Finite Element Method :-

To control the optical properties of materials has become a key issue in material engineering. Photonic crystals are periodic dielectric materials characterized by photonic band gaps (PBGs). A PBG can prohibit the propagation of electromagnetic waves (EM) whose frequency fall within the band gap region. These materials are expected to find many applications in optoelectronics and optical communications.

It was proposed that the emission of EM wave can be modified by enviornment such as metallic cavities, dielectric cavities etc which can be described by the photon density of states (PDOS) which is related to transition rate of fermi golden rule.

Many numerical methods have been developed and applied to the analysis and investigation of photonic crystals including finite element frequency domain - or finite element time domain method etc.

On the other hand, the finite element method (FEM) has proved to be a flexible and efficient numerical tool with which to design various types of microwave components with in-homogeneous and complex structures.

Finite element Method was originally developed for solving problems in solid state mechanics and widely used in all areas of computational physics and engineering. This is the most flexible method to solve differential equations numerically.

The basic concept of FEM can be thought of splitting the computational domain into individual small patches and finding local solutions that satisfy the differential equations within the boundary of this patch. By stitching the individual solutions on this patches back together, a global solution can be obtained.

Computational approach to calculate optical excitations

Optical processes in solids :- The way in which light interacts with material objects is determined by the optical properties of the materials.

Use of optical Materials

→ To design and build devices to manipulate light : mirrors, lenses, filters, polarizers, and a host of other gadgets.

→ we can measure the optical properties of some new material and obtain a wealth of information about the low energy excitations that govern the material's physics.

In general, semiconductors are materials, inorganic or organic which can control their conduction depending on chemical structure, temperature, illumination and presence of dopants. They have electrical conductivity between conductor and an insulator. In contrast to conductors, electrons in a semiconductor must obtain energy to cross the band gap and to reach the conduction band. Energy for the excitation can be obtained by different ways.

Thermal Excitation :-
Electron-hole pairs are constantly generated from thermal energy as well, in the absence of any external energy source. Thermal excitation does not require any other form of starting impulse. This phenomenon occurs also at room temperature. It is caused by impurities, irregularity in structure lattice or by dopant. It strongly depends on the Eg, so that for lower Eg

a number of thermally excited charge carriers increases. Since thermal excitation results in the detector noise, active cooling is required for some types of semiconductors. Detectors based on silicon have sufficiently low noise even by room temperature. This is caused by the large band gap of silicon ($E_g = 1.12\,eV$) which allows us to operate the detector at room temperature, but cooling is preferred to reduce noise.

Optical Excitation :- Note that, energy of a single photon of visible light spectrum is comparable with these band gaps. Photons of wave lengths 700nm - 400nm have energies of 1.77 ev, 3.10 ev. As a result, also visible light is able to excite electrons to the conduction band. Actually, this is the principle of photovoltaic panels that generate electric current.

A quantum $\hbar\omega$ or $h\nu$ of optical excitation will drive a solid out of thermal equilibrium provided that $\hbar\omega \gg KT$. Here, T is the temperature of the solid, and KT character-izes the mean energy of its thermally excited degrees of freedom. The condition is usually met, even far above room temperature, for optical interband transitions in semiconductors. During and after the absorption process a number of electronic and vibronic excited states will be populated and interact with each other. These excitations subsequently relax towards equi-librium, through exchange of momentum and energy with the rest of the system.

→ optically or electrically excited electrons and holes with large excess energies $\Delta E \gg KT$ will interact among themselves and with the low-lying excitations through very different processes, which nevertheless can be classified in two main categories : carrier-lattice and carrier-carrier interactions. The former class involves direct dissipation of excess energy into vibrational modes of the lattice, including also other excitations to which these lattice modes are coupled. The ~~lattice~~ later is short-form for the fact that the excited charge carriers, electrons and holes, interact mutually via the Coulomb interaction, and scatter off each other.

→ The rate of such collisions (e-e, e-h, h-h) depends on carrier density and may involve either single-electron or collective excitations, like plasmons and phonons. Both interaction mechanisms rapidly randomize momenta and energies of the optically excited non-equilibrium charge carriers.

→ Many of the relevant relaxation processes have characteristics times in the picosecond range so that a meaningful empirical analysis of the relaxation processes requires experimental probes with adequate time resolution. Steady progress in short-pulse electrical and optical techniques and notably the invention of laser light sources, has led to the enormous achievements in the field of optical spectroscopy and charge transport applied to semi-conductors.

Electronic Band structure and optical excitations

The optical properties of semiconductors in the near IR, visible and UV part of the spectrum are closely connected with their electronic band structure. All gross features of linear optical spectra in the range $E_g < \hbar\omega < 10\,eV$ can be readily inferred from (i) the energy band structure $E(K)$ and the density of states derived from it, ii) the corresponding wave functions $\psi(r)$ of crystal electrons and iii) the fermi equilibrium distribution function.

Many Ion electron system :-

$$H_0 = \sum_i \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{|r_i - r_j|} + \sum_K \frac{P_K^2}{2M_K} + \frac{1}{2}\sum_{K \neq L} \frac{e^2}{|R_K - R_L|} - \sum_{i,K} \frac{e^2}{|r_i - R_K|}$$

Schrodinger equation for many body problem

$$\mathcal{H} = \overbrace{-\sum \frac{\hbar^2}{2M_I}\nabla_I^2}^{\text{K.E of Ions}} \overbrace{- \sum \frac{\hbar^2}{2m_i}\nabla_i^2}^{\text{K.E of e's}} + \overbrace{\frac{e^2}{2}\sum_I \sum_{J, J \neq I} \frac{Z_I Z_J}{|R_I - R_J|}}^{\text{Ion-Ion Interaction}}$$

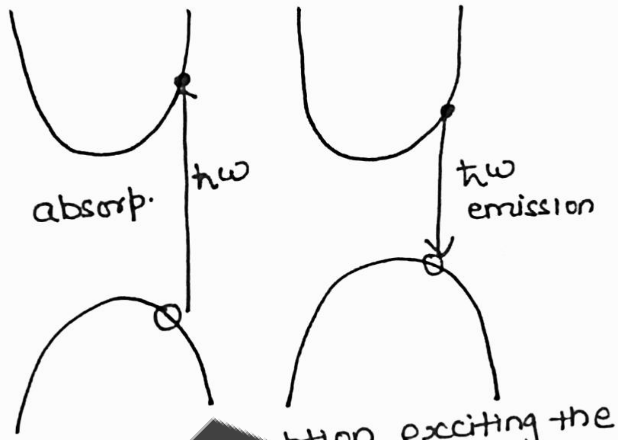
$$+ \underbrace{\frac{e^2}{2}\sum_i \sum_{j, j \neq i} \frac{1}{|r_i - r_j|}}_{\text{e-e interaction}} \underbrace{- e^2 \sum_I \sum_i \frac{Z_I}{|R_I - r_i|}}_{\text{e-Ion interaction}}$$

Solving the eigen value problem,

$$\mathcal{H}\,\Psi_n(R,r) = \mathcal{E}_n \Psi_n(R,r)$$

and using Born-Oppenheimer approximation, we can calculate the true wave function and ground state energy.

Transitions from occupied valence to unoccupied conduction band states (upward transitions) and their time-reversed counter-parts. (downward transitions)



light absorption exciting the crystal grond state.

Excitations in N electron system:

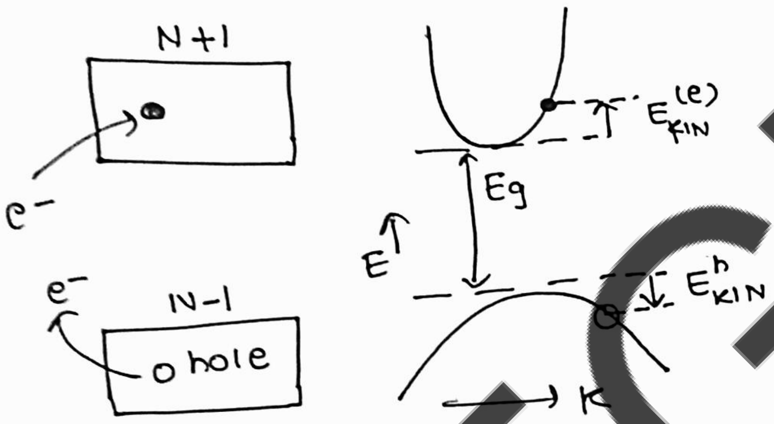


Figure shows creation of excited electron-hole pair state of the N-electron system. The energy wavevector diagram shows a valence band hole and a conduction band electron with kinetic-energies E_{kin}^{h} and E_{kin}^{e}.

Example - optical excitation in Boron Nitride (BN):-

BN appears to be the material of choice for emerging applications in optoelectronics, electron emitters and detectors due to its high chemical stability, thermal conductivity, melting temperature, resistivity, band gap (~6.5 eV), optical absorption near the band edge (~ 7.5×10^5 / cm).

Optical properties of BN :-

(a) Ultra-high bandgap :- Both theoretical and experi- -mental results indicate that the bandgap of BN is around 6.5 eV.

(b) High optical emission and absorption :- ($\sim 7.5 \times 10^5$/cm)

(c) Very large exciton energy - The exciton binding energies is about 0.7 eV in BN Bulk crystals and 2.1 eV in BN - monolayers.