Lecture 6 – Photons, electrons and other quanta

EECS 598-002 Winter 2006

Nanophotonics and Nano-scale Fabrication

P.C.Ku

From classical to quantum theory

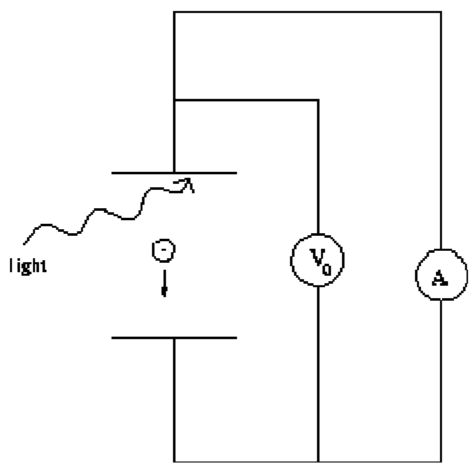
- In the beginning of the 20th century, experiments showed:
  - Particle nature of EM radiation
  - Wave nature of electrons

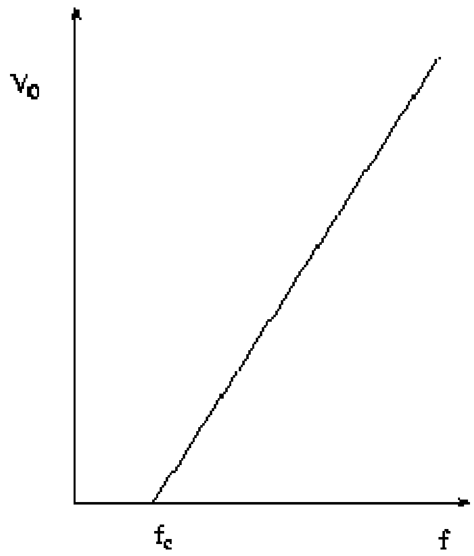
- In 1927, Heisenberg proposed the uncertainly principle which later on became the foundation of modern quantum mechanics (QM):

  Not all the physical quantities can be measured at the same time with however precision we would like. E.g. the more precisely we measure the position of a particle, the less precisely we will be able to measure its momentum.

Example: Photoelectric effect

- In the experiment, the light shines on a metal and knocks out the electrons on the metal surface. When we measured the stopping voltage V_0 to counteract the generated current, we found a cutoff frequency f_0. This can not be explained by the Maxwell's equations.





Quantum state and operators

- In the language of QM, the physics of a particle (or a system that is comprising of many particles) can be described by a state $\left|\Psi(t)\right\rangle$ (a vector in Hilbert space).

- The physical quantities (measurables) can be obtained by applying a suitable operator Ω to the state $\Omega\left|\Psi(t)\right\rangle$. This will yield one of the eigenvalues with probability P given by $P(\omega)=\left|\left\langle\omega|\Psi(t)\right\rangle\right|^2$. The measurement will also change the system to the new state $\left|\omega\right\rangle$.

e.g. In coordinate basis:

Position operator	$\vec{r}$
Momentum operator	$-i\hbar\nabla$
Total energy operator	$-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r}) \longrightarrow$ Hamiltonian

Dynamics of quantum states

- The evolution of the quantum state obeys the Schroedinger equation:

$$i\hbar \frac{d\left|\Psi(t)\right\rangle}{dt} = H\left|\Psi(t)\right\rangle$$

  where *H* is the Hamiltonian.

- For example, an electron in a time-independent potential V(r) is governed by:

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r})\right]\left|\Psi(t)\right\rangle = i\hbar\frac{d\left|\Psi(t)\right\rangle}{dt}$$

$$\left|\Psi(t)\right\rangle = \left|E\right\rangle e^{-iEt/\hbar}$$

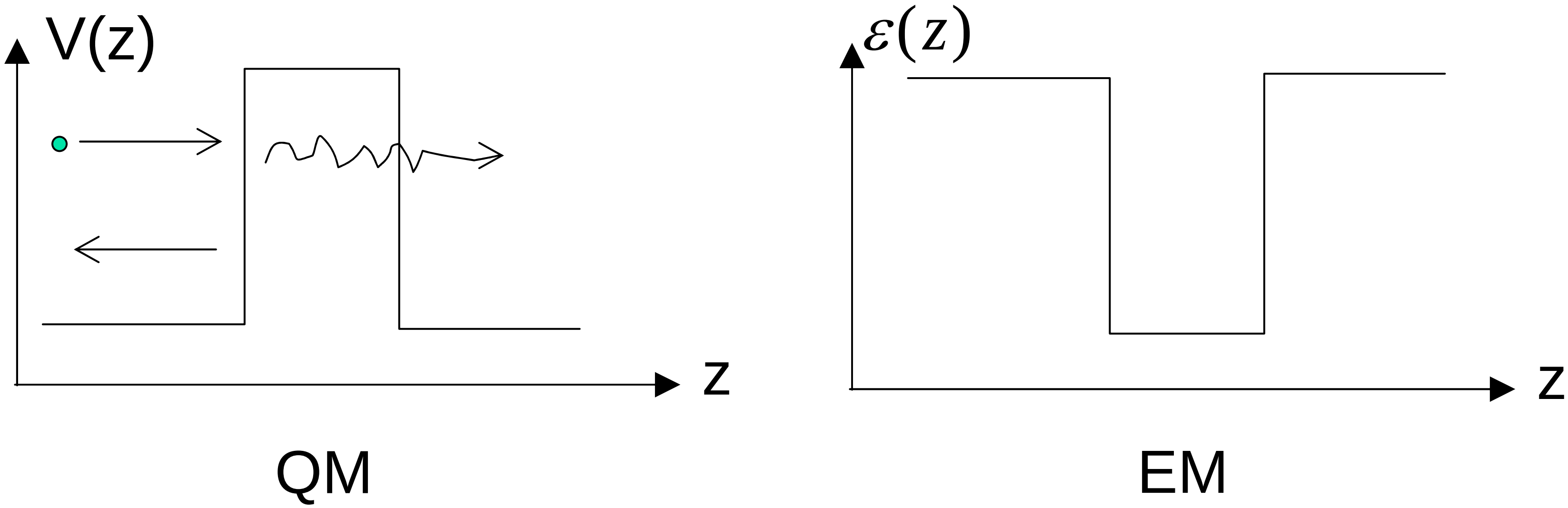
$$\Rightarrow \left[-\frac{\hbar^2\nabla^2}{2m}+\left(V(\vec{r})-E\right)\right]\left|E\right\rangle = 0$$

Comparison b/w QM and EM

Equation governing QM and EM have lots of mathematical similarities.

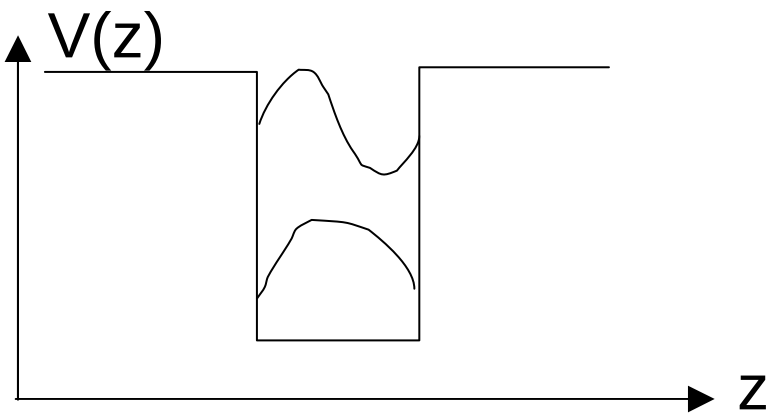
	QM	EM
Equation	$\left[\nabla^2 + \frac{2m}{\hbar^2}\left(E - V(\vec{r})\right)\right]\left\|E\right\rangle = 0$	$\left[\nabla^2 + \omega^2\mu_0\left(\varepsilon_0 + \varepsilon(r) - \varepsilon_0\right)\right]\begin{Bmatrix}\vec{E}\\ \vec{H}\end{Bmatrix} = 0$
Potential	$-V(\vec{r})$	$\varepsilon(r) - \varepsilon_0$
Eigenstate	$\left\|E\right\rangle$	$\vec{E}$ and $\vec{H}$
Eigenvalue	E	ω^2
Wavevector	$\sqrt{\frac{2m}{\hbar^2}\left(E - V(\vec{r})\right)}$	$\omega\sqrt{\mu_0\varepsilon(r)}$

First analogy: tunneling

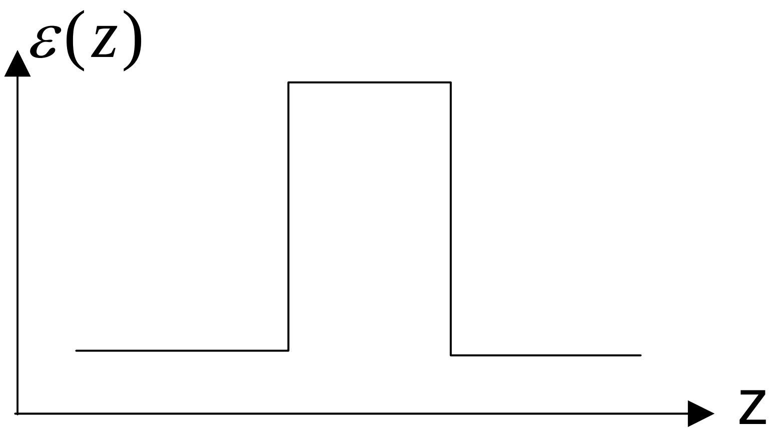


1. Electron experiences reflection and tunneling through the potential barrier. The wavefunction $|E\rangle$ is exponential decayed in the barrier.
2. The tunneling probability increases when the width of the potential barrier decreases.

Slab waveguide vs potential well

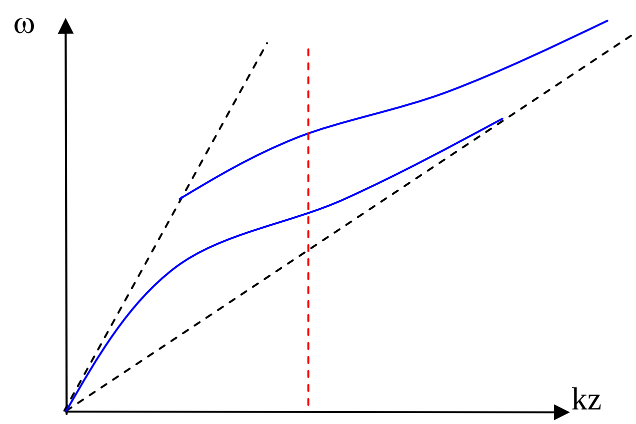


QM



EM

At a fixed K.E. in the x-y plane, the kinetic energy of an electron in the z direction is quantized.



Electrons in crystals

- When electron travels in a periodic potential (e.g. in the crystal), its eigenstate satisfies the Bloch's theorem.

$$\psi(\vec{r}) = u(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$

- The Bloch function $u(\vec{r})$ has the same periodicity as the crystal lattice.

- The spatial symmetry of the crystal lattice with respect to a fixed point determines the eigenfunctions of the electron.

- Because of the periodicity, the energy bandgap exists at certain k values.

Effective mass vs constitutive relation

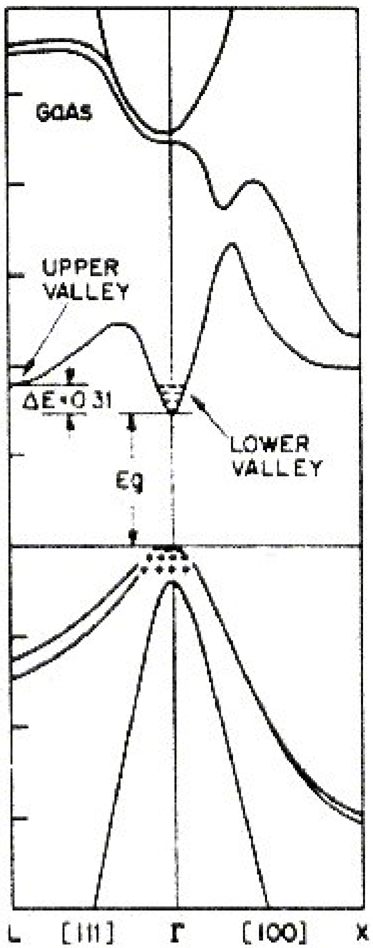
- Similar to the "macroscopic version" of the Maxwell's equations, we can also derive an "effective-mass" equation for electrons traveling in the lattice with the assumption that the electron interacts weakly with the lattice.

$$\left[-\frac{\hbar^2\nabla^2}{2m}+\left(V_{crystal}(\vec{r})+V_{macroscopic}(\vec{r})-E\right)\right]\left|E\right\rangle=0$$

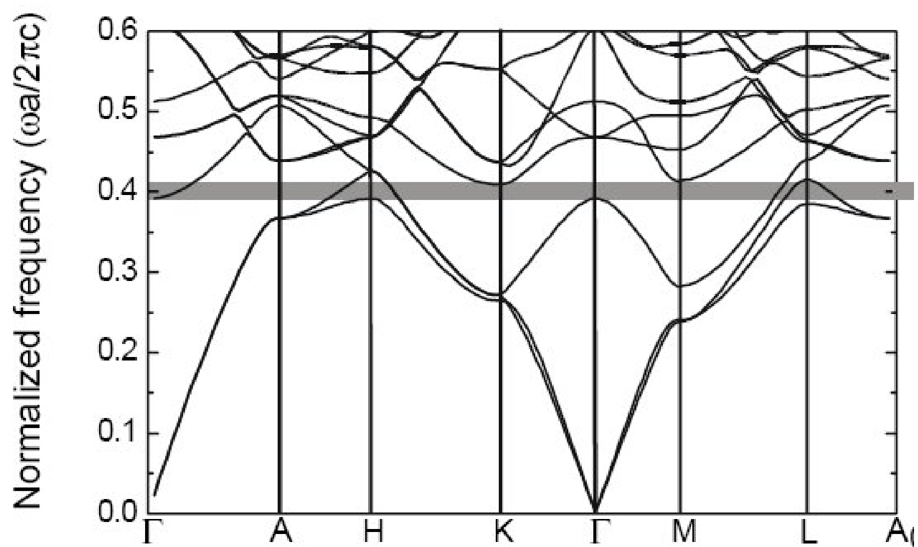
$$\rightarrow\left[-\frac{\hbar^2\nabla^2}{2m^*}+V_{macroscopic}(\vec{r})-E\right]\left|E\right\rangle=0$$

Example of a dispersion relation

Electron in periodic V(r)



EM wave in periodic ε(r)



Density of states

- Density of states g(E) is the total number of allowed-to-occupy states with frequencies between E and E+δE per unit volume.

$$g(E)=\frac{1}{V}\frac{dN(E)}{dE}$$

where $N(E)$ is the total number of states from 0 to E.

- In a potential well:

$$N(E)=\int_{E'<E} g(E')f(E')dE'=\sum_{k'} f(k')$$

$$=2\times\frac{1}{(\Delta k)^d}\int_{k'<k} f(k')d\vec{k}'=2\times\frac{1}{(\Delta k)^d}\int_{k'<k} A(k')f(k')dk'$$

$$g(E_n)=\left(\frac{1}{V}\right)\frac{2A(k)}{(\Delta k)^d}\frac{dk}{dE}=2\left(\frac{1}{2\pi}\right)^d A(k)\frac{dk}{dE}$$

$$d=\begin{cases}3\text{ dim} & A(k)=4\pi k^2\\ 2\text{ dim} & A(k)=2\pi k\\ 1\text{ dim} & A(k)=1\\ 0\text{ dim} & A(k)=\delta(k-k_n)\end{cases}$$

Density of states (cont.)

For electrons, $E = \hbar^2 k^2 / 2m$. For EM waves (photons), $E = \hbar\omega = \hbar c k$.

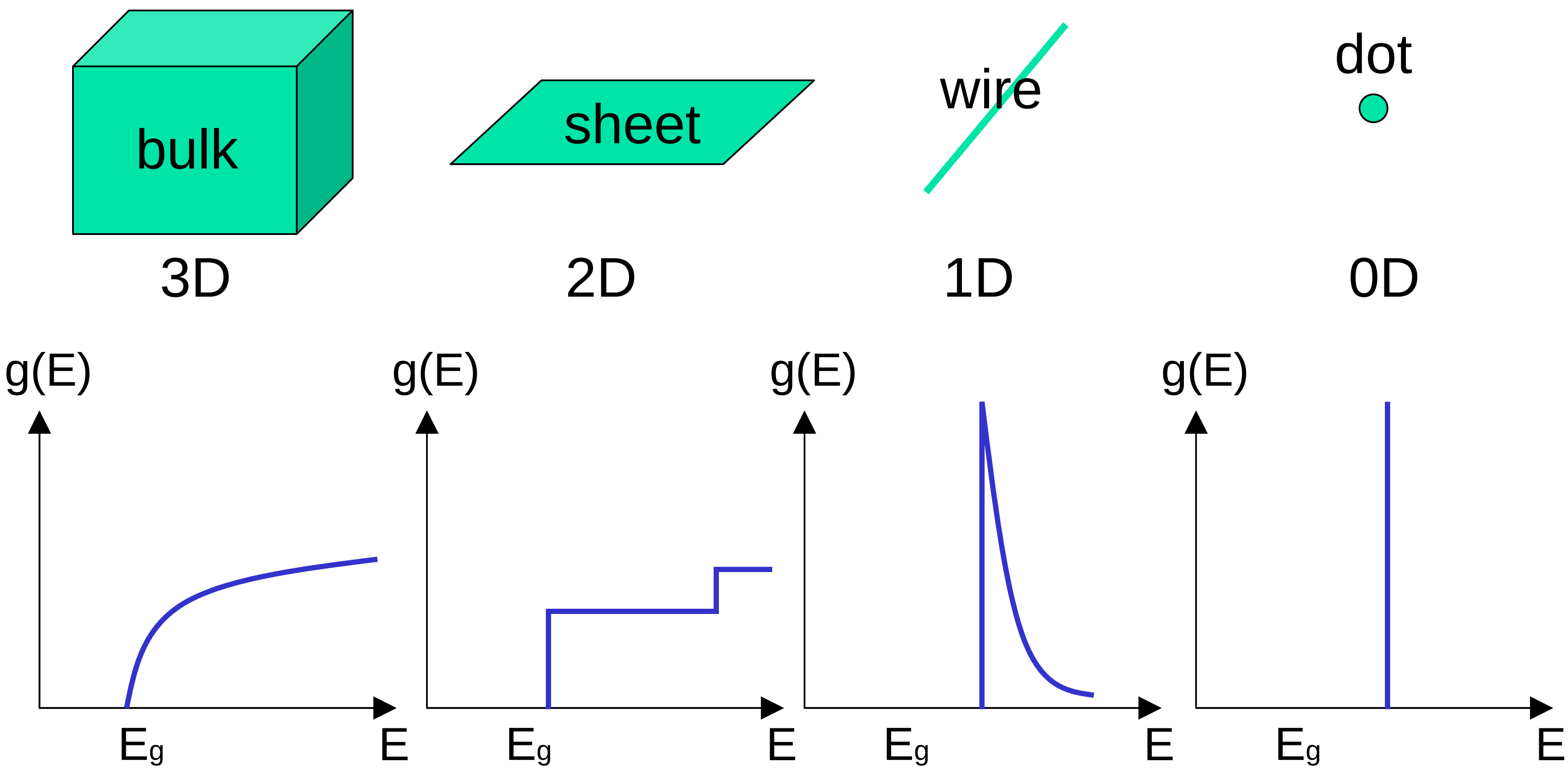
Note k can be discrete due to quantization.

For electrons: $\dfrac{dk}{dE} = \dfrac{m}{\hbar^2 k}$ (d>0) ; $g(E) = \sum_n g(E_n)$

$$
d = \begin{cases}
\text{3 dim} \quad g(E) = \dfrac{1}{2\pi^2}\left(\dfrac{2m}{\hbar^2}\right)^{3/2}\sqrt{E} \\
\text{2 dim} \quad g(E) = \dfrac{m}{\pi\hbar^2}\sum_n \theta(E - E_n) \\
\text{1 dim} \quad g(E) = \dfrac{1}{\pi}\left(\dfrac{m}{2\hbar^2}\right)^{1/2}\sum_n \dfrac{1}{\sqrt{E_n}} \\
\text{0 dim} \quad g(E) = 2\sum_n \delta(E - E_n)
\end{cases}
$$

Density of states for electrons

g(E) = Density of states



Occupation probability

- In thermal equilibrium, fermions (e.g. electrons) satisfy the Fermi-Dirac statistics (two fermions cannot stay in the same state):

$$f(E) = \frac{1}{\exp\left[(E - E_F)/k_B T\right] + 1}$$

- In thermal equilibrium, bosons (e.g. photons) satisfy the Bose-Einstein statistics:

$$f(E) = \frac{1}{\exp\left[(E - E_F)/k_B T\right] - 1}$$

From single-particle to many-particle system

- So far we have considered only the quantization of a single particle, namely the electron. This procedure (namely the uncertainly principle) applies to all particles that are governed by Newton's Laws classically.

- Similarly, we can also treat a multi-particle system as a whole and quantize the system at once. To treat the system classically, we can imagine the position and momentum of each particle form a field. The moving of a particle w.r.t. its equilibrium position looks like a perturbation of the field, i.e. wave.

Number operator

$$\hat{N} = \hat{a}^{+}\hat{a}$$

$$\hat{a}^{+}\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle$$

Creation operator

$$\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle$$

Annihilation operator

$$\hat{H} = \hbar\omega(\hat{a}^{+}\hat{a} + 1/2)$$

Hamiltonian operator

Photons

- Similar to the quantization of a many-particle system, EM wave can be thought as a perturbation of the EM field in space-time.

- Quantization of the EM field → photons

$$\left[\hat{D}_i(\vec{r},t),\hat{B}_j(\vec{r}\,',t)\right] = -i\hbar\varepsilon_{ijk}\frac{\partial}{\partial x_k}\delta(\vec{r}-\vec{r}\,')$$

- Properties of photons
  - Mass = 0
  - Charge = 0
  - Energy = h$\nu = \hbar\omega$
  - Momentum = $\hbar k$

When do we need concepts of photons?

- When do we need to treat the EM wave as photons?
  - When the momentum of each photon is comparable to that of the material upon which it impinge.
  - When the number of photons involved in the interaction is very small.

- Examples:
  - Photoelectric effect
  - Spontaneous emission

Density of states for photons in 3D

$$\frac{dk}{d\omega} = \frac{1}{c}$$

$$N(\omega) = \int_{\omega' < \omega} g(\omega') f(\omega') d\omega' = \sum_{k'} f(k')$$

$$= 2 \times \frac{1}{(\Delta k)^3} \int_{k' < k} f(k') d\vec{k}' = 2 \times \frac{1}{(\Delta k)^3} \int_{k' < k} 4\pi k'^2 f(k') dk'$$

$$g(\omega) = \left(\frac{k}{\pi}\right)^2 \frac{dk}{d\omega} = \frac{\omega^2}{\pi^2 c^3}$$

Other quanta

- Phonon
- Plasmon
- Surface plasmon

Classification of quanta

- Mass
  - Mass of the electron = 9.1E-31 kg
  - Mass of the photon = 0
- Charge
  - Electrons carry one unit of negative charge
  - Photons don't carry charges.
- Spin
  - Spin = 1/2 (electrons), 3/2, 5/2, … = fermions
  - Spin = 0, 1 (photons), 2, … = bosons. E.g. Excitons can carry integer spins.
- Dispersion relation
  - Particularly useful for quasi particles