complete Wavefunction for Infinite Potential Well



$$\Psi(\vec{r},t) = \phi'(x,y)\phi(z)e^{-i\omega t}$$

Electron confined in z, but free in x, y

$\Rightarrow$ Plane wave in x and y

$$\phi'(x,y) = \frac{1}{\sqrt{A}}e^{ik_x x + ik_y y}$$

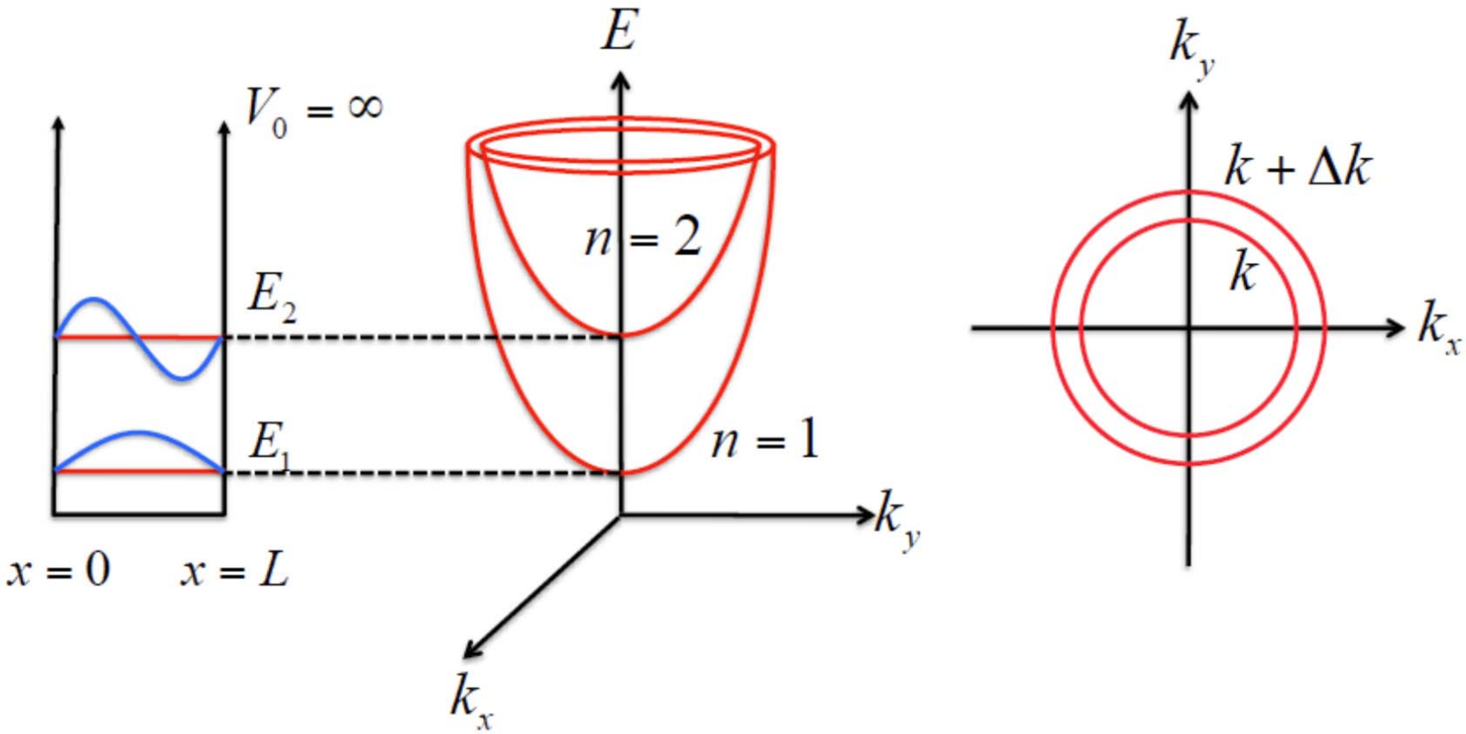
A: area (normalization const)

$$\Psi(\vec{r},t) = \sqrt{\frac{2}{L}}\frac{1}{\sqrt{A}}e^{ik_x x + ik_y y}\sin\left(\frac{n\pi}{L}z\right)$$

$$E_n = \frac{\hbar^2}{2m}\left[k_x^2 + k_y^2 + \left(\frac{n\pi}{L}\right)^2\right]$$

Energy quantized only in k_z direction

2-d Density of States



2-d Density of States

Consider the lowest band first (n=1):

Number of electron states between k and $k + \Delta k$ per unit volume

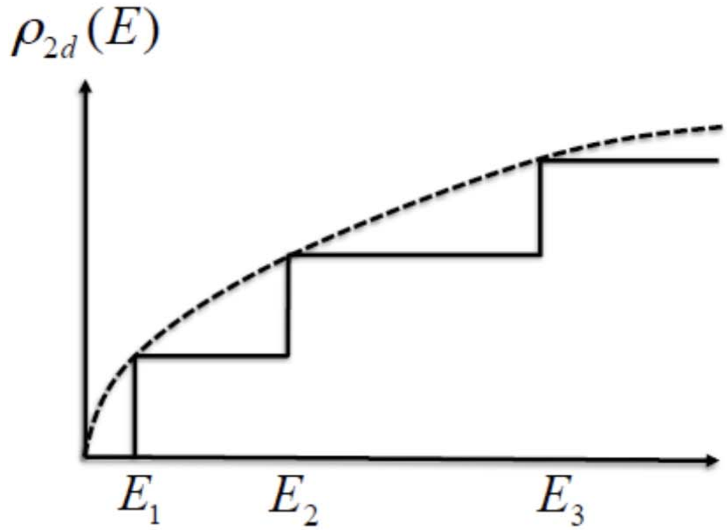
$$\rho_k(k)dk = \frac{2}{V}\cdot\frac{2\pi k dk}{\frac{2\pi}{L_x}\frac{2\pi}{L_y}} = \frac{2}{L_z}\frac{k}{2\pi}dk$$

$$E(k) = \frac{\hbar^2}{2m_e^*}\left[k^2 + \left(\frac{\pi}{L}\right)^2\right]$$

$$\rho_{2d}(E)dE = \rho_k(k)\frac{dk}{dE}dE = \left(\frac{2}{L_z}\frac{k}{2\pi}\right)\frac{1}{\frac{\hbar^2}{m_e^*}k}dE$$

$$\boxed{\rho_{2d}(E) = \frac{m_e^*}{\pi\hbar^2 L_z}}$$

2-d DOS for Multiple Energy Levels



$$
\begin{cases}
0 < E < E_1 & \rho_{2d}(E) = 0 \\
E_1 < E < E_2 & \rho_{2d}(E) = \dfrac{m_e^*}{\pi\hbar^2 L_z} \\
E_2 < E < E_3 & \rho_{2d}(E) = \dfrac{2m_e^*}{\pi\hbar^2 L_z} \\
E_3 < E < E_4 & \rho_{2d}(E) = \dfrac{3m_e^*}{\pi\hbar^2 L_z}
\end{cases}
$$

In general

$$
\rho_{2d}(E) = \frac{m_e^*}{\pi\hbar^2 L_z} \sum_{n=1}^{\infty} H(E - E_n)
$$

Step Function

2-d Electron/Hole Concentration

Electron and hole concentrations:

$$n = \int_{E_C}^{\infty} f_n(E)\rho_{e,2d}(E)dE$$

$$p = \int_{-\infty}^{E_V} f_p(E)\rho_{h,2d}(E)dE$$

At T = 0K, and for $E_1 < E < E_2$

$n =$

Example:

10-nm-wide GaAs quantum well

quasi-Fermi energy is 100 meV above E_1

2-d electron concentration

$m\_e := 0.067 \cdot m0$	$m\_e = 6.104 \times 10^{-32}\,kg$
$Lz := 10nm$	$Lz = 1 \times 10^{-8}\,m$
$\rho 2d := \dfrac{m\_e}{\pi \cdot h\_bar^2 \cdot Lz}$	$\rho 2d = 1.747 \times 10^{44}\,\dfrac{s^2}{kg \cdot m^5}$
$n := 100meV \cdot \rho 2d$	$n = 2.795 \times 10^{18} \cdot \dfrac{1}{cm^3}$
$n\_s := n \cdot Lz$	$n\_s = 2.795 \times 10^{12} \cdot \dfrac{1}{cm^2}$

2-d Electron/Hole Concentration

Electron and hole concentrations:

$$n = \int_{E_C}^{\infty} f_n(E)\rho_{e,2d}(E)dE$$

$$p = \int_{-\infty}^{E_V} f_p(E)\rho_{h,2d}(E)dE$$

At T = 0K, and for $E_1 < E < E_2$

$$n = (F_n - E_1)\cdot \rho_{e,2d}(E_1 < E < E_2)$$

$$n = (F_n - E_1)\frac{m_e^*}{\pi \hbar^2 L_z}$$

Example:

10-nm-wide GaAs quantum well quasi-Fermi energy is 100 meV above E_1

2-d electron concentration

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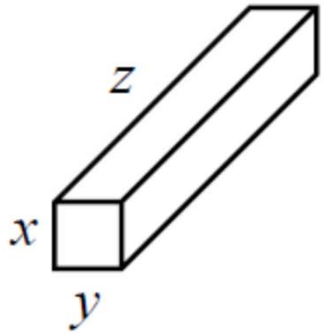
1-d Density of States



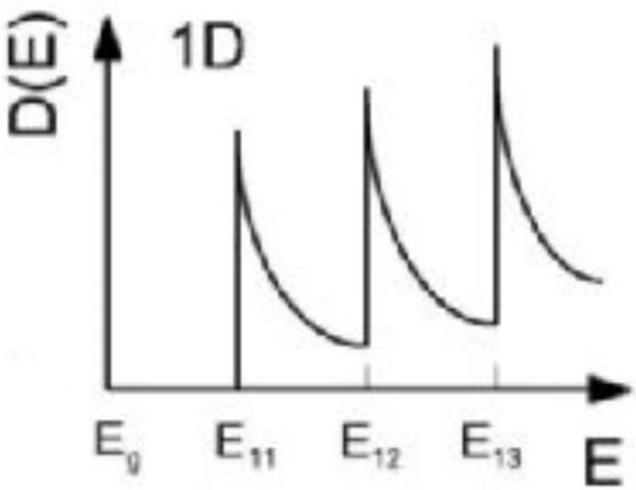
$$E_{m,n}(k_z) = \frac{h^2}{2m_e^*}\left(\left(\frac{m\pi}{L}\right)^2 + \left(\frac{n\pi}{L}\right)^2 + k_z^2\right)$$

$$dE_{m,n}(k_z) = \frac{h^2}{2m_e^*}2k_z \cdot dk_z = \frac{h^2 k_z}{m_e^*}dk_z$$

$$n = \frac{2}{V}\sum_{m,n}\int_{-\infty}^{\infty}\frac{dk_z}{\left(\frac{2\pi}{L_z}\right)} = \frac{2}{\pi L_x L_y}\sum_{m,n}\int_0^{\infty}dk_z$$

$$= \frac{2}{\pi L_x L_y}\sum_{m,n}\int_0^{\infty}\frac{m_e^*}{h^2 k_z}dE$$

$$= \frac{1}{\pi L_x L_y}\sqrt{\frac{2m_e^*}{h^2}}\sum_{m,n}\int_0^{\infty}\frac{1}{\sqrt{E - E_{mx} - E_{ny}}}dE$$

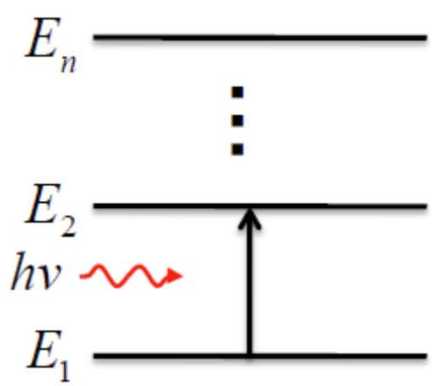


$$\boxed{\rho_{1D}(E) = \frac{1}{\pi L_x L_y}\sqrt{\frac{2m_e^*}{h^2}}\sum_{m,n}\frac{1}{\sqrt{E - E_{mx} - E_{ny}}}}$$

Fermi’s Golden Rule

Time-Dependent Perturbation

Consider a quantum mechanical system:



$$H_0\phi_n(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\phi_n(\vec{r},t)$$

$$\phi_n(\vec{r},t) = \phi_n(\vec{r})e^{-\frac{iE_nt}{\hbar}}$$

$\phi_n(\vec{r}) = |n\rangle$ an orthonormal set of eigenstates

$$\langle m|n\rangle = \int \phi_m^*(\vec{r})\phi_n(\vec{r})d\vec{r} = \delta_{mn}$$

Consider a single-frequency, time-varying stimulus

$$H'(\vec{r},t) = H'(\vec{r})e^{-iwt} + H'^{\dagger}(\vec{r})e^{iwt} \quad \text{for } t>0$$

$$H = H_0 + H'(\vec{r},t)$$

$$H\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

Assuming $|H'| \ll |H_0|$

The new wavefunction can be expressed as a linear combination of original eigenstates with time-varying coefficients:

$$\psi(\vec{r},t) = \sum_n a_n(t)\phi_n(\vec{r})e^{-iE_nt/\hbar}$$

$|a_n(t)|^2$: probability of electron at state $|n\rangle$ at time t

Time-Dependent Perturbation (cont'd)

$$H\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

$$(H_0 + H')\sum_n a_n(t)\phi_n(\vec{r})e^{-iE_nt/\hbar} = i\hbar\sum_n \frac{da_n(t)}{dt}\phi_n(t)e^{-iE_nt/\hbar} + i\hbar\sum_n a_n(t)\phi_n(\vec{r})\left(\frac{-iE}{\hbar}\right)e^{-iE_nt/\hbar}$$

$$H'\sum_n a_n(t)\left|n\right\rangle e^{-iE_nt/\hbar} = i\hbar\sum_n \frac{da_n(t)}{dt}\left|n\right\rangle e^{-iE_nt/\hbar}$$

Multiply both sides by $\left\langle m\right|$ (i.e., multiply by $\phi_m^*(\vec{r})$ and integrate over $\vec{r}$)

$$\sum_n a_n(t)\left\langle m\right|H'\left|n\right\rangle e^{-iE_nt/\hbar} = i\hbar\sum_n \frac{da_n(t)}{dt}\left\langle m|n\right\rangle e^{-iE_nt/\hbar} = i\hbar\frac{da_m(t)}{dt}e^{-iE_mt/\hbar}$$

$$\frac{da_m(t)}{dt} = \frac{1}{i\hbar}\sum_n a_n(t)H'_{mn}(t)e^{i\omega_{mn}t}$$

$$\omega_{mn} = \frac{E_m - E_n}{\hbar}$$

First-Order Perturbation

To track the order of perturbation, let

$$H = H_0 + \lambda H'$$

$$a_n(t) = a_n^{(0)}(t) + \lambda a_n^{(1)}(t) + \lambda^2 a_n^{(2)}(t) + \ldots$$

Group terms with the same order of λ:

$$\frac{da_m^{(0)}(t)}{dt} = 0 \Rightarrow a_m^{(0)}(t) = \text{constant}$$

$$\frac{da_m^{(1)}(t)}{dt} = \frac{1}{i\hbar} \sum_n a_n^{(0)}(t) H'_{mn}(t) e^{i\omega_{mn}t}$$

$$\frac{da_m^{(2)}(t)}{dt} = \frac{1}{i\hbar} \sum_n a_n^{(1)}(t) H'_{mn}(t) e^{i\omega_{mn}t}$$

First-Order Perturbation (Cont'd)

Initial state i at t=0 and final state f

$$\begin{cases} a_i^{(0)}(t) = 1 \\ a_m^{(0)}(t) = 0 \ \text{ if } \ m \neq i \end{cases}$$

$$\frac{da_f^{(1)}(t)}{dt} = \frac{1}{i\hbar} H'_{fi}(t) e^{i\omega_{mi}t} = \frac{1}{i\hbar}\left(H'_{fi} e^{-i\omega t} + H'^{\dagger}_{fi} e^{i\omega t} \right) e^{i\omega_{mi}t}$$

$$= \frac{1}{i\hbar}\left(H'_{fi} e^{i(\omega_{mi}-\omega)t} + H'^{\dagger}_{fi} e^{i(\omega_{mi}+\omega)t} \right)$$

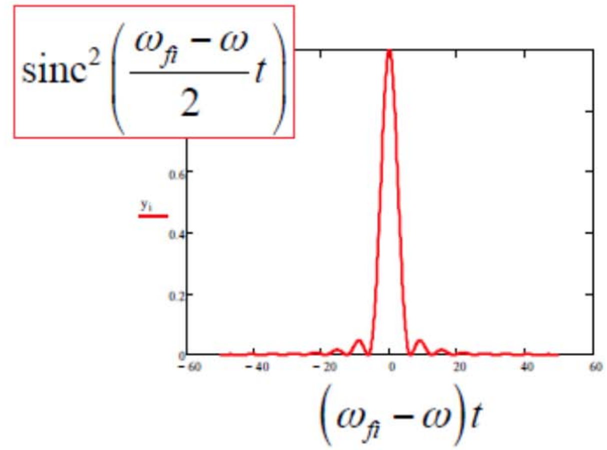
$$a_f^{(1)}(t) = \frac{-1}{\hbar}\left(H'_{fi} \frac{e^{i(\omega_{mi}-\omega)t} - 1}{\omega_{mi} - \omega} + H'^{\dagger}_{fi} \frac{e^{i(\omega_{mi}+\omega)t} - 1}{\omega_{mi} + \omega} \right)$$

We are only interested at frequencies near resonance:

$$\left| a_f^{(1)}(t) \right|^2 = \frac{4\left| H'_{fi} \right|^2}{\hbar^2} \frac{\sin^2\left(\frac{\omega_{mi} - \omega}{2} t \right)}{\left(\omega_{mi} - \omega \right)^2} + \frac{4\left| H'^{\dagger}_{fi} \right|^2}{\hbar^2} \frac{\sin^2\left(\frac{\omega_{mi} + \omega}{2} t \right)}{\left(\omega_{mi} + \omega \right)^2}$$

Fermi's Golden Rule

$$\frac{\sin^2\left(\frac{\omega_{fi}-\omega}{2}t\right)}{\left(\omega_{fi}-\omega\right)^2}=\frac{t^2}{4}\operatorname{sinc}^2\left(\frac{\omega_{fi}-\omega}{2}t\right)$$



$$\rightarrow\frac{\pi t}{2}\delta(\omega_{fi}-\omega)\quad \text{as}\ \ t\rightarrow\infty$$

$$\left|a_f^{(1)}(t)\right|^2=\frac{2\pi t\left|H'_{fi}\right|^2}{\hbar^2}\delta(\omega_{fi}-\omega)+\frac{2\pi t\left|H'^{\dagger}_{fi}\right|^2}{\hbar^2}\delta(\omega_{fi}+\omega)$$

Transition Rate:

$$W_{i\rightarrow f}=\frac{d}{dt}\left|a_f^{(1)}(t)\right|^2=\frac{2\pi\left|H'_{fi}\right|^2}{\hbar^2}\delta(\omega_{fi}-\omega)+\frac{2\pi\left|H'^{\dagger}_{fi}\right|^2}{\hbar^2}\delta(\omega_{fi}+\omega)$$

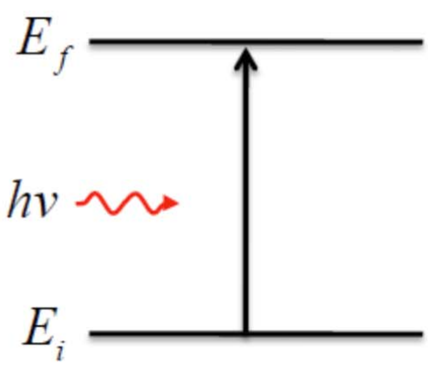
Note: $\delta(E_f-E_i-\hbar\omega)=\frac{1}{\hbar}\delta(\omega_f-\omega_i-\omega)$

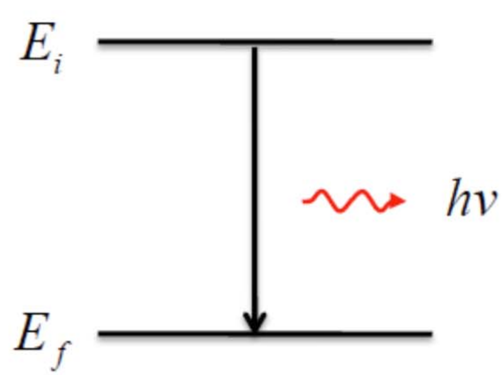
$$W_{i\rightarrow f}=\frac{2\pi\left|H'_{fi}\right|^2}{\hbar}\delta(E_f-E_i-\hbar\omega)+\frac{2\pi\left|H'^{\dagger}_{fi}\right|^2}{\hbar}\delta(E_f-E_i+\hbar\omega)$$

Physical Interpretation

$$W_{i\to f} = \frac{2\pi\left|H'_{fi}\right|^2}{\hbar}\delta(E_f - E_i - \hbar\omega) + \frac{2\pi\left|H'^{\dagger}_{fi}\right|^2}{\hbar}\delta(E_f - E_i + \hbar\omega)$$

$$\boxed{\begin{array}{c} E_f = E_i + \hbar\omega \\ \text{Absorption of a photon} \end{array}} \qquad \boxed{\begin{array}{c} E_f = E_i - \hbar\omega \\ \text{Emission of a photon} \end{array}}$$





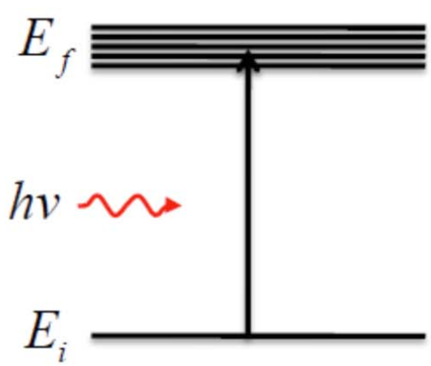
- **Conservation of energy**
- **Transition rate is proportional to the square of the “matrix element”**

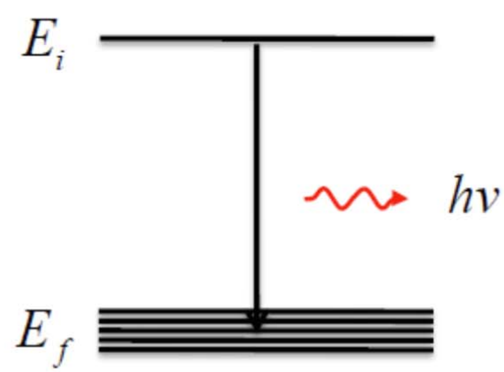
Distributed Final States

- If the final state is a distribution of states, the transition rate is proportional to the density of states of the final state:

$$W_{i\to f} = \frac{2\pi\left|H'_{fi}\right|^2}{\hbar}\rho_f\delta(E_f - E_i - \hbar\omega) + \frac{2\pi\left|H'^{\dagger}_{fi}\right|^2}{\hbar}\rho_f\delta(E_f - E_i + \hbar\omega)$$

$$\boxed{\begin{array}{c} E_f = E_i + \hbar\omega \\ \text{Absorption of a photon} \end{array}} \qquad \boxed{\begin{array}{c} E_f = E_i - \hbar\omega \\ \text{Emission of a photon} \end{array}}$$



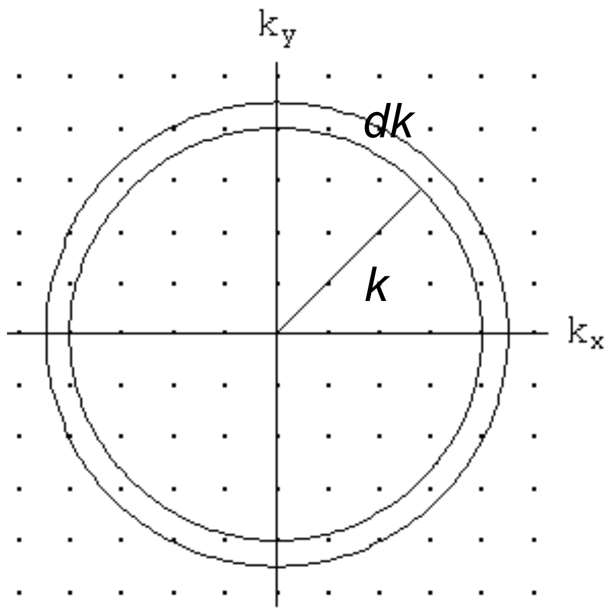


photon DOS in a box of vacuum

States in an LxLxL box:

$$E(x,t) = Ae^{i\omega t}\sin(\mathbf{k}\cdot\mathbf{r}) \quad \text{with} \quad \mathbf{k} = \frac{\pi}{L}(l,m,n)$$

l,m,n positive integers



Picture from http://britneyspears.ac

Number of states with |**k**| between k and k+dk:

$$N(k)dk = \frac{4}{8}\pi k^2 dk\left(\frac{L}{\pi}\right)^3 \cdot 2$$

l,m,n > 0
fill one octant

fudge 2 for polarization

As a function of frequency ω $(=ck)$:

$$N(\omega)d\omega = L^3\frac{\omega^2}{\pi^2 c^2}\frac{dk}{d\omega}d\omega = L^3\frac{\omega^2}{\pi^2 c^3}d\omega$$

Density of states in vacuum

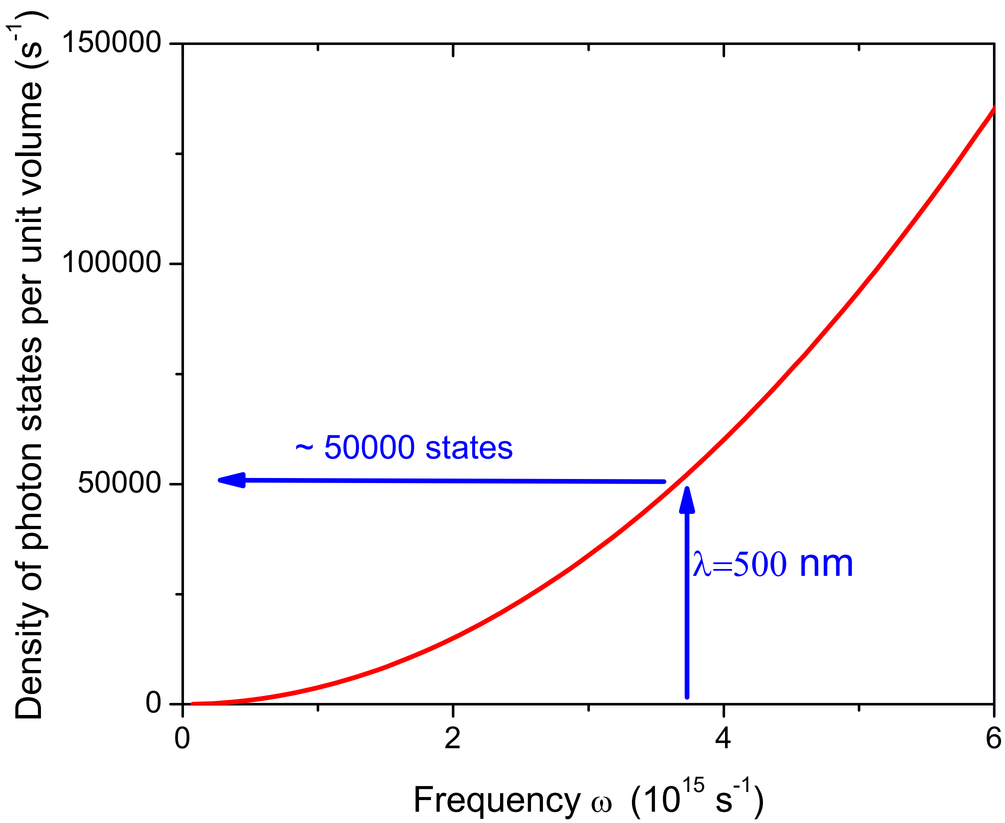
$$N(\omega)d\omega = L^3 \frac{\omega^2}{\pi^2 c^2} \frac{dk}{d\omega} d\omega = L^3 \frac{\omega^2}{\pi^2 c^3} d\omega$$

Example: How many photon states per m^3 of vacuum per 1 Hz @ λ=500 nm ?

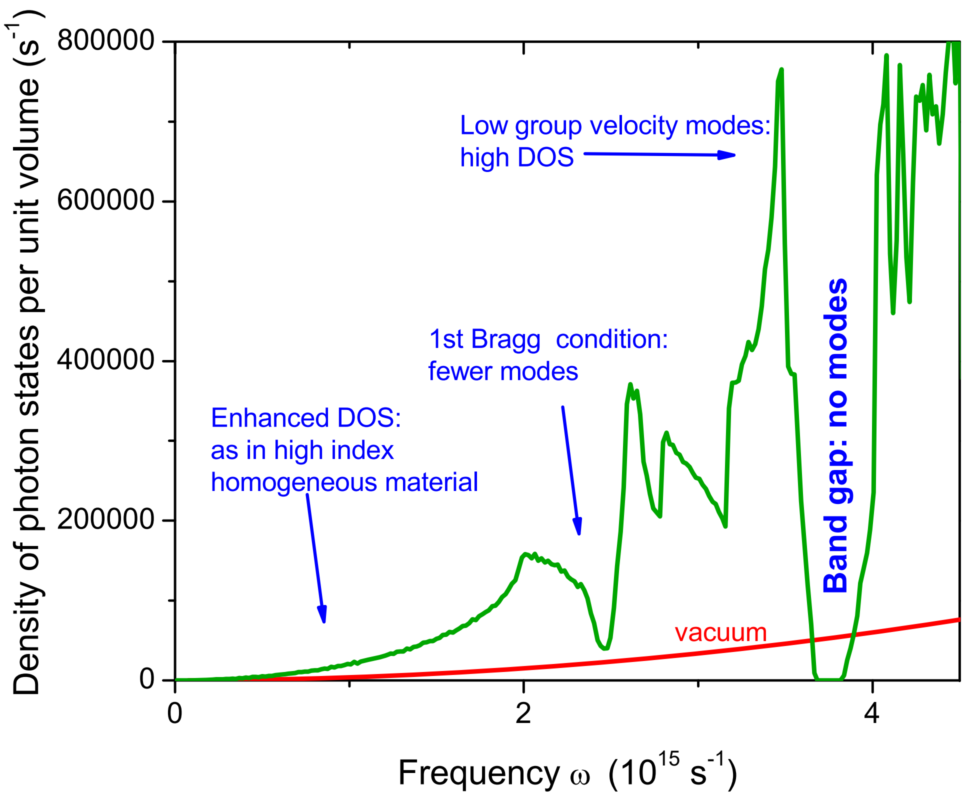
Density of states in vacuum

$$N(\omega)d\omega = L^3 \frac{\omega^2}{\pi^2 c^2}\frac{dk}{d\omega}d\omega = L^3 \frac{\omega^2}{\pi^2 c^3}d\omega$$

Example: ~50000 photon states per m^3 of vacuum per 1 Hz @ λ=500 nm

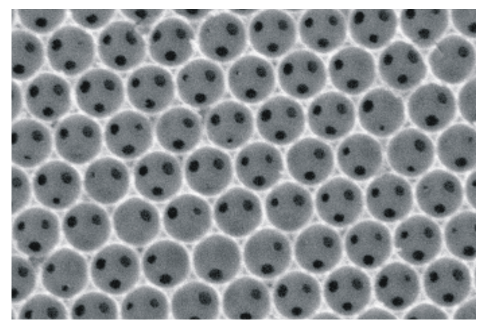


Controlling the DOS



Photonic band gap material

Example:
fcc close-packed
air spheres in n=3.5
Lattice spacing 400 nm



Photonic band gap: no states = no spontaneous emission

Enhanced DOS: faster spontaneous emission according to Fermi G. Rule

Local DOS

An emitter doesn't just count modes (as in DOS)

It also feels *local mode strength* $|E|^2$.

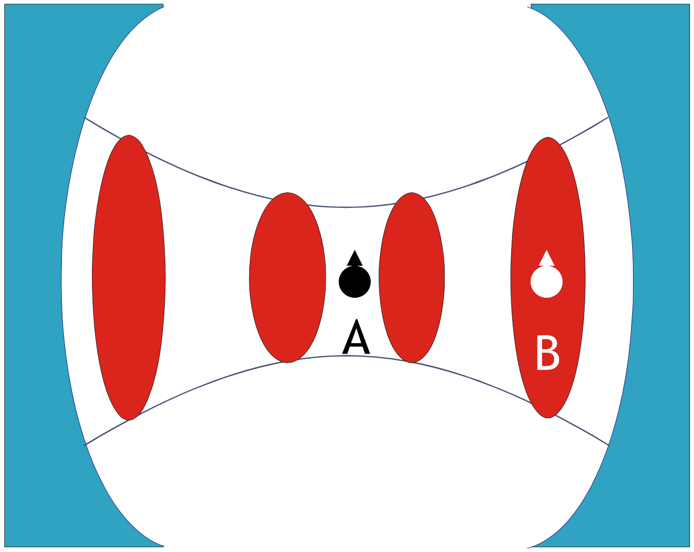
It can only emit into a mode if the mode is not zero at the emitter

DOS: just count states

$$N(\omega) = \sum_{\text{all modes } m} \delta(\omega_m - \omega)$$

Local DOS

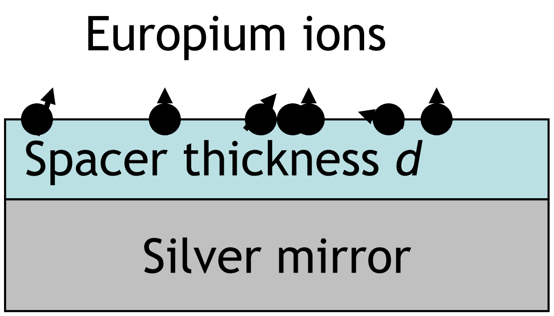
$$N(\mathbf{r},\mathbf{d},\omega) = \sum_{\text{all modes}} |\mathbf{d}\cdot\mathbf{E}_m(\mathbf{r})|^2 \, \delta(\omega_m - \omega)$$

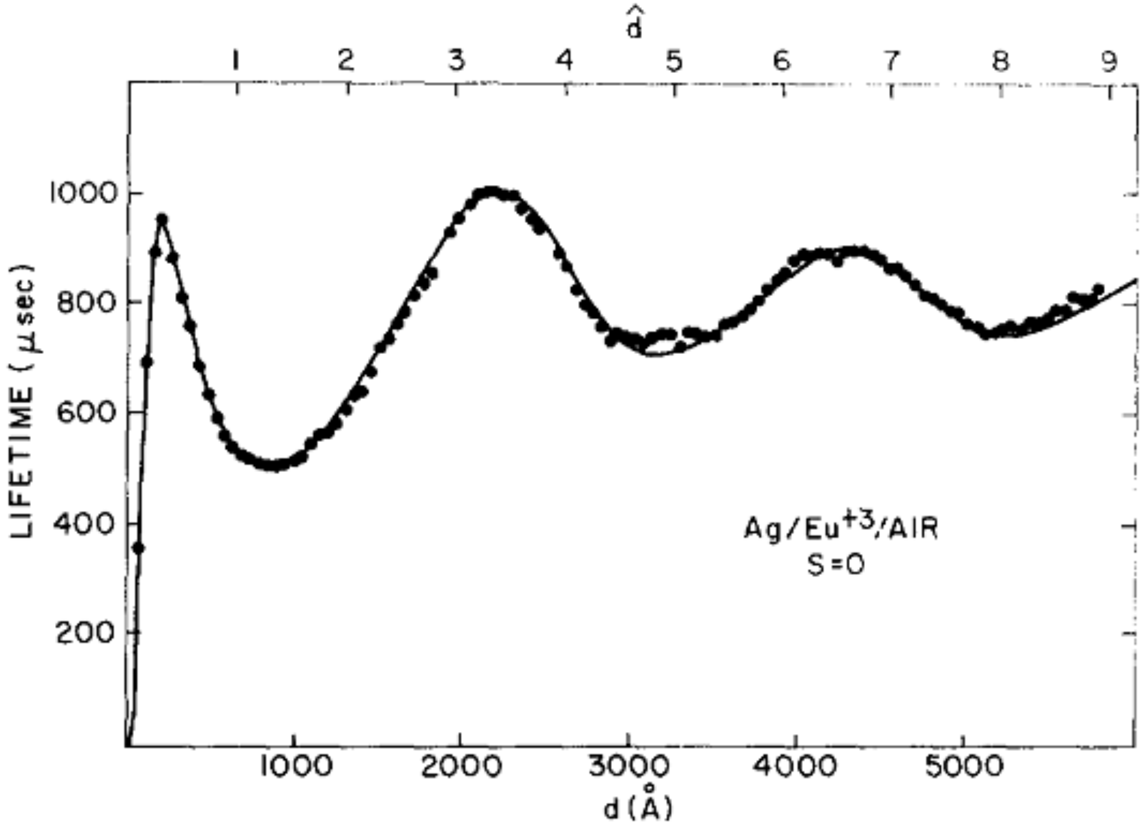


Atom at position A can not emit into cavity mode.

Atom at position B can emit into cavity mode.

LDOS: emission in front of a mirror





Drexhage (1966): fluorescence lifetime of Europium ions depends on source position relative to a silver mirror *(λ=612 nm)*