### **Handout 24**

# The Effective Mass Theorem and the Effective Mass Schrodinger Equation

### In this lecture you will learn:

- Electron states in crystals with weak potential perturbations
- The effective mass theorem
- The effective mass Schrodinger equation
- The donor and acceptor impurity levels in crystals
- G. H. Wannier, Phys. Rev., 52, 191 (1937).
- J. C. Slater, Phys. Rev., 76, 1592 (1949).
- J. M. Luttinger and W. Kohn, Phys. Rev., 97, 869 (1955).

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### **Perturbed Electrons in Energy Bands**

1) The quantum states of an electron in a crystal are given by Bloch functions that obey the Schrodinger equation:

$$\hat{H} \psi_{n,\vec{k}}(\vec{r}) = E_n(\vec{k}) \psi_{n,\vec{k}}(\vec{r})$$

where the wavevector  $\vec{k}$  is confined to the FBZ and "n" is the band index

2) Under a lattice translation, Bloch functions obey the relation:

$$\psi_{n,\vec{k}}(\vec{r}+\vec{R})=e^{i\vec{k}\cdot\vec{R}}\psi_{n,\vec{k}}(\vec{r})$$

Now we ask the following question: if an external potential is added to the crystal Hamiltonian,

$$\hat{H} + U(\vec{r})$$

then what happens? How do the electrons behave? How do we find the new energies and eigenstates?

$$\left[\hat{H} + U(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r})$$

The external potential could represent, for example, an applied E-field or an applied B-field, or potentials due to impurity atoms, or inhomogeneous nanostructures

#### **Some Preliminaries**

Statement of problem: Need to solve,

$$\left[\hat{H} + U(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r})$$

As always, we will start from a completely different point to solve the problem stated above

Recall that the energy bands are lattice-periodic in the reciprocal space,

$$E_n(\vec{k} + \vec{G}) = E_n(\vec{k})$$

When a function in real space is lattice-periodic, we can expand it in a Fourier series,

$$V(\vec{r} + \vec{R}) = V(\vec{r}) \implies V(\vec{r}) = \sum_{j} V(\vec{G}_{j}) e^{i\vec{G}_{j} \cdot \vec{r}}$$

 $\Rightarrow$  When a function is lattice-periodic in reciprocal space, we can also expand it in Fourier series of the form,

$$E_n(\vec{k} + \vec{G}) = E_n(\vec{k}) \implies E_n(\vec{k}) = \sum_j E_n(\vec{R}_j) e^{i \vec{R}_j \cdot \vec{k}}$$

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#### **A Brief Review**

$$E_n(\vec{k} + \vec{G}) = E_n(\vec{k}) \implies E_n(\vec{k}) = \sum_j E_n(\vec{R}_j) e^{i \vec{R}_j \cdot \vec{k}}$$

Recall the operator:

$$\hat{E}_n(-i\nabla) = \sum_j E_n(\bar{R}_j) e^{\bar{R}_j \cdot \nabla}$$

When we apply this operator to a Bloch function from the same band (i.e. the n-th band) we got:

$$\begin{split} \hat{E}_{n}(-i\nabla)\psi_{n,\bar{k}}(\bar{r}) &= \sum_{j} E_{n}(\bar{R}_{j}) e^{\bar{R}_{j} \cdot \nabla} \psi_{n,\bar{k}}(\bar{r}) \\ &= \sum_{j} E_{n}(\bar{R}_{j}) \psi_{n,\bar{k}}(\bar{r} + \bar{R}_{j}) \\ &= \sum_{j} E_{n}(\bar{R}_{j}) e^{i \, \bar{k} \cdot \bar{R}_{j}} \psi_{n,\bar{k}}(\bar{r}) \\ &= E_{n}(\bar{k}) \psi_{n,\bar{k}}(\bar{r}) \end{split}$$

The result above implies that the action of the operator  $\hat{E}_n(-i\nabla)$  on a Bloch function belonging to the same band is that of the Hamiltonian!

$$\boldsymbol{E}_{n}(-i\nabla)\psi_{n,\bar{k}}(\bar{r}) = \hat{H}\psi_{n,\bar{k}}(\bar{r}) = \boldsymbol{E}_{n}(\bar{k})\psi_{n,\bar{k}}(\bar{r})$$

### **Solution Strategy**

Now we come back to the problem:

$$\left[\hat{H} + U(\vec{r})\right]\psi(\vec{r}) = E \psi(\vec{r})$$

We want to see how the Bloch function  $\Psi_{n,\vec{k}_0}(\vec{r})$  is perturbed by the potential.

We write the solution as a superposition using Bloch functions from the same n-th band :

$$\psi(\vec{r}) = \sum_{\vec{k} \text{ near } \vec{k}_0} c(\vec{k}) \psi_{n,\vec{k}}(\vec{r})$$

to get,

$$\begin{split} & \left[ \hat{H} + U(\bar{r}) \right] \psi(\bar{r}) = E \, \psi(\bar{r}) \\ \Rightarrow & \left[ \hat{E}_n(-i\nabla) + U(\bar{r}) \right] \psi(\bar{r}) = E \, \psi(\bar{r}) \end{split}$$

where we have replaced the Hamiltonian operator by  $\hat{E}_n(-i\nabla)$ 

We are seeking a solution near a particular point  $\vec{k}_0$  in k-space. For example, near a band extremum. For  $\vec{k}$  near  $\vec{k}_0$  we can approximate all Bloch functions as,

$$\psi_{n,\vec{k}}(\vec{r}) = e^{i \, \vec{k} \cdot \vec{r}} \, u_{n,\vec{k}}(\vec{r}) \approx e^{i \, \vec{k} \cdot \vec{r}} \, u_{n,\vec{k}_0}(\vec{r}) = e^{i \, (\vec{k} - \vec{k}_0) \cdot \vec{r}} \, \psi_{n,\vec{k}_0}(\vec{r})$$

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### The Envelope Function

$$\begin{split} \psi(\vec{r}) &= \sum_{\vec{k} \text{ near } \vec{k}_{o}} c(\vec{k}) \psi_{n,\vec{k}}(\vec{r}) \\ &= \sum_{\vec{k} \text{ near } \vec{k}_{o}} c(\vec{k}) e^{i(\vec{k} - \vec{k}_{o}) \cdot \vec{r}} \psi_{n,\vec{k}_{o}}(\vec{r}) \\ &= \left[ \sum_{\vec{k} \text{ near } \vec{k}_{o}} c(\vec{k}) e^{i(\vec{k} - \vec{k}_{o}) \cdot \vec{r}} \right] \psi_{n,\vec{k}_{o}}(\vec{r}) \\ &= \phi(\vec{r}) \ \psi_{n,\vec{k}_{o}}(\vec{r}) \end{split}$$

The above expression shows that we are approximating the solution as a product of a Bloch function and another (unknown) function  $\phi(\vec{r})$  which is called the envelope function. By construction the envelope function is slowly varying in space (on atomic scale).

We use the above form of the solution in the equation,

$$\left[\,\hat{E}_{n}(-i\nabla) + U(\vec{r}\,)\,\right]\phi(\vec{r}\,)\,\psi_{n,\vec{k}_{0}}(\vec{r}\,) = E\,\phi(\vec{r}\,)\,\psi_{n,\vec{k}_{0}}(\vec{r}\,)$$

First we look at:

$$\hat{E}_n(-i\nabla) \phi(\vec{r}) \psi_{n,\vec{k}_0}(\vec{r})$$

## **The Effective Mass Schrodinger Equation**

$$\begin{split} \hat{E}_{n}(-i\nabla) \phi(\vec{r}) \psi_{n,\vec{k}_{o}}(\vec{r}) &= \sum_{j} E_{n}(\vec{R}_{j}) e^{\vec{R}_{j} \cdot \nabla} \phi(\vec{r}) \psi_{n,\vec{k}_{o}}(\vec{r}) \\ &= \sum_{j} E_{n}(\vec{R}_{j}) \phi(\vec{r} + \vec{R}_{j}) \psi_{n,\vec{k}_{o}}(\vec{r} + \vec{R}_{j}) \\ &= \sum_{j} E_{n}(\vec{R}_{j}) e^{i \vec{K}_{o} \cdot \vec{R}_{j}} \phi(\vec{r} + \vec{R}_{j}) \psi_{n,\vec{k}_{o}}(\vec{r}) \\ &= \psi_{n,\vec{k}_{o}}(\vec{r}) \sum_{j} E_{n}(\vec{R}_{j}) e^{i \vec{k}_{o} \cdot \vec{R}_{j}} \phi(\vec{r} + \vec{R}_{j}) \\ &= \psi_{n,\vec{k}_{o}}(\vec{r}) \sum_{j} E_{n}(\vec{R}_{j}) e^{i \vec{k}_{o} \cdot \vec{R}_{j}} e^{\vec{R}_{j} \cdot \nabla} \phi(\vec{r}) \\ &= \psi_{n,\vec{k}_{o}}(\vec{r}) \sum_{j} E_{n}(\vec{R}_{j}) e^{i (\vec{k}_{o} - i\nabla) \cdot \vec{R}_{j}} \phi(\vec{r}) \\ &= \psi_{n,\vec{k}_{o}}(\vec{r}) \hat{\Sigma}_{n} (\vec{k}_{o} - i\nabla) \phi(\vec{r}) \end{split}$$

This implies:

$$\begin{split} & \left[ \ \hat{\boldsymbol{E}}_{n}(-i\nabla) + \boldsymbol{U}(\vec{r}) \ \right] \phi(\vec{r}) \, \psi_{n,\vec{k}_{o}}(\vec{r}) = \boldsymbol{E} \, \phi(\vec{r}) \, \psi_{n,\vec{k}_{o}}(\vec{r}) \\ \Rightarrow & \psi_{n,\vec{k}_{o}}(\vec{r}) \left[ \ \hat{\boldsymbol{E}}_{n}(\vec{k}_{o} - i\nabla) + \boldsymbol{U}(\vec{r}) \ \right] \phi(\vec{r}) = \boldsymbol{E} \, \phi(\vec{r}) \, \psi_{n,\vec{k}_{o}}(\vec{r}) \end{split}$$

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### **The Effective Mass Theorem**

Finally we have the following equation for the envelope function:

$$\left[\hat{E}_{n}(\vec{k}_{o}-i\nabla)+U(\vec{r})\right]\phi(\vec{r})=E\ \phi(\vec{r})$$

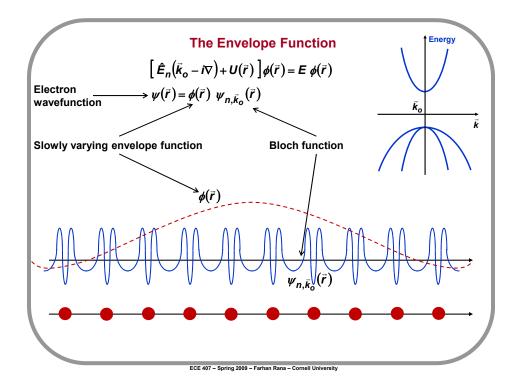
The effective mass theorem states the following:

a) In the presence of a weak perturbing potential the solution for electron states near  $\vec{k}_0$  in k-space can be represented as a product of a slowly varying envelope function and a Bloch function

$$\psi(\vec{r}) = \phi(\vec{r}) \ \psi_{n,\vec{k}_0}(\vec{r})$$

b) The slowly varying envelope function obeys the effective mass Schrodinger equation:

$$\left[\hat{E}_{n}(\vec{k}_{0}-i\nabla)+U(\vec{r})\right]\phi(\vec{r})=E\ \phi(\vec{r})$$



## The Effective Mass Schrodinger Equation: An Example

Consider a conduction energy band with the dispersion:

$$E_c(\vec{k}) = E_c + \frac{\hbar^2 (k_x - k_{ox})^2}{2m_{xx}} + \frac{\hbar^2 (k_y - k_{oy})^2}{2m_{yy}} + \frac{\hbar^2 (k_z - k_{oz})^2}{2m_{zz}}$$

Now suppose an external potential  $U(\vec{r})$  is present. The electron states near the conduction band bottom in the presence of the external potential are described by the effective mass equation:

$$\left[\hat{E}_{c}(\vec{k}_{O} - i\nabla) + U(\vec{r})\right]\phi(\vec{r}) = E \phi(\vec{r})$$

 $\left[\hat{E}_c(\bar{k}_o-i\nabla)+U(\bar{r})\right]\phi(\bar{r})=E\;\phi(\bar{r}) \qquad / \qquad / \qquad | \qquad \backslash$  Note that one has to make the following replacements in the energy dispersion relation:

The operator 
$$\hat{E}_c(\vec{k}_o - i\nabla)$$
 is then:

$$E_c(\bar{k}_o - i\nabla) = E_c - \frac{\hbar^2}{2m_{xx}} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{yy}} \frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_{zz}} \frac{\partial^2}{\partial z^2}$$

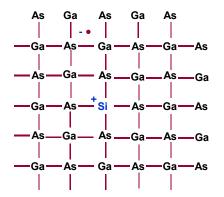
The effective mass Shrodinger equation becomes

$$\left[-\frac{\hbar^2}{2m_{xx}}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{yy}}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_{zz}}\frac{\partial^2}{\partial z^2} + E_c + U(\vec{r})\right]\phi(\vec{r}) = E\phi(\vec{r})$$

### **Donor Impurities in Semiconductors**

One of the earliest applications of the effective mass theorem was the donor and acceptor impurity states and energy levels in semiconductors

Consider a semiconductor (say GaAs) in which one Ga atom site is occupied by a Si atom, as shown:



- Silicon has one more electron in the outermost shell compared to Ga (4 in Si compared to 3 in Ga)
- Since only 3 electrons are needed to form co-valent bonds with the nearby As atoms, the extra electron does not participate in bonding and can drift away leaving behind a positively charged Si atom

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**Donor Impurities in Semiconductors: Effective Mass Equation** 

The positively charged Si atoms presents a Coulomb potential to the lattice. Therefore the potential energy is:

Attractive positive potential:  $U(\vec{r}) = -\frac{e^2}{4\pi \varepsilon_s |\vec{r}|}$ 

We need to figure out how the electron states and energy levels in the conduction band are modified because of this Coulomb potential

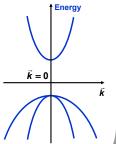
$$\left[\hat{H} + U(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r})$$

We are interested in how the states near the conduction band bottom get modified, so we assume

$$\psi(\vec{r}) = \phi(\vec{r}) \ \psi_{c,\vec{k}_0=0}(\vec{r})$$

And we know that the envelope function satisfies the effective mass Schrodinger equation

$$\left[\hat{E}_{c}(\vec{k}_{o} - i\nabla) + U(\vec{r})\right]\phi(\vec{r}) = E \phi(\vec{r})$$



## **Donor Impurities in Semiconductors: Effective Mass Equation**

$$\Rightarrow \left[ \hat{E}_c(-i\nabla) + U(\vec{r}) \right] \phi(\vec{r}) = E \phi(\vec{r})$$

We seek a solution near the conduction band bottom at 
$$\bar{k}_o = 0$$
:
$$\Rightarrow \left[ \hat{E}_c(-i\nabla) + U(\bar{r}) \right] \phi(\bar{r}) = E \phi(\bar{r})$$
The conduction band dispersion in GaAs implies:
$$E_c(\bar{k}) = E_c + \frac{\hbar^2 k^2}{2m_e} \Rightarrow E_c(\bar{k}_o - i\nabla) = E_c(-i\nabla) = E_c - \frac{\hbar^2 \nabla^2}{2m_e}$$
—Ga—As—Ga—As—Ga—
$$= E_c(\bar{k}) = E_c + \frac{\hbar^2 k^2}{2m_e} \Rightarrow E_c(\bar{k}_o - i\nabla) = E_c(-i\nabla) = E_c - \frac{\hbar^2 \nabla^2}{2m_e} = \frac{-\hbar^2 \nabla^2}{2$$

So we get the equation

$$\begin{bmatrix} E_c - \frac{\hbar^2 \nabla^2}{2m_e} - \frac{e^2}{4\pi \varepsilon_s r} \end{bmatrix} \phi(\vec{r}) = E \phi(\vec{r})$$

$$\Rightarrow \begin{bmatrix} -\frac{\hbar^2 \nabla^2}{2m_e} - \frac{e^2}{4\pi \varepsilon_s r} \end{bmatrix} \phi(\vec{r}) = (E - E_c) \phi(\vec{r})$$

The above equation looks like the Schrodinger equation for an electron in a hydrogen atom with the exceptions that:



i)The mass is the effective mass  $m_e$  instead of the free-electron mass m

ii)The dielectric constant is  $\varepsilon_{\rm s}$  instead of  $\varepsilon_{\rm o}$ 

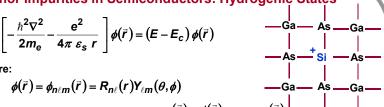
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### **Donor Impurities in Semiconductors: Hydrogenic States**

$$\left[ -\frac{\hbar^2 \nabla^2}{2m_e} - \frac{e^2}{4\pi \varepsilon_s r} \right] \phi(\bar{r}) = (E - E_c) \phi(\bar{r})$$

Solutions are:

$$\phi(\vec{r}) = \phi_{n\ell m}(\vec{r}) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi)$$



Remember that the actual wavefunction is:  $\psi(\vec{r}) = \phi(\vec{r}) \psi_{c,\vec{k}_0=0}(\vec{r})$  Where:

- 1) n is a positive integer  $\geq 1$  (n = 1,2,.....)
- 2)  $\ell$  is a postive integer < n  $(\ell = 0,1,2,.....(n-1)$  for s, p, d, f, .....)
- 3) m is an integer such that  $|m| \le \ell$   $(m = -\ell, ..., -1, 0, +1, .... + \ell)$

The corresponding energy eigenvalues are:

$$E - E_c = -\frac{E_o}{n^2} \longrightarrow n = 1,2,3....$$

$$\Rightarrow E = E_c - \frac{E_o}{n^2}$$

$$\Rightarrow E = E_c - \frac{E_o}{n^2}$$

$$= \frac{m_e}{2\hbar^2} \left(\frac{e^2}{4\pi\varepsilon_s}\right)^2$$

### **Donor Impurities in Semiconductors: Hydrogenic States**

$$E = E_c - \frac{E_o}{n^2} \qquad n = 1, 2, 3 \dots$$

Ground state (lowest energy state):

$$\Rightarrow$$
  $n=1$   $\ell=0$   $m=0$ 

$$E = E_c - E_c$$

$$\phi_{1s}(\vec{r}) = \phi_{n=1}|_{\ell=0} m=0 (\vec{r}) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

$$E = E_c - \frac{E_o}{n^2} \qquad n = 1,2,3.....$$

$$E_o = \frac{m_e}{2\hbar^2} \left(\frac{e^2}{4\pi\varepsilon_s}\right)^2$$

$$= (13.6 \text{ eV}) \left(\frac{m_e}{m}\right) \left(\frac{\varepsilon_o}{\varepsilon_s}\right)^2$$

$$\Rightarrow n = 1 \quad \ell = 0 \quad m = 0$$

$$\Rightarrow n = 1 \quad \ell = 0 \quad m = 0$$

$$E = E_c - E_o$$

$$\phi_{1s}(\vec{r}) = \phi_{n=1} \ell = 0 \quad m = 0 \quad \begin{cases} a_o = \left(\frac{4\pi\varepsilon_s}{e^2}\right) \frac{\hbar^2}{m_e} \\ = (0.53 \text{ A}) \left(\frac{\varepsilon_s}{\varepsilon_o}\right) \left(\frac{m}{m_e}\right) \end{cases}$$

$$= (0.53 \text{ A}) \left(\frac{\varepsilon_s}{\varepsilon_o}\right) \left(\frac{m}{m_e}\right)$$
Effective Bohr radius

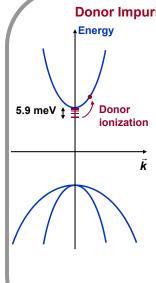
**Effective Bohr radius** 

In GaAs:  $m_{\rm e}$  = .067 m and  $\varepsilon_{\rm s}$  = 12.4  $\varepsilon_{\rm o}$ 

$$E = E_c - E_o = E_c - (13.6 \text{ eV}) \left(\frac{m_e}{m}\right) \left(\frac{\varepsilon_o}{\varepsilon_s}\right)^2 \approx E_c - 5.9 \text{ meV}$$

$$a_{\rm o} = (0.53 \text{ A}) \left(\frac{\varepsilon_{\rm s}}{\varepsilon_{\rm o}}\right) \left(\frac{m}{m_{\rm e}}\right) \approx 98 \text{ A}$$
 Very large!

## **Donor Impurities in Semiconductors: Hydrogenic States** $E = E_c - \frac{(13.6 \text{ eV})}{n^2} \left(\frac{m_e}{m}\right) \left(\frac{\varepsilon_o}{\varepsilon_s}\right)^2 \approx E_c - \frac{5.9 \text{ meV}}{n^2}$ $a_{\rm o} = (0.53 \text{ A}) \left(\frac{\varepsilon_{\rm s}}{\varepsilon_{\rm o}}\right) \left(\frac{m}{m_{\rm e}}\right) \approx 98 \text{ A}$ $\phi_{1s}(\vec{r}) = \phi_{n=1}|_{\ell=0} m=0 (\vec{r}) = \frac{1}{\sqrt{\pi a_o^3}} e^{-r/a_o}$ 其 ‡ 5.9 meV 1.42 eV The positively charge donor atoms create new quantum states whose energies are slightly below the conduction band edge and whose wavefunctions are localized near the donor atom $\psi(\vec{r}) = \phi_{1s}(\vec{r}) \ \psi_{c,\vec{k}_0=0}(\vec{r})$



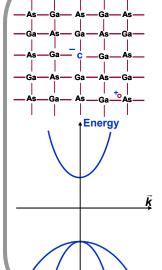
- **Donor Impurities in Semiconductors: N-Type Doping** 
  - At very low temperatures the electron resides in the donor energy level and the donor atom is neutral
  - At room temperature, the electron in the donor energy level can acquire enough energy to jump to the conduction band

When this happens the donor is said to have ionized

- Once in the conduction band the electron can move around and is no longer localized at the donor atom
- Donor impurities can therefore be used to dope semiconductors n-type

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## Acceptor Impurities in Semiconductors: P-Type Doping



Consider a semiconductor (say GaAs) in which one As atom site is occupied by a carbon atom, as shown:

- C has one less electron in the outermost shell compared to As (4 in C compared to 5 in As)
- Since 4 electrons are needed to form covalent bonds with the nearby Ga atoms, the required electron is taken from the valence band resulting in a negatively charged C atom and a hole in the valence band

Solution:  $\psi(\vec{r}) = \phi(\vec{r}) \ \psi_{hh,\bar{k}_0=0}(\vec{r})$ 

$$\Rightarrow \left[ \hat{E}_{hh}(-i\nabla) + U(\vec{r}) \right] \phi(\vec{r}) = E \phi(\vec{r})$$

Negative repulsive potential:  $U(\vec{r}) = +\frac{e^2}{4\pi \varepsilon_s |\vec{r}|}$ 

hh-band dispersion:  $E_{hh}(\vec{k}) = E_V - \frac{\hbar^2 k^2}{2m_{hh}}$ 

$$\Rightarrow E_{hh}(-i\nabla) = E_V + \frac{\hbar^2 \nabla^2}{2m_{hh}}$$

### **Acceptor Impurities in Semiconductors: P-Type Doping**

The effective mass Schrodinger equation becomes:

$$\left[ E_V + \frac{\hbar^2 \nabla^2}{2m_{hh}} + \frac{e^2}{4\pi \varepsilon_s |\vec{r}|} \right] \phi(\vec{r}) = E \phi(\vec{r})$$

Rearrange:

$$\left[ -\frac{\hbar^2 \nabla^2}{2m_{hh}} - \frac{e^2}{4\pi \varepsilon_s |\vec{r}|} \right] \phi(\vec{r}) = (-E + E_v) \phi(\vec{r})$$

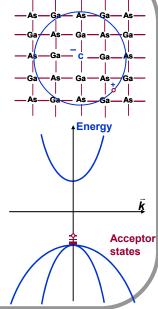
Again we end up with a Schrodinger-like equation for a Hydrogen atom which has the solution:

$$\phi(\vec{r}) = \phi_{n\ell m}(\vec{r}) = R_{n\ell}(r)Y_{\ell m}(\theta, \phi)$$

$$-E + E_{v} = -\frac{E_{o}}{n^{2}}$$

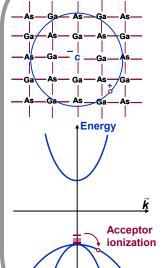
$$\Rightarrow E = E_{v} + \frac{E_{o}}{n^{2}}$$

$$= (13.6 \text{ eV}) \left(\frac{m_{hh}}{m}\right) \left(\frac{\varepsilon_{o}}{\varepsilon_{s}}\right)^{2}$$



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## **Acceptor Impurities in Semiconductors: P-Type Doping**

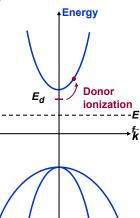


- Acceptor atom gives rise to hydrogenic energy levels near the valence band maximum
- At very low temperatures the hole resides in the acceptor energy level and the acceptor atom location is overall neutral
- At room temperature, the hole in the acceptor energy level can acquire enough energy to jump to the valence band

When this happens the acceptor is said to have ionized

- Once in the valence band the hole can move around and is no longer localized at the acceptor atom
- Acceptor impurities can therefore be used to dope semiconductors p-type





In the grand canonical ensemble the probability of a system to have total particles N and total energy E is:

$$P(N,E) = A e^{-(E-E_f N)/KT}$$

The donor level can have the following possible states:

1) No electrons present

$$P(N=0,E=0) = A$$

2) One spin-up electron present

$$P(N = 1, E = E_d) = A e^{-(E_d - E_f)/KT}$$
3) One spin-down electron present

$$P(N = 1, E = E_d) = A e^{-(E_d - E_f)/KT}$$

4) Two or more electrons present

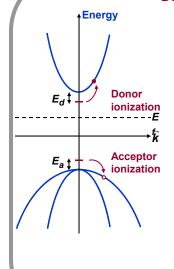
$$P(N > 1, E) = 0$$
 Coulomb repulsion does not allow it

Sum of all probabilities

Sum of all probabilities should equal unity: 
$$\Rightarrow A \left[ 1 + 2 e^{-(E_d - E_f)/KT} \right] = 1 \Rightarrow A = \frac{1}{1 + 2 e^{-(E_d - E_f)/KT}}$$

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### **Donor Ionization Statistics**



Probability that the Probability that the donor level is ionized donor level has no electrons P(N=0,E=0)

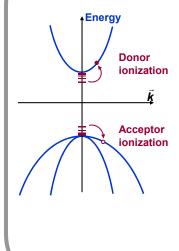
If the total donor impurity concentration is  $N_d$  then the concentration of ionized donors N<sup>+</sup><sub>d</sub> is equal to:

$$N_d^+ = \frac{N_d}{1 + 2 e^{-(E_d - E_f)/KT}}$$

For acceptors we have a similar relation:

$$N_a^- = \frac{N_a}{1 + 2 e^{(E_a - E_f)/KT}}$$





Consider a semiconductor that is doped with both donor and acceptor impurity atoms

• The total charge must be zero:

$$N_d^+ - N_a^- + p - n = 0$$

The above equation can be used to find the position of the equilibrium Fermi level since every term depends on the Fermi level position (one equation in one unknown)

$$N_d^+ = \frac{N_d}{1 + 2 e^{-(E_d - E_f)/KT}}$$

$$N_a^- = \frac{N_a}{1 + 2 e^{(E_a - E_f)/KT}}$$