Physics of Semiconductors and Nanostructures

ECE 4070 / MSE 6050
Spring, 2019

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ECE & MSE, Cornell University
ECE 4070/MSE 6050, Physics of Semiconductors and Nanostructures: The Physics Enabling Big Data

Cornell University, Spring 2019

Silicon Transistors

Electron waves

Microprocessors and Memories

Lasers, LEDs, Solar Cells

Atoms

Semiconductors

Logic

Memory

Communications

You probably cannot stop hearing that we are living in the age of “Big Data”. But what exactly is this data? How and where is it created? How and where is it stored? How is it manipulated to create meaning? And how are massive chunks of data moved around at the speed of light?

This course is the red pill that will show you how deep the physics of “Big Data” goes. Answers to all these questions are tied to the physics of electrons in semiconductor materials.

Lecturer: Debdeep Jena (djena@cornell.edu)
Classes: TR 11:40 am-12:55 pm, Phillips Hall 403

Website: https://djena.engineering.cornell.edu/2019_ece4070_mse6050.htm
Prerequisites: Basic notions of quantum mechanics and statistical physics
Microsoft Plumbs Ocean’s Depths to Test Underwater Data Center

By JOHN MARKOFF  JAN. 31, 2016

Ben Cutler, left, and Norman Whitaker, both of Microsoft Research, with the “Leona Philpot,” a prototype underwater data center, at the company’s headquarters in Redmond, Wash. Matt Lutton for The New York Times
Transistors Will Stop Shrinking in 2021, Moore’s Law Roadmap Predicts

By Rachel Courtland
Posted 22 Jul 2016 | 16:00 GMT

The trajectory of transistor feature sizes (the physical gate length of transistors in high-performance logic is shown here) could take a sharp turn in 2021.

Illustration: Erik Vrielink
Debdeep Jena (djena@cornell.edu)

It all began with Light…

- 3 Pillars of Information systems are: “Computation, Memory, and Communication”
It all began with Light

• 3 Pillars of Information systems are: “Computation, Memory, and Communication”
Course Outline: 4 Modules

• Module I: Fundamentals
  • Chapters 1 - 7

• Module 2: Semiconductor Bands, Doping, and Heterostructures
  • Chapters 8-14

• Module 3: Quantum Electrostatics and Transport in Semiconductors & Devices
  • Chapters 15-24

• Module 4: Photonics with Semiconductors
  • Chapters 25-30
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The Electron

?
The Electron

Electron mass

\[ m_e = 9.1 \times 10^{-31} \text{ kg} \]

Electron charge

\[ q = 1.6 \times 10^{-19} \text{ Coulomb} \]

Fig. 1.2 J. J. Thomson discovered the electron in 1896 @ the Cavendish Laboratory. He was awarded the 1906 Nobel prize in Physics. Seven of his students went on to win Nobel prizes.
Classical Physics

\[ F = m \frac{d^2 x}{dt^2} \]

\[ \vec{F} = q (\vec{E} + \vec{v} \times \vec{B}) \]

\[ \frac{n(E_2)}{n(E_1)} = e \frac{E_2 - E_1}{kT} \]

Boltzmann

\[ \nabla \cdot \vec{E} = \frac{\rho}{\varepsilon_0} \]
\[ \nabla \cdot \vec{B} = 0 \]
\[ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \]
\[ \nabla \times \vec{B} = \mu_0 \vec{j} + \mu_0 \frac{\partial \vec{D}}{\partial t} \]
Electrons in the Classical World

Path is deterministic

\[ F = \frac{dp}{dt} \]

Path is deterministic

\[ F = q(E + v \times B) \]
Properties of Metals

Periodic Table of Elements

Metals are:
- good conductors of electricity,
- good conductors of heat, and
- reflective and shiny.

Fig. 2.3 Ohm’s law is $V = IR$, or equivalently $J = \sigma E$. 

Debdeep Jena (djena@cornell.edu)
Properties of Metals

Data compiled by Rusen Yan
Properties of Metals

Metals are:

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![Diagram of electron gas moving in response to an electric field in a metal.](image)

**Fig. 2.4** Electron gas moving in response to an electric field in a metal.

\[ J = qnv = \frac{nq^2\tau}{m_e} E = \sigma E \quad \iff \quad \sigma = \frac{nq^2\tau}{m_e} \]

**Conductivity**

\[ \mu = \frac{q\tau}{m_e} \]

**Mobility**

![Graph of Ohm's law: V = IR.](image)

**Fig. 2.3** Ohm’s law is \( V = IR \), or equivalently \( J = \sigma E \).
## Properties of Metals

### Table 1.1
FREE ELECTRON DENSITIES OF SELECTED METALLIC ELEMENTS

<table>
<thead>
<tr>
<th>ELEMENT</th>
<th>Z</th>
<th>n (×10^22/cm^3)</th>
<th>r_e(Å)</th>
<th>r_s/α₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li (78 K)</td>
<td>1</td>
<td>4.70</td>
<td>1.72</td>
<td>3.25</td>
</tr>
<tr>
<td>Na (5 K)</td>
<td>1</td>
<td>2.65</td>
<td>2.08</td>
<td>3.93</td>
</tr>
<tr>
<td>K (5 K)</td>
<td>1</td>
<td>1.40</td>
<td>2.57</td>
<td>4.86</td>
</tr>
<tr>
<td>Rb (5 K)</td>
<td>1</td>
<td>1.15</td>
<td>2.75</td>
<td>5.20</td>
</tr>
<tr>
<td>Cs (5 K)</td>
<td>1</td>
<td>0.91</td>
<td>2.98</td>
<td>5.62</td>
</tr>
<tr>
<td>Cu</td>
<td>1</td>
<td>8.47</td>
<td>1.41</td>
<td>2.67</td>
</tr>
<tr>
<td>Ag</td>
<td>1</td>
<td>5.86</td>
<td>1.60</td>
<td>3.02</td>
</tr>
<tr>
<td>Au</td>
<td>1</td>
<td>5.90</td>
<td>1.59</td>
<td>3.01</td>
</tr>
<tr>
<td>Be</td>
<td>2</td>
<td>24.7</td>
<td>0.99</td>
<td>1.87</td>
</tr>
<tr>
<td>Mg</td>
<td>2*</td>
<td>8.61</td>
<td>1.41</td>
<td>2.65</td>
</tr>
<tr>
<td>Ca</td>
<td>2</td>
<td>4.61</td>
<td>1.73</td>
<td>3.27</td>
</tr>
<tr>
<td>Sr</td>
<td>2</td>
<td>3.55</td>
<td>1.89</td>
<td>3.57</td>
</tr>
<tr>
<td>Ba</td>
<td>2</td>
<td>3.15</td>
<td>1.96</td>
<td>3.71</td>
</tr>
<tr>
<td>Nb</td>
<td>2</td>
<td>5.56</td>
<td>1.63</td>
<td>3.07</td>
</tr>
<tr>
<td>Fe</td>
<td>2</td>
<td>17.0</td>
<td>1.12</td>
<td>2.12</td>
</tr>
<tr>
<td>Mn (α)</td>
<td>2</td>
<td>16.5</td>
<td>1.13</td>
<td>2.14</td>
</tr>
<tr>
<td>Zn</td>
<td>2</td>
<td>13.2</td>
<td>1.22</td>
<td>2.30</td>
</tr>
<tr>
<td>Cd</td>
<td>2</td>
<td>9.27</td>
<td>1.37</td>
<td>2.59</td>
</tr>
<tr>
<td>Hg (78 K)</td>
<td>2</td>
<td>8.65</td>
<td>1.40</td>
<td>2.65</td>
</tr>
<tr>
<td>Al</td>
<td>3</td>
<td>18.1</td>
<td>1.10</td>
<td>2.07</td>
</tr>
<tr>
<td>Ga</td>
<td>3</td>
<td>15.4</td>
<td>1.16</td>
<td>2.19</td>
</tr>
<tr>
<td>In</td>
<td>3</td>
<td>11.5</td>
<td>1.27</td>
<td>2.41</td>
</tr>
<tr>
<td>Ti</td>
<td>3</td>
<td>10.5</td>
<td>1.31</td>
<td>2.48</td>
</tr>
<tr>
<td>Sn</td>
<td>4</td>
<td>14.8</td>
<td>1.17</td>
<td>2.22</td>
</tr>
<tr>
<td>Pb</td>
<td>4</td>
<td>13.2</td>
<td>1.22</td>
<td>2.30</td>
</tr>
<tr>
<td>Bi</td>
<td>5</td>
<td>14.1</td>
<td>1.19</td>
<td>2.25</td>
</tr>
<tr>
<td>Sb</td>
<td>5</td>
<td>16.5</td>
<td>1.13</td>
<td>2.14</td>
</tr>
</tbody>
</table>

* At room temperature (about 300 K) and atmospheric pressure, unless otherwise noted. The radius r_e of the free electron sphere is defined in Eq. (1.2). We have arbitrarily chosen one value of Z for those elements that display more than one chemical valence. The Drude model gives no theoretical basis for the choice. Values of n are based on data from R. W. G. Wyckoff, Crystal Structures, 2nd ed., Interscience, New York, 1963.

### Table 1.3
DRUDE RELAXATION TIMES IN UNITS OF 10^-14 SECOND

<table>
<thead>
<tr>
<th>ELEMENT</th>
<th>77 K</th>
<th>273 K</th>
<th>373 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>7.3</td>
<td>0.88</td>
<td>0.61</td>
</tr>
<tr>
<td>Na</td>
<td>17</td>
<td>3.2</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>18</td>
<td>4.1</td>
<td></td>
</tr>
<tr>
<td>Rb</td>
<td>14</td>
<td>2.8</td>
<td></td>
</tr>
<tr>
<td>Cs</td>
<td>8.6</td>
<td>2.1</td>
<td></td>
</tr>
<tr>
<td>Cu</td>
<td>21</td>
<td>2.7</td>
<td>1.9</td>
</tr>
<tr>
<td>Ag</td>
<td>20</td>
<td>4.0</td>
<td>2.8</td>
</tr>
<tr>
<td>Au</td>
<td>12</td>
<td>3.0</td>
<td>2.1</td>
</tr>
<tr>
<td>Be</td>
<td></td>
<td>0.51</td>
<td>0.27</td>
</tr>
<tr>
<td>Mg</td>
<td>6.7</td>
<td>1.1</td>
<td>0.74</td>
</tr>
<tr>
<td>Ca</td>
<td>2.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sr</td>
<td>1.4</td>
<td>0.44</td>
<td></td>
</tr>
<tr>
<td>Ba</td>
<td>0.66</td>
<td>0.19</td>
<td></td>
</tr>
<tr>
<td>Nb</td>
<td>2.1</td>
<td>0.42</td>
<td>0.33</td>
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<tr>
<td>Fe</td>
<td>3.2</td>
<td>0.24</td>
<td>0.14</td>
</tr>
<tr>
<td>Mn (α)</td>
<td>2.4</td>
<td>0.49</td>
<td>0.34</td>
</tr>
<tr>
<td>Zn</td>
<td>2.4</td>
<td>0.56</td>
<td></td>
</tr>
<tr>
<td>Cd</td>
<td>0.71</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hg</td>
<td>6.5</td>
<td>0.80</td>
<td>0.55</td>
</tr>
<tr>
<td>Al</td>
<td>0.84</td>
<td>0.17</td>
<td></td>
</tr>
<tr>
<td>Ga</td>
<td>1.7</td>
<td>0.38</td>
<td>0.25</td>
</tr>
<tr>
<td>In</td>
<td>0.91</td>
<td>0.22</td>
<td>0.15</td>
</tr>
<tr>
<td>Ti</td>
<td>1.1</td>
<td>0.23</td>
<td>0.15</td>
</tr>
<tr>
<td>Sn</td>
<td>0.57</td>
<td>0.14</td>
<td>0.099</td>
</tr>
<tr>
<td>Pb</td>
<td>0.072</td>
<td>0.023</td>
<td>0.016</td>
</tr>
<tr>
<td>Bi</td>
<td>0.27</td>
<td>0.055</td>
<td>0.036</td>
</tr>
</tbody>
</table>

* Relaxation times are calculated from the data in Tables 1.1 and 1.2, and Eq. (1.8). The slight temperature dependence of n is ignored.

\[ \sigma = \frac{n q^2 T}{m_e} \]

From: Solid State Physics, Ashcroft and Mermin
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Optical Reflectivity

Optical Reflectivity

\[ \Gamma_r = \frac{E_r}{E_i} = \frac{\sqrt{\varepsilon_0} - \sqrt{\varepsilon(\omega)}}{\sqrt{\varepsilon_0} + \sqrt{\varepsilon(\omega)}} \]

Oscillating electric field

\[ qE_0 e^{i\omega t} = m_e \frac{dv}{dt} - \frac{m_e v}{\tau} \]

“Optical” Conductivity

\[ \sigma(\omega) = \frac{\sigma_0}{1 - i\omega \tau} \]

Dielectric value depends on the frequency

\[ \varepsilon(\omega) = \varepsilon_0 [1 + i \frac{\sigma(\omega)}{\omega \varepsilon_0}] \]

Spectral reflectance curves for aluminium (Al), silver (Ag), and gold (Au) metal mirrors at normal incidence. From Wikipedia
The classical Drude model

Paul Drude (1900)

Electrons move and scatter every \( \tau \) seconds

\[
m \frac{dv}{dt} = qE - \frac{mv}{\tau}
\]

steady state: \( \frac{d}{dt}(\ldots) \to 0 \)

\[
v = \frac{q\tau}{m}E = \mu E
\]

\[
J = qnv = \frac{nq^2\tau}{m}E = \sigma E \implies \sigma_0 = \frac{nq^2\tau}{m}
\]

Oscillating field:

\[
E(t) = E e^{i\omega t} \quad m \frac{dv}{dt} = qE e^{i\omega t} - \frac{mv}{\tau}
\]

\[
v(t) = v(0)e^{i\omega t}
\]

DC field:

\[
\sigma(\omega) = \frac{\sigma_0}{1 + i\omega\tau} = \frac{\sigma_0}{1 + (\omega\tau)^2} - i \frac{\omega\tau\sigma_0}{1 + (\omega\tau)^2}
\]

Re(\(\sigma(\omega)\)) \quad Im(\(\sigma(\omega)\))

DC conductivity

AC conductivity

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Thermal Conductivity

\[ J_{\text{heat}} = \frac{1}{3} c v u^2 \tau (-\nabla T) \]
The Weidemann-Franz Law for metals

Data compiled by Rusen Yan

\[
\frac{\kappa}{\sigma T} = \frac{3}{2} \left( \frac{k_B}{q} \right)^2 \Rightarrow \frac{\kappa}{\sigma T} = \mathcal{L}
\]

Ratio of Boltzmann Constant and Electron Charge, which are fundamental constants and do not depend on the metal.
Electronic specific heat is much smaller than $nk_B$

- Classical Mechanics and Thermodynamics is not adequate to explain electron statistics.
- Electrons must follow the Pauli Exclusion principle, and are subject to the laws of quantum mechanics.
Planck’s Blackbody Radiation: Birth of ‘Quantum’

Rayleigh-Jean
UV catastrophe
5800 K

Planck’s law

5800 K (Sun)

4500 K

3000 K

\[ \omega \left( 10^{12} \text{ rad/s} \right) \]

\[ u_{\omega} (\omega) \left( \text{eV.s/m}^3 \right) \]

\[ u_{\lambda}(\lambda) \left( \text{eV.s/m}^3 \right) \]

Rayleigh-Jean
UV catastrophe
5800 K

Planck’s law

5800 K (Sun)

4500 K

3000 K

\[ \lambda \left( \text{nm} \right) \]
Classical physics unable to explain light spectrum

Rayleigh-Jeans Classical Result

Experimental Blackbody @ temperature T

Planck's Result with the Quantum Hypothesis

\[ E = n \cdot (\hbar \nu) \]

[Spectral Density of Radiation]

\[ \sim \nu^2 (k_B T) \]

\[ \sim k_B T \]

\[ \frac{\nu^3}{e^{\frac{\nu}{k_B T}} - 1} \]
Einstein explains the Photoelectric effect

Fig. 3.35 The photoelectric effect.
Experiment: Light is a wave... or a particle?

"WAVE"

many photons

laser one...

double slit

Tune down the intensity!

Intensity

Intensity

screen with an array of detectors

Recover this!

Keep doing this again and again

one photon

laser one...

Click!

only one detector clicks!

"PARTICLE"
Experiment: Light is a wave... or a particle?

**Planck's hypothesis for photons to explain expts:**

\[ p = \hbar k \]

\[ k = (2\pi/\lambda)\hat{n}, \text{ } \hat{n} \text{ the direction of propagation} \]

\[ \omega = c|k| \text{ with } c \text{ the speed of light} \]

\[ E = \hbar \omega \]

**Einstein: look downstairs!**

\[ p = mv/\sqrt{1 - (v/c)^2} \]

- The only way an object of mass \( m = 0 \) can have momentum is if its speed \( v = c \), or the speed of light.
- A photon is exactly such an object. No mass, all energy, and a finite momentum!
Bohr’s Quantum Theory for Electrons

\[ E = \frac{p^2}{2m_e} - \frac{q^2}{4\pi\epsilon_0 R} \]

\[ \int p\,dx = n\hbar \quad p_n 2\pi R_n = n\hbar \implies p_n R_n = n\hbar. \]

\[ \frac{m_e v_n^2}{R_n} = \frac{q^2}{4\pi\epsilon_0 R_n^2} \implies p_n = \frac{q^2 m_e}{4\pi\epsilon_0 \hbar} \cdot \frac{1}{n} = \frac{\hbar}{a_B} \cdot \frac{1}{n} \]

\[ R_n = n^2 \left( \frac{4\pi\epsilon_0 \hbar^2}{q^2 m_e} \right) = n^2 a_B \]

\[ E_n = \frac{p_n^2}{2m_e} - \frac{q^2}{4\pi\epsilon_0 R_n} = \frac{1}{2} \frac{\hbar^2}{m_e a_B^2} \cdot \frac{1}{n^2} - \frac{\hbar^2}{m_e a_B^2} \cdot \frac{1}{n^2} = -\frac{\hbar^2}{2m_e a_B^2} \cdot \frac{1}{n^2} \]

\[ E_{n_2} - E_{n_1} = \frac{m_e q^4}{2(4\pi\epsilon_0)^2 \hbar^2} \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \]

\[ \text{Ry} = 13.6\text{eV} \]
Particle... or wave?

de Broglie’s hypothesis:
\[ \lambda = \frac{h}{|\mathbf{p}|} \]
holds for objects with mass too, not just photons.

When electrons are waves:
\[ qV = E = \frac{p^2}{2m_0}, \text{ but } \lambda = \frac{h}{p}, \text{ which} \]
\[ \lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mqV}}. \]
You can change the wavelength of electrons with voltage.
Particle... or wave?

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but \( \lambda = \frac{h}{p} \), which

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You can change the wavelength of electrons with voltage.
An electron is a particle... or a wave?
An electron is a particle... or a wave?

Guowang Li (Results from our lab!)

De Broglie: \( \lambda = \frac{2\pi \hbar}{|p|} \)

For both waves, and particles!

Electron beam incident on a crystal (RHEED)

Atomic structure of a crystal (grating!)

Electron diffraction pattern on a screen

Figure 2.7: RHEED patterns of (a) smooth surface and (b) crystalline but rough of GaN surface.
Wave and particle ➔ need for a wavefunction

Quantum states (electrons, photons) behave as waves AND particles. How do we describe them quantitatively?

- The state of the free quantum particle cannot be represented by independent ‘numbers’ \((x, p_x)\).
- We need a function whose amplitude oscillates in space, yet its magnitude never goes to zero.
- The complex exponential \(e^{ikx}\) satisfies these requirements, and respects the uncertainty relation.
By linear superposition of complex exponentials, we can create ‘particle’ like or ‘wave’ like states as desired for the problem.

Drawing on Fourier series, we realize that we can create any wavefunction shape to capture the correct physics of the problem. Note the corresponding reciprocal space weight distribution.

The best we can do to locate a "particle" is a 'wave packet'.

\[ \psi(x) = \sum_{p} A_p e^{i\frac{px}{\hbar}} \]

is an allowed "wavefunction".

• Drawing on Fourier series, we realize that we can create any wavefunction shape to capture the correct physics of the problem. Note the corresponding reciprocal space weight distribution.
Math preliminaries before the physics...

\[ \psi_p(x) = A e^{ipx/\hbar} \]

\[ \hat{p} = -i\hbar \frac{\partial}{\partial x} \]

\[ \hat{p} \psi_p(x) = (\hbar k) \psi_p(x) \]

\[ x\hat{p} - \hat{p}x = [x, \hat{p}] = i\hbar. \]

Wavefunction ties \( x \) and \( p \) together. Must respect the uncertainty principle.

Obervables are mathematical operators. They act on the wavefunction to extract info.

The states of definite value of an operator are called the eigenstates of that operator.

Unlike classical mechanics, some operators fail to commute!

THE EXCHANGE RELATION
\[ PQ - QP = h/2\pi i \]

Non-commuting actions...
Ref: Gamow, Thirty years that shook physics.

Debdeep Jena (djena@cornell.edu)
Definite momentum, and definite location states

A state of definite location $x_0$:
Must be an eigenstate of operator $\hat{x}$, with eigenvalue $x_0$:

$$ x\psi_{x_0}(x) = x_0\psi_{x_0}(x) \implies \psi_{x_0}(x) = \delta(x - x_0) $$

Definite in real space $\rightarrow$ spread out in momentum

A state of definite momentum $p$:
Must be an eigenstate of operator $-i\hbar(d/dx)$, with eigenvalue $p$:

$$ \hat{p}_x \psi_p(x) = p_x \psi_p(x) \implies -i\hbar \frac{d}{dx} \psi_p(x) = p_x \psi_p(x) $$

$$ \psi_p(x) = Ae^{i\frac{px}{\hbar}} = Ae^{ik_xx} $$

Definite in momentum $\rightarrow$ spread out in real space

States of definite location and definite momentum are unique in quantum mechanics.

Debdeep Jena (djena@cornell.edu)
States of definite energy: Schrödinger equation

States of definite energy are not unique, because they depend on the 'potential' \( V(x) \)

In classical mechanics, the energy of a particle is:

\[
E_{cl} = \frac{p^2}{2m} + V(r)
\]

In quantum mechanics, \( r \) & \( p \) cannot be simultaneously determined because \([x,p]=i\hbar\).
Thus, we must solve an equation to obtain the energy.

\[
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi_E(x) = E \psi_E(x).
\]

The Schrödinger equation gives us the prescription to find the states of definite energy.

\[
\left[ \frac{\hat{p}^2}{2m} + V(r) \right] |\psi\rangle = E |\psi\rangle
\]
Quantum states are vectors in the Hilbert space.

Any wavefunction \( \psi(x) = \sum_n A_n \phi_n(x) \) is an allowed state.

\[ |\psi\rangle = \sum_n A_n |n\rangle \]

\[ \langle m|n\rangle = \delta_{mn} \]

\[ A_n = \langle n|\psi\rangle \]

\[ |\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle = \sum_n |n\rangle \langle n|\psi\rangle \]

\[ \sum_n |n\rangle \langle n| = 1 \]

It is useful here to draw an analogy to the decomposition of a vector into specific coordinates. The ‘hybrid’ state function \( \psi(x) \) is pictured as a vector \( |\psi\rangle \) in an abstract space. The definite momentum wavefunctions \( \psi_n(x) \) are pictured as the ‘coordinate’ vectors \( |n\rangle \) in that space of vectors. This set of vectors is called the basis. Since there are an infinite set of integers \( n = 0, \pm 1, \pm 2, \ldots \), the vector space is infinite dimensional. It is called the Hilbert space. One may then consider the coefficients \( A_n \) as the length of the projections of the state on the basis states. The abstract picture allows great economy of expression by writing \( |\psi\rangle = \sum_n A_n |n\rangle \). The orthogonality of the basis states
By projecting states, get various representations

- We can think of the states as vectors.
- The ‘inner product’ is a complex number generated by projection to the appropriate space.
- This number is the wavefunction – it can be found in real space, momentum space, etc...

\[ \langle x | \psi \rangle = \psi(x) \]
\[ \langle k | \psi \rangle = \psi(k) \]
\[ \langle x | k_x \rangle = \frac{e^{ik_x x}}{\sqrt{2\pi}} \]

\[ \langle \psi_2 | \psi_1 \rangle = \int_{-\infty}^{\infty} dx \langle \psi_2 | x \rangle \langle x | \psi_1 \rangle = \int_{-\infty}^{\infty} dx \psi_2^*(x) \psi_1(x) \]
### The particle in a box

The energy spectrum is discrete, zero energy **NOT** allowed!

\[ V(x) = 0, \quad 0 \leq x \leq L \]
\[ V(x) = \infty, \quad x < 0, x > L \]

The major change is that \( \psi(x) = 0 \) in regions where \( V(x) = \infty \).

\[ \psi(x) = A e^{ikx} + B e^{-ikx} \rightarrow \psi(0) = 0 = A + B, \psi(L) = A e^{ikL} + B e^{-ikL} = 0 \]

\[ \frac{A}{B} = -e^{-i2kL} = -1 \rightarrow 2kL = 2n\pi \rightarrow k_n = \frac{n\pi}{L}, \quad n = \pm 1, \pm 2, \pm 3, \ldots \]

Note that \( n = 0 \) is **not allowed**, because then \( \psi(x) = 0 \) and there is no particle wavefunction after normalization over the length \( L \) is

\[ \psi(n, x) = \sqrt{\frac{2}{L}} \sin(n\frac{\pi}{L}x) = \sqrt{\frac{2}{L}} \sin(k_nx) \]

\[ E_n = n^2 \left(\frac{\pi \hbar}{2m_eL^2}\right)^2 = n^2 \frac{\hbar^2}{8m_eL^2} \]
The harmonic oscillator

The energies are

\[ E_n = \hbar \omega \left( n + \frac{1}{2} \right). \]

The corresponding wave functions are

\[ \psi_n(x) = \frac{1}{\sqrt{2^n n! \pi^{1/4}}} \cdot \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} \cdot e^{-m \omega x^2 / 2\hbar} \cdot H_n \left( \sqrt{m \omega / \hbar} x \right), \]

and

\[ H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left( e^{-x^2} \right). \]

The energy levels are equally spaced.

Zero energy is not allowed.

\[ V(x) = \frac{1}{2} m \omega^2 x^2 \]

Can solve the problem using raising and lowering operators.

\[ a = \sqrt{\frac{m \omega}{2\hbar}} (\hat{x} + i \frac{m \omega}{m \omega \hat{p}}) \]

\[ a^\dagger = \sqrt{\frac{m \omega}{2\hbar}} (\hat{x} - i \frac{m \omega}{m \omega \hat{p}}) \]

\[ \hat{x} = \sqrt{\frac{\hbar}{2m \omega}} (a^\dagger + a) \]

\[ \hat{p} = i \sqrt{\frac{m \omega \hbar}{2}} (a^\dagger - a) \]
The hydrogen atom

**Energy levels**

The energy levels of hydrogen, including fine structure, are given by the Sommerfeld expression:

\[
E_{jn} = -\frac{m_e c^2}{2} \left[ 1 + \left( \frac{\alpha}{n-j-\frac{1}{2} + \sqrt{(j + \frac{1}{2})^2 - \alpha^2}} \right)^2 \right]^{-1/2} - 1
\]

\[
\approx -\frac{m_e c^2 \alpha^2}{2n^2} \left[ 1 + \frac{\alpha^2}{n^2} \left( \frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) \right],
\]

where \(\alpha\) is the fine-structure constant and \(j\) is the "total angular momentum" quantum number, which is equal to \(l \pm 1/2\) depending on the direction of the electron spin. The factor in square brackets in the last expression is nearly one; the extra term arises from relativistic effects (for details, see #Features going beyond the Schrödinger solution).

The value

\[
\frac{m_e c^2 \alpha^2}{2} = \frac{0.51 \text{ MeV}}{2 \cdot 137^2} = 13.6 \text{ eV}
\]

**Wavefunction**

The normalized position wavefunctions, given in spherical coordinates are:

\[
\psi_{n\ell m}(r, \vartheta, \varphi) = \sqrt{\left( \frac{2}{na_0} \right)^3 \frac{(n - \ell - 1)!}{2n(n + \ell)!}} e^{-\rho/2} \rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho) Y_{\ell m}(\vartheta, \varphi)
\]

where:

.. math::

   \rho = \frac{2r}{na_0},

\(a_0\) is the Bohr radius,

\(L_{n-\ell-1}^{2\ell+1}(\rho)\) is a generalized Laguerre polynomial of degree \(n - \ell - 1\), and

\(Y_{\ell m}(\vartheta, \varphi)\) is a spherical harmonic function of degree \(\ell\) and order \(m\). Note that the generalized Laguerre polynomials are defined differently by different authors. The usage here is consistent with the definitions used by Messiah\(^8\) and Mathematica\(^9\). In other places, the Laguerre polynomial includes a factor of \((n + \ell)!\)\(^{10}\) or the generalized Laguerre polynomial appearing in the hydrogen wave function is \(L_{n+\ell}^{2\ell+1}(\rho)\) instead.\(^{11}\)

The quantum numbers can take the following values:

\[
n = 1, 2, 3, \ldots \\
\ell = 0, 1, 2, \ldots, n - 1 \\
m = -\ell, \ldots, \ell.
\]

\[ \Delta x \Delta p \geq \frac{\hbar}{2} \]

\[ F = -\nabla V(r) = \frac{dp}{dt} \]

Path is deterministic

\[ i\hbar \frac{\partial |\psi\rangle}{\partial t} = \left[ \frac{\hat{p}^2}{2m} + V(r, t) \right] |\psi\rangle \]

Path respects uncertainty relation
States of definite energy are stationary states

The energy eigenvalues of the time-independent Schrödinger equation are states of definite energy. Their probability density does not change with time → they are called stationary states. This is analogous to the 1st law of classical mechanics: quantum states of definite energy will continue to remain in those states unless perturbed by a potential.

The energy eigenvalues of the time-independent Schrödinger equation are states of definite energy.

Their probability density does not change with time → they are called stationary states.

This is analogous to the 1st law of classical mechanics: quantum states of definite energy will continue to remain in those states unless perturbed by a potential.
The classical Drude model

Paul Drude (1900)

Electrons move and scatter every tau seconds

dc field:

\[ m \frac{dv}{dt} = qE - \frac{mv}{\tau} \]

steady state: \( \frac{d}{dt} (\ldots) \to 0 \)

\[ v = \frac{q \tau}{m} E = \mu E \]

\[ J = qnv = \frac{nq^2 \tau}{m} E = \sigma E \implies \sigma_0 = \frac{nq^2 \tau}{m} \]

dc conductivity

Oscillating field:

\[ E(t) = E e^{i\omega t} \]

\[ m \frac{dv}{dt} = qE e^{i\omega t} - \frac{mv}{\tau} \]

\[ v(t) = v(0) e^{i\omega t} \]

ac conductivity

\[ \sigma(\omega) = \frac{\sigma_0}{1 + i \omega \tau} = \frac{\sigma_0}{1 + (\omega \tau)^2} - i \frac{\omega \tau \sigma_0}{1 + (\omega \tau)^2} \]

Re(\(\sigma(\omega)\)) Im(\(\sigma(\omega)\))
Quantum mechanical current

\[ |\Psi(x, t)|^2 = \Psi^* \Psi \]

Probability density in space and time

\[ \frac{\partial |\Psi(x, t)|^2}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi \]

Change in probability density with time

\[ \frac{\partial |\Psi(x, t)|^2}{\partial t} = \Psi^* \left( \frac{\hat{p}^2 / 2m + V}{i \hbar} \right) \Psi + \Psi \left( \frac{\hat{p}^2 / 2m + V}{-i \hbar} \right) \Psi^* \]

Use time-dependent Schrödinger equation

\[ \frac{\partial |\Psi(x, t)|^2}{\partial t} = \frac{1}{2mi \hbar} (\Psi^* \hat{p}^2 \Psi - \Psi \hat{p}^2 \Psi^*) \]

Since \( \hat{p} = -i \hbar \nabla_r \)

\[ \frac{\partial |\Psi(x, t)|^2}{\partial t} = -\nabla_r \cdot \left[ \frac{1}{2m} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*) \right] \]

In the form of a continuity equation \( \rightarrow \) read off the current density!

Continuity equation

\[ \partial \rho / \partial t = -\nabla_r \cdot \mathbf{j} \]

\[ \mathbf{j} = \frac{1}{2m} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*) \]

Quantum mechanical probability current density

\[ \frac{d}{dt} \left( \int_{\text{space}} d^3r |\Psi|^2 \right) = -\int_{\text{space}} d^3r \nabla \cdot \mathbf{j} = -\int \mathbf{j} \cdot d\mathbf{S} = 0 \]

Satisfies the conservation of number of particles
Electric current of quantum states

\[ J = \frac{q}{2m_e} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*) \]

For most semiconductors we know the bandstructure, but not the Bloch functions. Go through the derivation to recast the current in terms of the bandstructure, or the group-velocity (see notes).

\[ \mathbf{v}_g(k) = \nabla_k E(k) / \hbar \]

- Group velocity of electron in state \(|k>\)

**General expression for charge current density in \(d\)-dimensions**

\[ J_d = \frac{q g_s g_v}{L^d} \sum_k \mathbf{v}_g(k) T(k) [f_L(k) - f_R(k)] \]

**VERY useful result: current in \(d\)-dimensions!**

\[ J_d = \frac{q g_s g_v}{(2\pi)^d} \int d^d k \times \mathbf{v}_g(k) T(k) [f_L(k) - f_R(k)] \]

General expression for charge current density in \(d\)-dimensions
Identity crisis: Indistinguishable particles

2 particles: total energy: $E_1 + E_2 \Rightarrow$ time evolution $= e^{i(E_1 + E_2)t}$

Since $i\hbar \frac{\partial}{\partial t} \psi = E \psi$, $\psi \sim \psi_1 \cdot \psi_2$

$\psi(x_1, x_2) = \psi_a(x_1) \psi_b(x_2)$

This is OK for distinguishable particles such as a proton and an electron. But NOT OK for indistinguishable particles such as two electrons! For example, $|\psi|^2$ should not change on swapping $x_1 \leftrightarrow x_2$.

How must we then write the wavefunction for two identical particles?
The restriction that we cannot put two electrons in the same energy state leads to the elements. The same restriction leads to a periodic variation of the physical properties of the elements.
Resolution of identity crisis: Bosons & Fermions

This is necessary for indistinguishable particles.

\[ P(x_2, x_1) = P(x_1, x_2) \rightarrow |\psi(x_2, x_1)|^2 = |\psi(x_1, x_2)|^2. \]

\[ \psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) \]

\[ \psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) + \psi_a(x_2)\psi_b(x_1) \]

\[ \psi(x_2, x_1) = \psi(x_1, x_2) \]

\[ \psi(x_1, x_1) = \psi(x_1, x_1) \]

\[ \psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) - \psi_a(x_2)\psi_b(x_1) \]

\[ \psi(x_2, x_1) = -\psi(x_1, x_2), \]

\[ \psi(x_1, x_1) = -\psi(x_1, x_1) \rightarrow \psi(x_1, x_1) = 0. \]

The Pauli exclusion principle!

The Bose-Einstein distribution! Particles are called **Bosons**. Examples: Photons, Phonons

\[ f_{BE}(E) = \frac{1}{e^{\frac{E-\mu}{kT}} - 1} \]

The Fermi-Dirac distribution! Particles are called **Fermions**. Examples: Electrons, Protons

\[ f_{FD}(E) = \frac{1}{e^{\frac{E-E_F}{kT}} + 1} \]

• Note: Why not \[ \psi(x_2, x_1) = e^{i\phi}\psi(x_1, x_2) \] ? Majorana particles \( \rightarrow \) later…

Debdeep Jena (djena@cornell.edu)
The Fermi-Dirac and Bose-Einstein distributions asymptotically approach the classical limit at high energies.

- Fermi-Dirac occupation function for any energy orbital is less than 1.
Some properties of the Fermi-Dirac Function

- The Fermi-function at T=0 K is a step function that is 1 below the Fermi energy, and 0 above.
- The derivative of the Fermi function is of central importance in transport phenomena. Because of the exclusion principle, it defines the energy states that can participate in transport.

\[ -\frac{\partial f_0}{\partial E} = +\frac{\partial f_0}{\partial \mu} = \frac{\beta}{4 \cosh^2 \left(\frac{\beta (E-\mu)}{2}\right)} \]

\[ \lim_{T \to 0} [-\frac{\partial f_0}{\partial E}] = \lim_{T \to 0} [+\frac{\partial f_0}{\partial \mu}] = \delta (E - \mu) \]

**Fig. 4.6 Illustration of the temperature dependence of the Fermi-Dirac distribution, and its derivative.**
The Fermi-Difference Function

- Two electrodes with different Fermi levels cause a difference in the Fermi functions for electrons that are in equilibrium with them.
- The Fermi difference function is rectangular, and defines the effect of voltages on transport properties.

\[ f(u) - f(v) = \left[ f(u) + f(v) - 2f(u)f(v) \right] \times \tanh\left( \frac{u-v}{2} \right) \geq 0 \]

\[ \int_0^\infty \text{d}E \left[ f_0(\mu_1) - f_0(\mu_2) \right] \approx (\mu_1 - \mu_2). \]

Fig. 4.7 Illustration of the temperature dependence of the Fermi-difference distribution. The difference is a window between \( \mu_2 - \mu_1 \) that becomes increasingly rectangular as the temperature drops.
Fermi-Dirac Integrals

\[ F_j(\eta) = \frac{1}{\Gamma(j + 1)} \int_0^\infty du \frac{u^j}{1 + e^{u-\eta}} \]

\[ \int_0^\infty dE f_0(E - \mu) = \int_0^\infty \frac{dE}{1 + e^{\beta(E-\mu)}} = \frac{1}{\beta} \ln(1 + e^{\beta\mu}) \]

Fermi-Dirac integrals are of central importance in the physics of semiconductors and nanostructures.

- Fermi-Dirac integrals are of central importance in the physics of semiconductors and nanostructures.

Debdeep Jena (djena@cornell.edu)
Quantum Equipartition of Energy

\[
\langle E \rangle_{1d} = \frac{\int_{-\infty}^{+\infty} dv_x \cdot \left( \frac{1}{2} m v_x^2 \right) \cdot \frac{1}{e^{\frac{1}{2} \frac{m v_x^2 - \mu}{k_B T}} + 1}}{\int_{-\infty}^{+\infty} dv_x \cdot \frac{1}{e^{\frac{1}{2} \frac{m v_x^2 - \mu}{k_B T}} + 1}} = \frac{1}{2} k_B T \cdot \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}. 
\]

- The equipartition of energy relation is modified from the Maxwell-Boltzmann form.
Quantum version of the Equipartition of Energy

\[
\langle E \rangle_{1d} = \frac{\int_{-\infty}^{\infty} dv_x \cdot \left(\frac{1}{2} mv_x^2 \right) \cdot e^{-\frac{1}{2} \frac{mv_x^2}{k_B T}}}{\int_{-\infty}^{\infty} dv_x \cdot e^{-\frac{1}{2} \frac{mv_x^2}{k_B T}}} = \frac{1}{2} k_B T.
\]

\[
\langle E \rangle_{3d} = \frac{\int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \cdot \left(\frac{1}{2} m (v_x^2 + v_y^2 + v_z^2) \right) \cdot e^{-\frac{1}{2} \frac{m (v_x^2 + v_y^2 + v_z^2)}{k_B T}}}{\int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \cdot e^{-\frac{1}{2} \frac{m (v_x^2 + v_y^2 + v_z^2)}{k_B T}}} = \frac{1}{2} k_B T + \frac{1}{2} k_B T + \frac{1}{2} k_B T = \frac{3}{2} k_B T.
\]

\[
\langle E \rangle_{1d} = \frac{\int_{-\infty}^{\infty} dv_x \cdot \left(\frac{1}{2} mv_x^2 \right) \cdot \frac{1}{e^{\frac{1}{2} \frac{mv_x^2-\mu}{k_B T}} + 1}}{\int_{-\infty}^{\infty} dv_x \cdot \frac{1}{e^{\frac{1}{2} \frac{mv_x^2-\mu}{k_B T}} + 1}} = \frac{1}{2} k_B T \cdot \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}
\]

\[
\langle E \rangle_{3d} = \frac{3}{2} k_B T \cdot \frac{F_{3/2}(\eta)}{F_{1/2}(\eta)}
\]

- Fermi-Dirac integrals are of central importance in the physics of semiconductors and nanostructures

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Electrons in the quantum world

We will now apply quantum statistics (e.g. the Fermi-Dirac distribution) and quantum mechanics (the Schrodinger equation) to electrons and investigate how properties alien to classical mechanics emerge from these monumental changes.

- solve the Schrodinger equation exactly to obtain the wavefunction $\psi(x)$,
- the allowed momentum $p_x$,
- the allowed energy eigenvalues $E$,
- the quantum current $J$,
- the Density of States $g(E)$, and
- the total energy $\mathcal{U}$, average energy $u$, and energy density $u_v$ of many electrons.
The free electron has a parabolic energy distribution. All energies and all momenta are allowed.

The quantum mechanical current has direct analogy to the classical current.

We have defined a group velocity for a state as the slope of the energy/momentum curve.

\[ V(x) = 0 \text{ for the free electron} \]

Superposition state of a right-and a left-going electron wave.

De-Broglie relation in action for the free electron.

Energy is momentum squared by twice mass, all kinetic, no potential.
Particle on a Ring: Quantum Confinement

- Particle on a ring has a parabolic energy distribution.
- Discrete energies and momenta are allowed.
- The quantum mechanical current has direct analogy to the classical current.

Boundary conditions force quantized values of $k$

$$\psi(x + L) = \psi(x) \rightarrow e^{ik(x+L)} = e^{ikx} \rightarrow e^{ikL} = 1 \rightarrow kL = 2n\pi$$

$$\psi_n(x) = A e^{ik_n x}$$

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}$$

$$k_n = \frac{2\pi}{L} n, n = 0, \pm 1, \pm 2, \ldots$$

$$p_n = \hbar k_n = \frac{\hbar}{2\pi} \frac{2\pi}{L} n = n \frac{\hbar}{L}$$

$$L_n = r \times p = \hbar k_n \times \frac{L}{2\pi} \hat{z} = \frac{2\pi \hbar}{L} n \times \frac{L}{2\pi} \hat{z} \rightarrow L_n = n\hbar$$

$$E_n = \frac{\hbar^2 k_n^2}{2m_e} = n^2 \frac{(2\pi \hbar)^2}{2m_e L^2} = n^2 \frac{\hbar^2}{2m_e L^2}$$
Quantum Confinement & Density of States

- Quantum confinement can be used to engineer the energy levels of nanostructures.
- The Density of states can be expressed in momentum or in energy space.

\[ E_n = \frac{\hbar^2 k_n^2}{2m_e} = n^2 \frac{(2\pi \hbar)^2}{2m_eL^2} = n^2 \frac{\hbar^2}{2m_eL^2} \]

- The smaller the circle, the larger the allowed energies \( (L \downarrow \Rightarrow E_n \uparrow) \), and
- The smaller the mass, the larger the allowed energies \( (m \downarrow \Rightarrow E_n \uparrow) \).

\[ g_s g_v \frac{2dk}{2\pi L} = G_{1d}(E)dE \quad \Rightarrow \quad g_{1d}(E) = \frac{G_{1d}}{L} = \frac{2g_s g_v}{2\pi \frac{dE}{dk}} \quad \Rightarrow \]

\[ g_{1d}(E) = \frac{g_s g_v}{2\pi} \left( \frac{2m_e}{\hbar^2} \right)^{1/2} \frac{1}{\sqrt{E}} \]

The Density of States is the number of quantum states allowed between energies \( E \) and \( E + dE \).
Fermi Energy, Fermi velocity & their quantum origin

Because of the Pauli exclusion principle and the Fermi-Dirac distribution, the presence of many electrons in a metal gain significant energy and velocity even at T=0 K. This is a most remarkable consequence of quantum theory!

The Fermi energy is a remarkable consequence of the exclusion principle!

Typical values for metals

Many-Electron Effect:
Temperature-dependence of Carrier Density

\[ n_{1d}(T) = \frac{g_s g_v}{L} \sum_k f(k) = \frac{g_s g_v}{L} \int_{-\infty}^{+\infty} \frac{dk}{2\pi L} \frac{1}{1 + e^{\frac{\hbar^2 k^2}{2m_e} - E_{1d}(T) \frac{k_b T}{k_b T}}} \]  \hspace{1cm} (5.22)

The dimensionless variables \( u = \frac{\hbar^2 k^2}{2m_e} / k_b T \) and \( \eta = E_{1d}(T) / k_b T \) convert the carrier density at any temperature to

\[ n_{1d}(T) = g_s g_v \left( \frac{2\pi m_e k_b T}{\hbar^2} \right)^{\frac{1}{2}} F_{-\frac{1}{2}} \left( \frac{E_F}{k_b T} \right) = N_{c1d} F_{-\frac{1}{2}} (\eta), \]  \hspace{1cm} (5.23)
From Ballistic conductance to Ohm’s Law

\[ R_0 \sim \frac{h}{2q^2} \]

\[ G_0 \sim \frac{2q^2}{h} \]

\[ R = \rho \frac{L}{A} \]

\[ G = \sigma \frac{A}{L} \]

For \( L \gg \lambda_{mfp} \) and 3D: \( M \sim k_F^2 A \)

\[ \rightarrow R \sim \frac{h}{2q^2} \cdot \frac{1}{k_F^2 A} \cdot \frac{L}{\lambda_{mfp}} \] (Ohm’s Law)

For \( L \ll \lambda_{mfp} \) and 3D: \( M \sim k_F^2 A \)

\[ \rightarrow R \sim \frac{h}{2q^2} \cdot \frac{1}{k_F^2 A} \] (Sharvin resistance)
“Ballistic” Transport & Quantized Conductance

Experiments:

FIG. 1. (a) Schematic layer structure of the heterostructure. (b) Improvement of plateau quantization with the application of a small magnetic field. Linear conductance $G(V_g)$ is plotted at magnetic field $B=0.1\ T$, $0.2\ T$, $0.5\ T$, and $1\ T$. Traces are shifted vertically for clarity. Inset: micrograph of the QPC. The gap between the two split gates is $80\ nm$ at its narrowest point. All experimental data shown in this letter were measured at $300\ mK$.

Appl. Phys. Lett. 86, 073108 (2005);

FIG. 44. Point contact conductance as a function of gate voltage at $0.6\ K$, demonstrating the conductance quantization in units of $2e^2/h$. The data are obtained from the two-terminal resistance after subtraction of a background resistance. The constriction width increases with increasing voltage on the gate (see inset). Taken from B. J. van Wees et al., Phys. Rev. Lett. 60, 848 (1988).
‘Ohmic’ Contacts as Fermi Fillers

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Most general expression for ‘Current Density’ in ‘d’ dimensions:

$$J_d = q \times \frac{g_s g_v}{L^d} \sum_k v_g(k) f(k),$$

where

- $g_s = \text{spin degeneracy}$
- $g_v = \text{valley degeneracy}$
- $v_g = \frac{1}{\hbar} \nabla \mathcal{E}(k)$ is the group velocity
- $f(k)$ is the Fermi-Dirac function

Example: 1D current flow at $T = 0$ K:

$$J_1 = I = I \rightarrow - I \leftarrow$$

$$I \rightarrow = \frac{2q}{\hbar} E_{F1}$$

$$I \leftarrow = \frac{2q}{\hbar} E_{F2}$$

$$\rightarrow I = I \rightarrow - I \leftarrow = \frac{2q^2}{\hbar} V_D$$
Ballistic Transport in 1 Dimension

\[ n_{1d}(T) = \frac{8sgsv}{L} \sum_k f(k) = \frac{8sgsv}{L} \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \frac{1}{L} \frac{\frac{\hbar^2k^2}{2me} - E_{Fd}^1(T)}{1 + e^{\frac{\frac{\hbar^2k^2}{2me} - E_{Fd}^1(T)}{k_BT}}} \]  

(5.22)

The dimensionless variables \( u = (\frac{\hbar^2k^2}{2me})/k_BT \) and \( \eta = E_{Fd}^1(T)/k_BT \) convert the carrier density at any temperature to

\[ n_{1d}(T) = gsgv(\frac{2\pi mek_BT}{\hbar^2})^{\frac{1}{2}} F_{-\frac{1}{2}}(\frac{E_F}{k_BT}) = N_c^{1d} F_{-\frac{1}{2}}(\eta), \]  

(5.23)

\[ \eta_s = \frac{E_{FS}}{k_BT}, \eta_d = \frac{E_{Fd}}{k_BT}, \text{ and } v_d = \frac{qV}{k_BT} \]

\[ E_{FS} - E_{Fd} = qV \]

\[ \eta_s - \eta_d = v_d \]

Fig. 5.5 Quantum picture of current flow in the 1D k-space due to a difference in the occupation functions of right-going and left-going eigenstates. The left contact is called the source, and the right contact the drain.

\[ n_{1d} = \frac{1}{2} N_c^{1d}(T) [F_{-\frac{1}{2}}(\eta_s) + F_{-\frac{1}{2}}(\eta_d)] \]

\[ J_{1d}^{R} = J_{1d}^{L} = \frac{qgs^v}{2\pi \hbar} (k_BT) \ln(\frac{1 + e^{\eta_s}}{1 + e^{\eta_d}}). \]
Ballistic Transport in 1 Dimension

Fig. 5.5 Quantum picture of current flow in the 1D k-space due to a difference in the occupation functions of right-going and left-going eigenstates. The left contact is called the source, and the right contact the drain.

\[ \eta_s - \eta_d = v_d, \text{ and } n_{1d} = \frac{1}{2} N_c^{1d}(T)[F_{-\frac{1}{2}}(\eta_s) + F_{-\frac{1}{2}}(\eta_d)] \]

\[ J^{1d} = J^{1d}_R - J^{1d}_L = \frac{qG_sG_v}{2\pi\hbar}(k_B T) \ln\left(\frac{1 + e^{\eta_s}}{1 + e^{\eta_d}}\right) \]

Fig. 5.8 The left plot shows the calculated normalized Fermi level \( \eta_F = E_F/k_B T \) at \( V = 0 \), and the split normalized Fermi levels \( \eta_s \) and \( \eta_d \) for nonzero normalized voltages \( v_d = qV/k_B T \) for two values of 1D electron density at 300 K. The red curves are for \( n_{1d} = 5 \times 10^7 / \text{cm} \), and the blue for \( n_{1d} = 10^6 / \text{cm} \). The right plot shows the resulting quantum mechanical current flowing in response to the voltage for six values of 1D electron densities ranging from \( 0.1 - 5.0 \times 10^7 / \text{cm} \). For example, at a 1D electron density of \( n_{1d} = 10^7 / \text{cm} \), the maximum (or saturation) current is \( \sim 70 \mu A \). The middle \( E(k) \) figures show the changes in the corresponding occupied electron states for \( n_{1d} = 5 \times 10^7 / \text{cm} \) for three different voltages.
\[ \eta_s - \eta_d = v_d, \text{ and } n_{1d} = \frac{1}{2} N_c^{1d}(T)[F_{-\frac{1}{2}}(\eta_s) + F_{-\frac{1}{2}}(\eta_d)] \]

\[ J_{1d} = \frac{q^2}{h} \cdot N_c^{0d} \cdot \frac{k_b T}{q} \cdot [F_0(\frac{E_{Fs} - E_c}{k_b T}) - F_0(\frac{E_{Fs} - E_c - qV}{k_b T})] \]

where \( N_c^{0d} = g_s g_v = g_s g_v(\frac{2\pi m_e k_b T}{h^2})^0 \)

\[ J_d = \frac{q^2}{h} \cdot N_c^{d-1} \cdot \frac{k_b T}{q} \cdot [F_{d-1}^{-\frac{1}{2}}(\frac{E_{Fs} - E_c}{k_b T}) - F_{d-1}^{-\frac{1}{2}}(\frac{E_{Fs} - E_c - qV}{k_b T})]. \]

\[ n_d = N_c^d F_{d-2}(\eta), \text{ where } N_c^d = g_s g_v(\frac{2\pi m_e k_b T}{h^2})^\frac{d}{2} \]

\[ J^{1d} = J_{R}^{1d} - J_{L}^{1d} = \frac{q g_s g_v}{2\pi h} (k_B T) \ln \left( \frac{1 + e^{\eta_s}}{1 + e^{\eta_d}} \right). \]

**Fig. 5.5** The free electron band edge DOS \( N_c^d \) for \( d = 1, 2, 3 \) in units of 1/cm for 1d, 1/cm² for 2d, and 1/cm³ for 3d.
Electrons in 2D

**Fig. 5.5** Periodic boundary conditions in 2D leads to a Torus.

\[
\psi(\mathbf{r}) = \frac{1}{\sqrt{L^2}} e^{i(k_x x + k_y y)} = \frac{1}{\sqrt{A}} e^{i\mathbf{k} \cdot \mathbf{r}}
\]

\[
\mathbf{k} = (k_{n_x}, k_{n_y}) = \frac{2\pi}{L} (n_x, n_y) \quad \Rightarrow \quad \mathbf{p} = \hbar \mathbf{k}, |\mathbf{p}| = \frac{\hbar}{L} \sqrt{n_x^2 + n_y^2}
\]

\[
E(k_x, k_y) = \frac{\hbar^2}{2m_e} (k_{n_x}^2 + k_{n_y}^2) = E(n_x, n_y) = (n_x^2 + n_y^2) \frac{\hbar^2}{2m_e L^2} = \frac{\hbar^2 |\mathbf{k}|^2}{2m_e}
\]

\[
g_s g_v \frac{2\pi k dk}{\left(\frac{2\pi}{L}\right)^2} = G_{2d}(E)dE \quad \Rightarrow \quad \frac{G_{2d}(E)}{L^2} = \frac{g_{2d}(E)}{2\pi \hbar^2} \Theta(E)
\]

\[
g_s g_v \frac{\pi k_F^2}{\left(\frac{2\pi}{L}\right)^2} = N \quad \Rightarrow \quad k_F = \sqrt{\frac{4\pi n}{g_s g_v}}
\]

If \( g_s = 2 \) and \( g_v = 1 \)

\[
k_F = \sqrt{2\pi n}
\]

\[
n \sim 10^{12}/\text{cm}^2 \quad k_F \sim 2.5 \times 10^8/\text{m} \quad \lambda_F = \frac{2\pi}{k_F} \sim 25 \text{ nm}
\]

\[
n \sim 10^{16}/\text{cm}^2 \quad \lambda_F \sim 0.25 \text{ nm}
\]
Electrons in 2D

Fig. 5.5 Periodic boundary conditions in 2D leads to a Torus.

\[ n = \int_0^{\infty} dE \cdot g_{2d}(E) \cdot f(E) = \frac{g_sg_v m_e k_BT}{2\pi\hbar^2} \ln(1+e^{\frac{E_F}{k_BT}}) \implies E_F = k_BT \ln(e^{\frac{n}{n_q}} - 1) \]

\[ \mathcal{U} = \int_0^{\infty} dE \cdot E \cdot G_{2d}(E) \cdot f(E) \implies u_{2d} = \frac{\mathcal{U}}{N} = \frac{\int_0^{\infty} dE \cdot E \cdot G_{2d}(E) \cdot f(E)}{\int_0^{\infty} dE \cdot G_{2d}(E) \cdot f(E)} = \frac{1}{2} E_F \]

\[ u_v(2d) = \frac{1}{2} n E_F \]

\[ J(k) = \frac{q}{2m_e} (\psi^* \hat{p} \psi - \psi \hat{p} \psi^*) = q \cdot \frac{1}{A} \cdot \frac{\hbar k}{m_e} = q \left( \frac{1}{A} \right) v_g(k) \]

Quantum Mechanical Current
Electrons in 2D

\[ g_{2d}(E) = \frac{g_s g_v m_e}{2\pi \hbar^2} \Theta(E). \]

Fig. 5.9 Periodic boundary conditions in 2D leads to a Torus.

Fig. 5.10 Energy eigenvalues and density of states for free electrons in 2 dimensions.

Fig. 5.13 Group velocity of 2D electrons in the k–space, and its relation to transport in real space.
Electrons in 2D

Fig. 5.13 Group velocity of 2D electrons in the $k$–space, and its relation to transport in real space.
Electrons in 3D

\[ \psi(\mathbf{r}) = \frac{1}{\sqrt{L^3}} e^{i(k_x x + k_y y + k_z z)} = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}} \]

\[ \mathbf{k} = (k_{n_x}, k_{n_y}, k_{n_z}) = \frac{2\pi}{L} (n_x, n_y, n_z) \Rightarrow \mathbf{p} = \hbar \mathbf{k}, |\mathbf{p}| = \frac{\hbar}{L} \sqrt{n_{x}^2 + n_{y}^2 + n_{z}^2} \]

\[ E(k_x, k_y, k_z) = \frac{\hbar^2}{2m_e} (k_{n_x}^2 + k_{n_y}^2 + k_{n_z}^2) = (n_x^2 + n_y^2 + n_z^2) \frac{\hbar^2}{2m_e L^2} = \frac{\hbar^2 |\mathbf{k}|^2}{2m_e} \]

\[ g_s g_v \frac{4\pi k^2 dk}{(\frac{2\pi}{L})^3} = G_{3d}(E) dE \Rightarrow \frac{G_{3d}(E)}{L^3} = g_{3d}(E) = g_s g_v \frac{2m_e}{\hbar^2} \left( \frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{E} \]

\[ g_s g_v \frac{4}{3} \pi k_F^3 \left( \frac{2\pi}{L} \right)^3 = N \Rightarrow k_F = \left( \frac{6\pi^2 n}{g_s g_v} \right)^{\frac{1}{3}} \]

If \( g_s = 2 \) and \( g_v = 1 \)

\[ k_F = \left( \frac{3\pi^2 n}{g_s g_v} \right)^{\frac{1}{3}} \]

3D Fermi Wavevector

\[ n \sim 10^{24} \text{/cm}^3 \quad k_F \sim 3 \times 10^{10} \text{/m} \quad \lambda_F \sim 0.2 \text{ nm} \]
Electrons in 3D

\[ n = \int_{0}^{\infty} dE \cdot g_{3d}(E) \cdot f(E) = \frac{g_s g_v}{4\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} \int_{0}^{\infty} dE \cdot \sqrt{E} \cdot f(E) = n_{3d} F_{\frac{1}{2}}(\eta) \]

\[ u = \int_{0}^{\infty} dE \cdot E \cdot G_{3d}(E) \cdot f(E) \]

\[ u_{3d} = \frac{u}{N} = \frac{\int_{0}^{\infty} dE \cdot E \cdot G_{3d}(E) \cdot f(E)}{\int_{0}^{\infty} dE \cdot G_{3d}(E) \cdot f(E)} = \frac{3}{5} E_F \]

\[ u_v(3d) = \frac{3}{5} n E_F \]

Average energy density of a 3D Fermi Gas
Electrons in 3D

\[ g_{3d}(E) = \frac{g_s g_v}{4\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^3 \sqrt{E}. \]

**Fig. 5.15** An electron in a 3D box of side \( L \) can have wavevectors \( \mathbf{k} = (k_x, k_y, k_z) = \frac{2\pi}{L} (n_x, n_y, n_z) \) which form a discrete grid in the 3D \( \mathbf{k} \)-space. When \( N \) electrons are filled in the box, the \( \mathbf{k} \)-states are filled inside the Fermi sphere such that the states on the Fermi sphere surface have energy \( E_F \). The density of states for free electrons in 3 dimensions showing the \( \sqrt{E} \) dependence, the Fermi level, and the average energy of the electron distribution.
Ballistic Transport in 1, 2, and 3 Dimensions

\[ n_{1d} = 5 \times 10^6 / \text{cm} \]

\[ n_{2d} = 5 \times 10^{13} / \text{cm}^2 \]

\[ n_{3d} = 10^{20} / \text{cm}^3 \]

\[ m_c^* = 0.2m_e, g_s = 2, g_v = 1 \]
Semiconductor Physics Summary

Densities of states for free electrons in one, two, and three dimensions.

\[ n_{1D}(E) = \frac{1}{\pi h} \sqrt{\frac{2m}{E}} \]

\[ n_{2D}(E) = \frac{m}{\pi h^2} \]

\[ n_{3D}(E) = \frac{m^{\frac{3}{2}} 2mE}{\pi^2 h^3} \]

Fermi-Dirac Integrals

\[ F_i(\eta) \]

\[ \eta \ll -1 \] approx.

\[ \eta \gg +1 \] approx.

\[ \eta \]

\[ i = -2 \]

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Physics of Semiconductor Nanostructures Summary

Table 1: Quantum Electronic, Photonic, and Statistical Properties of Conduction and Valence Band Electrons in Semiconductor Nanostructures.

- \( E_c \) is the band edge, and \( m_c^* \) the effective mass of the conduction band. \( E_v \) is the band edge, and \( m_v^* \) the effective mass of the valence band.
- For low dimensions, \( E_c \) and \( E_v \), and the bandgap \( E_g = E_v - E_c \) include the quantum confinement energies if present.
- \( h \) is Planck’s constant, \( \hbar = \frac{h}{2\pi} \), \( k_B \) is the Boltzmann constant, and \( q \) the electron charge.
- \( g_s \) is the spin degeneracy, and \( g_v \) the valley degeneracy.
- \( f_{j}(q) = \frac{1}{E_{j}^{(i+1)}} \int_{0}^{E_{j}} dE_{j} \) is the Fermi-Dirac integral of order \( j \) and \( \Gamma(-...) \) is the Gamma function.
- \( E_{g} \) is the Fermi level at equilibrium. \( E_{g} \) is the source quasi-Fermi level and \( E_{g} \) the drain quasi-Fermi level.
- Similarly, \( E_{b} \) is the conduction band quasi-Fermi level and \( E_{c} \) the valence band quasi-Fermi level.
- \( I_{p} \) is the photon energy of frequency \( v \), and \( L_{c}, L_{v}, L_{b} \) are the dimensions of the semiconductor nanostructure.
- \( A \) and \( B \) are the Einstein parameters, \( A = h v / (e n) \), the wavelength of the photon in vacuum, and \( b \) the refractive index of the semiconductor.
- \( f_{j}(E_{2}) = 1 / [1 + e^{E_{2} - E_{j}/k_{B}T}] \) is the Fermi-Dirac occupation function of state \( E_{2} \) = \( E_{c} + \frac{E_{g}}{2} \) in the conduction band.
- \( f_{j}(E_{1}) = 1 / [1 + e^{E_{1} - E_{j}/k_{B}T}] \) is the Fermi-Dirac occupation function of state \( E_{1} \) = \( E_{v} - \frac{E_{g}}{2} \) in the valence band.
- \( E_{2} - E_{1} = h v = E_{g} + \frac{E_{g}}{2} \) is the energy of the photon emitted when the electron transitions from \( E_{2} \rightarrow E_{1} \) radiatively.
- The Einstein parameters \( A \) and \( B \) coefficients are related by \( A = \frac{B}{2} \).
- The photon density is \( p_{\gamma} = L_{p}/(c/n) \) in eV/cm², \( c \) is the speed of light in a medium of refractive index \( n \), and \( L_{p} = E_{2}^{3}/2\eta \) in W/cm² is the Poynting energy density with electric field amplitude \( E_{0} \) and wave impedance \( \eta \).
Prelim 1 for ECE 4070 / MSE 6050

- Tuesday March 5th 2019
- Time: 7:30 – 9:00 pm
- In Phillips Hall 219 (Note: different from class location!)

- No restrictions on books/notes/calculators/computers etc.
- Bring pen/pencil – exam books will be provided.
- Questions: conceptual, no heavy number crunching will be needed.
- Previous year questions fairly representative of what to expect.
- Topics covered: Chapters 1-5 from the Notes.

Exams and Grades:
An assignment every 1.5 weeks. Total of 6-8 homework assignments per semester. Exams: 2 Evening Prelim Exams and 1 Final Exam. Here is the approximate breakup of scores that will go towards your final grade:

35% Assignments
15% Prelim 1 [Tuesday March 5th, 2019]
20% Prelim 2 [Thursday April 11th, 2019]
30% Final [Wednesday May 15th, 2019]
Tight-Binding Bandstructure

Energy Bands of Si, Ge, and GaAs for Reference

ECE 4070 / MSE 6050
Energy Bandstructures of the most common Semiconductors
Semiconductors: Quantum Energy Eigenvalues

- Calculated by the Empirical Pseudopotential Method
The Nearly Free Electron Model for Any FCC Lattice

Fig. 9.5 Nearly Free Electron Bandstructure for the FCC Lattice. Silicon, Ge, GaAs, Diamond, and many semiconductors have a FCC real-space lattice with 2-atom bases. The nearly free electron bandstructure shown here is representative of all semiconductors that share the same real-space lattice.
Electrons in a Crystal are not Exactly Free…

- The Periodic Potential for electrons in a crystal

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Electrons in a Crystal are not Exactly Free…

- The Periodic Potential in a crystal causes standing waves for electrons.
- It splits the allowed energies into bands separated by gaps.
Electrons in a Crystal are not Exactly Free...

- The Periodic Potential in a crystal causes standing waves for electrons.
- It splits the allowed energies into bands separated by gaps
- To explain the quantitative details, we must learn perturbation theory of quantum mechanics

Fig. 8.3 Bandgap opening in the energy spectrum of a free electron upon perturbation by a periodic potential.
Background: The expansion principle

We learn early on that any well-behaved\(^1\) function \(f(x)\) can be expressed as a sum over a complete set of trigonometric functions (or complex exponentials) by the Fourier theorem

\[ f(x) = \sum_k a_k e^{ikx}. \]

Note that any complete set of eigenfunctions \([\ldots, e^{ikx}, \ldots]\) works! To find the Fourier coefficients, we use the ‘filtering’ property of complex exponentials

\[ a_{kn} = \int dx f(x)e^{-iknx}. \]

If we tweak the function \(f(x) \to f(x) + \delta(x) = h(x)\), then

\[ h(x) = \sum_k a'_k e^{ikx} \]

is still a valid expansion; the Fourier coefficients will be tweaked from \(a_k \to a'_k\). But note that the perturbed function can still be expanded in terms of the original complete set of eigenfunctions. This idea leads to the Expansion Principle in quantum mechanics.

In quantum mechanics, any quantum state ‘vector’ \(|\Psi\rangle\) may be expanded as a linear superposition of the eigenvectors of any Hermitian operator

\[ |\Psi\rangle = \sum_n a_n |n\rangle. \]

This is the Expansion Principle of quantum mechanics. For most problems, the Hermitian operator of choice is the Hamiltonian operator \(\hat{H} = (\hat{p}^2/2m_0) + V(\mathbf{r})\), but it need not be. We choose the Hamiltonian operator since there exist a few problems for which we know the set of exact eigenvectors \([\ldots, |n-1\rangle, |n\rangle, |n+1\rangle, \ldots]\). These sets of eigenvectors are complete. We also discussed in chapter 2 that this choice of eigenstates are stationary, which makes life easier.

---

\(^1\)Well-behaved in the sense that it is integrable.

Be sure to understand and appreciate this powerful statement!
Background: Operators = Matrices

\[ |\Psi\rangle = \sum_n a_n |n\rangle \]
\[ a_1 \\
\begin{array}{c}
|\Psi\rangle = \begin{bmatrix}
a_1 \\
a_2 \\
a_3 \\
\vdots
\end{bmatrix} = \begin{bmatrix}
(1|\Psi) \\
(2|\Psi) \\
(3|\Psi) \\
\vdots
\end{bmatrix} \rightarrow \langle \Psi | = \begin{bmatrix}
a_1^* \\
a_2^* \\
a_3^* \\
\vdots
\end{bmatrix} \rightarrow \langle \Psi | \Psi \rangle = 1 \]
\[ \sum_n |a_n|^2 = 1 \]

\[ \langle m|n \rangle = \delta_{mn} \]
\[ \sum_n |n\rangle \langle n| = 1. \]
\[ \int dx |x\rangle \langle x| = 1 \]

Fig. 6.3 Three ways of saying the same thing. The operator \( A \) rotates a state vector \( |\Psi\rangle \) into \( |\Phi\rangle \). The pictorial depiction is equivalent to the algebraic operator equation, which in turn is equivalent to the matrix form \([A][\Psi] = [\Phi] \).
Background: Operators = Matrices

\[ |\Psi\rangle = \sum_n a_n |n\rangle \]

\[
\begin{bmatrix}
    a_1 \\
    a_2 \\
    a_3 \\
    \vdots
\end{bmatrix}
= \begin{bmatrix}
    \langle 1 | \Psi \rangle \\
    \langle 2 | \Psi \rangle \\
    \langle 3 | \Psi \rangle \\
    \vdots
\end{bmatrix}
\rightarrow \langle \Psi | = \begin{bmatrix}
    a_1^* & a_2^* & a_3^* & \cdots
\end{bmatrix}
\rightarrow \langle \Psi | \Psi \rangle = 1
\]
\[
\sum_n |a_n|^2 = 1
\]

\[ \langle m | n \rangle = \delta_{mn} \]

\[ \sum_n |n\rangle \langle n| = 1 \]

\[ \int dx |x\rangle \langle x| = 1 \]

Consider now an operator \( \hat{A} \) acts on the state vector \( |\Psi\rangle \). It will try to ‘rotate’ the state vector in the Hilbert state to a state \( |\Phi\rangle \), which is written as

\[ \hat{A} |\Psi\rangle = |\Phi\rangle \]

By the expansion principle, we can expand the new state \( |\Phi\rangle = \sum_m b_m |m\rangle \). Then, if we project this state on \( |m\rangle \), we have

\[ \langle m | \Phi \rangle = \langle m | \hat{A} |\Psi\rangle \rightarrow b_m = \sum_n a_n \langle m | \hat{A} |n\rangle = \sum_n A_{mn} a_n. \quad (11.6) \]

We see that the operator is equivalent to a matrix \( \hat{A} \equiv A_{mn} \). The elements of the equivalent matrix are the terms \( A_{mn} = \langle m | \hat{A} |n\rangle \), obtained by the operator acting on eigenstates on both sides. They are called matrix elements for this reason.
Background: Hamiltonian Operator as a Matrix

\[ \hat{H} |n\rangle = E_n |n\rangle \]

For eigenstates

\[ |\Psi\rangle = \sum_n a_n |n\rangle \]

\[ \hat{H} \sum_n a_n |n\rangle = E \sum_n a_n |n\rangle \]

\[ \sum_n \langle m | \hat{H} |n\rangle a_n = E a_m \]

The most important operator is the Hamiltonian operator, which ‘extracts’ the energy of the state it is acting on. If the state happens to be an eigenstate, the Hamiltonian operator extracts its energy eigenvalue: \( \hat{H} |n\rangle = E_n |n\rangle \). Visualize \( \hat{H} |n\rangle \) as a new vector whose ‘direction’ is the same as the eigenvector \( |n\rangle \), but the length determined by the eigenvalue \( E_n \). So the action of the Hamiltonian operator leaves the ‘direction’ of the eigenvector \( |n\rangle \) unaffected.

Matrix form of Schrodinger eqn.

\[ \begin{bmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix} = E \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix} \]

The strangest property of matrices is that they do not necessarily commute. Which is to say that in general for square matrices, \( AB \neq BA \). As a mathematical object, therefore they are quite distinct from real or complex numbers. Matrices thus form the natural objects for non-commutative algebra. Therefore they are central to the tenets of quantum mechanics, which is built upon the non-commutativity of operators.

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Background: Spectral decomposition of $H$

$$A[x] = \lambda[x] \rightarrow [A - \lambda I][x] = 0$$

Map to equivalent problem in matrix algebra:

$$A = UDU^{-1}$$

Solve, form diagonal matrix with e'vals:

$$D = \begin{bmatrix} 
\lambda_1 & 0 & \cdots \\
0 & \lambda_2 & \cdots \\
\vdots & \vdots & \ddots 
\end{bmatrix}$$

Form unitary transformation matrix with e'vectors:

$$U = \begin{bmatrix} 
[x_1] & [x_2] & \cdots 
\end{bmatrix}$$

Property of Traces of matrices:

$$\text{Tr}[AB] = \text{Tr}[BA]$$

$$\text{Tr}[U^{-1}UD] = \text{Tr}[D] = \sum_n E_n$$

Spectral decomposition of matrix A

Eigenvalue problem of a matrix

Spectral decomposition of the Hamiltonian operator (diagonalization)
Background: Spectral decomposition enables...

\[ A = U D U^{-1} \]

\[ A^N = U D^N U^{-1} \]

\[ e^A = 1 + A + \frac{1}{2!} A^2 + \ldots = U e^D U^{-1} = U \begin{bmatrix} \lambda_1^2 & 0 & \ldots \\ 0 & \lambda_2^2 & \ldots \\ \vdots & \vdots & \ddots \end{bmatrix} U^{-1}. \]

Functions of matrices

\[ e^A e^B = e^{B+[A,B]+\frac{1}{2!}[A,[A,B]]+\ldots} \]

Baker-Hausdorff formulae

\[ e^A B e^{-A} = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \frac{1}{3!} [A, [A, [A, B]]] + \ldots \]

Jacobi formula

\[ \text{Det}[e^A] = e^{\text{Trace}[A]} \]

Consider 2 state vectors

Inner product is a number

\[ \langle \Phi | \Psi \rangle = \sum_n a_n b_n^*, \text{ we get a number} \]

Trace is invariant!

\[ \text{Tr}[\langle \Psi | \Phi \rangle] = \text{Tr}[\langle \Phi | \Psi \rangle] = \sum_n a_n b_n^* \]

Outer product is the density matrix
Evaluation of Matrices

Fig. 6.4 Examples of 2x2, 3x3, and 5x5 Matrix eigenvalue and eigenfunction calculations in Mathematica. The 2x2 Hamiltonian is general and one of the most important in all of quantum mechanics. The 3x3 matrix is a numerical example, and the 5x5 matrix of a 5-site circular ring tight-binding Hamiltonian model. Note that the eigenvectors (or eigenfunction coefficients $a_n$) are evaluated for each eigenvalue, which is very nice.
Background: Green’s Function Matrices

To construct operators of the form $\hat{A} = \sum a_n |n\rangle\langle n|$:

$$\hat{G}(E) = \sum_n \frac{|n\rangle\langle n|}{E - E_n}$$

**Definition of the Green’s function operator**

$E_n$ is the eigenvalue of state $|n\rangle$

$$\hat{G}(E)|m\rangle = \sum_n \frac{|n\rangle\langle n|}{E - E_n} |m\rangle = \sum_n \frac{|n\rangle\langle n|}{E - E_n} (E - \hat{H}^0) |\psi\rangle = \sum_n |n\rangle\langle n| |\psi\rangle = |\psi\rangle$$

**Action of $\hat{G}(E)$ on a state $|m\rangle$**

$$\hat{G}(E)(E - \hat{H}^0)|\psi\rangle = \sum_n \frac{|n\rangle\langle n|}{E - E_n} (E - \hat{H}^0)|\psi\rangle = \sum_n |n\rangle\langle n| |\psi\rangle = |\psi\rangle$$

**Action of $\hat{G}(E)$ on the Schrodinger equation yields identity**

$$\hat{G}(E) = (E - \hat{H}^0)^{-1}$$

**Green’s function operator is the inverse operator of $E - \hat{H}^0$**

Formal solution of the perturbation problem using Green’s functions: elegant, but analytically not too useful…

$$(E - \hat{H}^0)|\psi\rangle = 0$$

**Perturbation $W$ changes the Hamiltonian**

$$\hat{H}^0 \rightarrow \hat{H}^0 + \hat{W}$$

$$(E - \hat{H}^0 - \hat{W})|\phi\rangle = 0$$

**Eigenstates have changed because of the perturbation $W$**

$$|\psi\rangle \rightarrow |\phi\rangle$$

Using $G(E)$, we can write the new eigenstate in terms of the old (known) eigenstates and eigenvalues

$$\hat{G}^{-1}(1 - \hat{G}\hat{W})|\phi\rangle = \hat{G}^{-1}|\psi\rangle \implies |\phi\rangle = (1 - \hat{G}\hat{W})^{-1}|\psi\rangle$$

$$|\phi\rangle = (1 + \hat{G}\hat{W} + \hat{G}\hat{W}\hat{G}\hat{W} + \hat{G}\hat{W}\hat{G}\hat{W}\hat{G}\hat{W} + ...) |\psi\rangle$$

**Lippmann-Schwinger equation, or Dyson equation**

Debdeep Jena (djena@cornell.edu)
Time-independent perturbation theory

Unperturbed (solved) problem: We know the eigenvalues & eigenstates

\[ H^0 |n\rangle = \mathcal{E}_n^0 |n\rangle \]

\[ H = H^0 + W \]

\[ (H^0 + W) |\psi\rangle = \mathcal{E} |\psi\rangle \]

\[ |\psi\rangle = \sum_{n} a_n |n\rangle \]

\[ a_n = \langle n | \psi \rangle \]

Perturbed Hamiltonian, new eigenstates

Expansion principle!

Unperturbed problem: We know the eigenvalues & eigenstates

\[ \mathcal{E} = \sum_{n=1}^{N} a_n |n\rangle \]

Perturbed problem:

Find \{l_n', \mathcal{E}_n' \}

\[ a_n \] are aff. of \[ W \]

The central problem of time-independent perturbation theory

Matrix solution of the perturbation problem: diagonalize & get solns.

\[ H^{mn} = \langle m | H | n \rangle \]

Matrix elements include the perturbation
Degenerate perturbation theory

\[ \sum_n a_n \langle m | (H^0 + W) | n \rangle = E a_m. \]

\[
\begin{bmatrix}
  E_1 + W_{11} & W_{12} & W_{13} & \ldots & W_{1N} \\
  W_{21} & E_2 + W_{22} & W_{23} & \ldots & W_{2N} \\
  W_{31} & W_{32} & E_3 + W_{33} & \ldots & W_{3N} \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  W_{N1} & W_{N2} & W_{N3} & \ldots & E_N + W_{NN}
\end{bmatrix}
\begin{bmatrix}
  a_1 \\
  a_2 \\
  a_3 \\
  \vdots \\
  a_N
\end{bmatrix}
= E
\begin{bmatrix}
  a_1 \\
  a_2 \\
  a_3 \\
  \vdots \\
  a_N
\end{bmatrix}
\]
Time-independent perturbation theory

\[
\begin{bmatrix}
H_{11} & H_{12} & \cdots & H_{1N} \\
H_{21} & H_{22} & \cdots & H_{2N} \\
\vdots & \vdots & \ddots & \vdots \\
H_{N1} & H_{N2} & \cdots & H_{NN}
\end{bmatrix}
\times
\begin{bmatrix}
a_1 \\
a_2 \\
\vdots \\
a_N
\end{bmatrix}
= \mathcal{E}
\begin{bmatrix}
a_1 \\
a_2 \\
\vdots \\
a_N
\end{bmatrix}
\begin{bmatrix}
H_{11} - \mathcal{E} & H_{12} & \cdots & H_{1N} \\
H_{21} & H_{22} - \mathcal{E} & \cdots & H_{2N} \\
\vdots & \vdots & \ddots & \vdots \\
H_{N1} & H_{N2} & \cdots & H_{NN} - \mathcal{E}
\end{bmatrix}
= 0
\]

Solve these for solutions to the perturbation problem. Exact solution is an infinite matrix! How to truncate?

\[
|m\rangle \leftrightarrow |n\rangle \\
|\mathcal{E}_m - \mathcal{E}_n| \\
W_{mn} = \langle m|W|n\rangle \\
\Delta \mathcal{E}_{ix} = \frac{|W_{ix}|^2}{\mathcal{E}_x - \mathcal{E}_i}
\]

Strength of interaction between states depends on:

- Their energy separation
- The matrix element between them
- \((\text{Matrix element})^2/\text{Energy difference}\)

Example: 2-Level system

\[
\begin{bmatrix}
H_{11} - \mathcal{E} & H_{12} \\
H_{21} & H_{22} - \mathcal{E}
\end{bmatrix}
= 0
\]

\[
\mathcal{E}_\pm = \frac{1}{2}(H_{11} + H_{22}) \pm \sqrt{\frac{1}{4}(H_{11} - H_{22})^2 + |H_{12}|^2}
\]

\[
a_1 = \frac{H_{12}}{\sqrt{|H_{12}|^2 + (\mathcal{E} - H_{11})^2}} \\
a_2 = \frac{\mathcal{E} - H_{11}}{\sqrt{|H_{12}|^2 + (\mathcal{E} - H_{11})^2}}
\]

\[
|\psi\rangle = a_1|1\rangle + a_2|2\rangle
\]
Analytical time-independent perturbation theory

\[ H^0 |u\rangle = \mathcal{E}_u |u\rangle \]

\[ |u\rangle \rightarrow |u\rangle + |\phi\rangle = |\psi\rangle \]

Select out an unperturbed state \( u \)

\[ |\psi\rangle = |u\rangle + \sum_{m \neq u} \sum_{n \neq m} \frac{\langle m | W | n \rangle}{\mathcal{E} - \mathcal{E}'_m} |n\rangle |\phi\rangle \]

Eigenvalues and eigenstates after perturbation

\[ \mathcal{E} \approx \mathcal{E}_u + \langle u | W | u \rangle + \sum_{m \neq u} \frac{|\langle m | W | u \rangle|^2}{\mathcal{E} - \mathcal{E}'_m} \]

Define...

\[ \mathcal{E}'_u = \mathcal{E}_u + \langle u | W | u \rangle \]
\[ \mathcal{E}'_m = \mathcal{E}_m + \langle m | W | m \rangle \]

iff this condition holds, in rhs...

\[ |\Delta \mathcal{E}^{(1)} + \Delta \mathcal{E}^{(2)}| \approx |\mathcal{E} - \mathcal{E}'_u| < < |\mathcal{E}_m - \mathcal{E}_u| \]

\[ \mathcal{E} \approx \mathcal{E}'_u + \sum_{m \neq u} \frac{|\langle m | W | u \rangle|^2}{\mathcal{E} - \mathcal{E}'_m} \]

\[ \mathcal{E} \approx \mathcal{E}'_u + \sum_{m \neq u} \frac{|\langle m | W | u \rangle|^2}{\mathcal{E}_u - \mathcal{E}'_m} \]

Brillouin-Wigner (BW) Perturbation theory

Rayleigh-Schrodinger (RS) Perturbation theory

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Level repulsion and Avoided Crossing

| \langle m | W | u \rangle^2 | \frac{1}{\mathcal{E}_u - \mathcal{E}_m} < 0 |
| \langle m | W | u \rangle^2 | \frac{1}{\mathcal{E}_u - \mathcal{E}_m} > 0 |

“Level repulsion”: Perturbative energy interactions between different states is repulsive

\[ \mathcal{E} \approx \mathcal{E}_u + \sum_{m \neq u} \frac{|\langle m | W | u \rangle|^2}{\mathcal{E}_u - \mathcal{E}_m} \]

Responsible for “curvature” of bands, and effective masses of band-edge electron states. Small bandgap semiconductors have small band-edge effective masses.

“Avoided Crossing”: Two unperturbed states that are not degenerate cannot be made degenerate (cross) by perturbation. This is because the interaction is repulsive in energy eigenvalues.

This observation holds independent of the sign of the perturbation, because the 2nd order energy correction has the square of the matrix element.
Perturbation Theory Example: Particle in a Box

Introduce a small perturbation to the particle in a box.

States with maximum wavefunction at the center will be perturbed the most. States with low energy will be perturbed more than states of high energy.
Perturbation Theory Example: Particle in a Box

Original eigenvalues

1\textsuperscript{st} order perturbation

\[ W_{nn} = \langle n|W(x)|n \rangle = \frac{2W_0}{L} \int_{L/2}^{L} dx \sin^2 \left( \frac{n \pi}{L} x \right) \]

Matrix Elements

\[ W_{nm} = \langle n|W(x)|m \rangle = \frac{2W_0}{L} \int_{L/2}^{L} dx \sin \left( \frac{n \pi}{L} x \right) \sin \left( \frac{m \pi}{L} x \right) \]

2\textsuperscript{nd} order perturbation

\[ E_1' \approx E_1 + E_0 + \sum_{m=3,5,\ldots} \frac{E_3^2}{1 - m^2 - \frac{E_0}{E_1}} \approx E_1 + E_0 - \frac{E_0^2}{8E_1} \]

Direct Matrix Method for perturbation solution

\[ \hat{H}^0 + W = \begin{pmatrix} 1 & 2 & 3 \\ E_1 + E_0 & 0 & E_0 \\ E_0 & 0 & E_3 + E_0 \end{pmatrix} \]

Perturbed ground state wavefunction

\[ \psi(x) = \psi_1(x) + \sum_{m=3,5,\ldots} \frac{E_0}{E_1(1 - m^2 - \frac{E_0}{E_1})} \psi_m(x) \]

Perturbation pushes out wavefunction probability
A Periodic Potential for the Electron on a Ring

• The central problem of the physics of semiconductors is that of an electron in a crystal.
• A crystal is a periodic array of atoms.
• The quantum mechanical electron experiences a periodic potential \( V(x+a) = V(x) \).
• What are the allowed eigenvalues and eigenfunctions?
• All answers to semiconductor physics are hidden in the solution of this problem.

Fig. 8.2 The electron on a ring experiences a periodic potential.

Fig. 8.5 Rudolph Peierls while working with Heisenberg was the first to produce the famous energy dispersion of a free electron perturbed by a periodic potential. His plot is reproduced in Figure 8.6.

Fig. 8.6 Rudy Peierls' iconic plot of the energy dispersion of a free electron in a periodic potential from his 1930 paper.
Example: Opening of a bandgap in a crystal

Unperturbed problem is the 'electron on a ring': E'states, E'Vals:

\[
\langle x|k \rangle = \psi(x, k) = \frac{1}{\sqrt{L}} e^{ikx}
\]

\[
E_0(k) = \frac{\hbar^2 k^2}{2m_0}
\]

\[
\langle k_m|k_n \rangle = \int dx \langle k_m|x \rangle \langle x|k_n \rangle = \int dx \psi^*(x, k_m)\psi(x, k_n) = \frac{1}{L} \int_0^L dx e^{i2\pi(n-m)x} = \delta_{n,m}
\]

unperturbed E'states are orthogonal

\[
W(x) = -2UG \cos(Gx) = -UG(e^{iGx} + e^{-iGx})
\]

Perturbation potential

States most strongly perturbed: +G/2, -G/2. F= E_0(G/2) is their unperturbed energy.

\[
E_0(G/2) = \frac{\hbar^2 G^2}{8m_0} = F
\]

Perturbing potential only couples state k with k+G, k-G with strength -UG

Solve to get the eigenvalues and the eigenfunctions

Form the 2-state Hamiltonian

\[
E_{\pm} = \frac{H_{11} + H_{22}}{2} \pm \sqrt{\left( \frac{H_{11} - H_{22}}{2} \right)^2 + |H_{12}|^2}
\]

\[
\begin{bmatrix}
H_{11} & H_{12} \\
H_{21} & H_{22}
\end{bmatrix}
\]

\[
\hat{H}^0 + W = \begin{pmatrix}
\frac{+G}{2} & F \\
\frac{-G}{2} & -UG
\end{pmatrix}
\]

\[
\begin{bmatrix}
| + \frac{G}{2} \rangle \\
| - \frac{G}{2} \rangle
\end{bmatrix}
\]
**Bandgap, band-edge states, effective masses**

\[ \hat{H}^0 + W = \begin{pmatrix} + \frac{G}{2} + k' & - \frac{G}{2} + k' \\ \frac{G}{2} + k' & - \frac{G}{2} + k' \end{pmatrix} \begin{pmatrix} E_0( + \frac{G}{2} + k') - U_G \\ - U_G & E_0( - \frac{G}{2} + k') \end{pmatrix} \]

\[ (F - E)^2 - U_G^2 = 0 \]

\[ E_+ = F \pm U_G \]

\[ E_+ - E_- = 2U_G \]

**Bandgap at +/- G/2**

**Near band-edge states**

\[ |\psi\rangle = \sum_n a_n |n\rangle \quad |\pm\rangle = a_{1\pm} + \frac{G}{2} + a_{2\pm} - \frac{G}{2} \]

\[ a_{1+} = -1/\sqrt{2}, \quad a_{2+} = +1/\sqrt{2}, \quad a_{1-} = -1/\sqrt{2}, \quad a_{2-} = -1/\sqrt{2}. \]

\[ \langle x|+\rangle = \psi_+(x) = \left( - \frac{1}{\sqrt{2}} \cdot \frac{e^{iGx}}{\sqrt{L}} \right) + \left( + \frac{1}{\sqrt{2}} \cdot \frac{e^{-iGx}}{\sqrt{L}} \right) = -i \sqrt{\frac{2}{L}} \sin(\frac{Gx}{2}) \]

\[ \langle x|-\rangle = \psi_-(x) = \left( - \frac{1}{\sqrt{2}} \cdot \frac{e^{iGx}}{\sqrt{L}} \right) + \left( + \frac{1}{\sqrt{2}} \cdot \frac{e^{-iGx}}{\sqrt{L}} \right) = \sqrt{\frac{2}{L}} \cos(\frac{Gx}{2}) \]

\[ |\psi_+(x)|^2 = (2/L) \sin^2(Gx/2) \quad |\psi_-(x)|^2 = (2/L) \cos^2(Gx/2) \]

**2-state Hamiltonian for states near +/- G/2**

**Perturbed eigenstates**

\[ E_\pm(k') \approx (F \pm U_G) + \left( 1 \pm \frac{2F}{U_G} \right) \frac{\hbar^2 k'^2}{2m^*_c} \]

\[ E_c(k') \approx E_c(0) + \frac{\hbar^2 k'^2}{2m^*_c} \]

**Conduction band**

**Valence band**

**Figure 13.3:** Probability pileups of band-edge states.
Bandgap, band-edge states, effective masses

- The effective mass at any $k$ is proportional to the curvature of the energy band at that $k$
- States at the Brillouin Zone edges 1=2 and 3=4.
- After the opening of the bandgap, $E(k+G) = E(k)$, the allowed energies are periodic in $k$-space.

Fig. 8.17 1D bandstructure plotted in a periodic $k$-space.
Bands, Gaps, Metals vs Insulators

Fig. 8.10 Energy gaps open at \( k = n \frac{\pi}{a} \), which is identical to the conditions when the electron wavelengths become resonant with twice the lattice constant, i.e. \( n\lambda = 2a \). This is analogous to Bragg's law of diffraction for a wave incident at an angle \( \theta \) on a crystal of period \( d \), when the law reads \( n\lambda = 2d\sin\theta \).

Because the width of each band in the \( k \)-space is \( G = \frac{2\pi}{a} \), and the separation between two allowed states is \( \frac{2\pi}{L} \) where \( L \) is the macroscopic length, the number of states in each band is \( N = L/a \), equal to the number of atoms in the crystal. Since each allowed state can hold 2 electrons of opposite spin, each band can hold 2N electrons. We can plot all energies within \( -\frac{G}{2} \leq k \leq +\frac{G}{2} \) and index them as \( E_n(k) \) where \( n \) indicates a reciprocal lattice vector. Because of the opening of the bandgaps, when an electron in an allowed band moves in response to \( F = \frac{dk}{dt} \), it cannot jump to the higher band when its \( k \to \pm\frac{G}{2} \) under moderate forces\(^5\). In that case, the electron remains in the same band, but enters it from \( k = -\frac{G}{2} \). This is because they are actually the same point in the reduced zone scheme.
Bandgap, band-edge states, effective masses

\[ v_g = \frac{1}{\hbar} \frac{\partial E(k)}{\partial k} \]

Group velocity of state \( k = \) slope of the band at that \( k \)

\[ J = q \frac{g_s}{L} \sum_k v_g(k) f(k) \]

Quantum current carried by electrons in a band

\[ J_{\text{filled}} = q \frac{g_s}{L} \sum_k v_g(k) f(k) = 0 \]

Current carried by a filled (or empty) band is zero

Filled bands carry no net current.

\[ J = \left( -q \right) \frac{g_s}{L} \sum_k v_g(k) [1 - f(k)] \]

- Current is carried in an almost filled band by HOLES.
- Holes behave as POSITIVE charges.
- Hole conduction causes a POSITIVE sign in the Hall Effect.
- Holes behave as POSITIVE charges in Field Effect.
Metals, Insulators and Semimetals

**Fig. 8.17** Impossibility of band overlaps in 1D, and possible overlaps in 2 and 3D crystals.
Higher order interactions and Bloch Theorem

**Glimpses of the Bloch Theorem**

The wavefunction in a periodic potential: Is in the form of a Bloch function!

\[ \psi_k(x) \approx e^{ikx} u_k(x) \]
\[ u_k(x + a) = u_k(x) \]

However, note that the Bloch function is an **EXACT** result, meaning a non-perturbative one. But it is useful to see that perturbation theory hints at its existence.

\[ |k'\rangle \approx |k\rangle + \frac{\langle k + G|W|k\rangle}{E(k) - E(k + G)} |k + G\rangle + \frac{\langle k - G|W|k\rangle}{E(k) - E(k - G)} |k - G\rangle \]

\[ \psi_k(x) = \langle x|k\rangle \approx e^{ikx} \frac{1}{\sqrt{L}} - \frac{U_G}{E(k) - E(k + G)} \frac{e^{i(k+G)x}}{\sqrt{L}} - \frac{U_G}{E(k) - E(k - G)} \frac{e^{i(k-G)x}}{\sqrt{L}} u_k(x) \]

\[ \psi_k'(x) \approx e^{ikx} \left[ \frac{1}{\sqrt{L}} - \left( \frac{U_G}{E(k) - E(k + G)} \right) \frac{e^{iGx}}{\sqrt{L}} - \left( \frac{U_G}{E(k) - E(k - G)} \right) \frac{e^{-iGx}}{\sqrt{L}} \right] u_k(x) \]
Bloch Functions of Electrons in Periodic Potentials

**Fig. 9.1** Bloch functions

\[ \psi_k(x) = e^{ikx} u_k(x), \text{ where } u_k(x + a) = u_k(x) \]

**Fig. 9.2** The Bloch function is a plane wave modulated by a function periodic in the lattice constant.
The most general Matrix Element for Bloch States of Electrons in Crystals

\[ \langle k' | V(x) | k \rangle = \int_0^L dx \cdot e^{i(k' - k)x} \cdot \left[ V(x) u^*_k(x) u_k(x) \right] = \sum_G c_G \delta_{k' - k, G} \sum_G c_G e^{iGx} \]

"When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in a metal so as to avoid a mean free path of the order of atomic distances. Such a distance was much too short to explain the observed resistances... To make my life easy, I began by considering wave functions in a one-dimensional periodic potential. By straight Fourier analysis I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation \[ [\psi_k(x) = e^{i k x} u_k(x)] \]. This was so simple that I didn’t think it could be much of a discovery, but when I showed it to Heisenberg he said right away: ‘That’s it!’ Well that wasn’t quite it yet, and my calculations were only completed in the summer when I wrote my thesis on The Quantum Mechanics of Electrons in Crystal Lattices.” [F. Bloch 1976]

Fig. 8.12 Felix Bloch showed mathematically that electron waves can propagate in a crystal with no scattering, by introducing a wavefunction that electrons experiencing a periodic potential must satisfy. Bloch was awarded the Nobel Prize in physics in 1952 for his work on nuclear magnetic resonance.
The Nearly Free Electron Bandstructure Model

**Fig. 8.13** The nearly free electron bandstructure. The model is where there is a lattice, but no crystal potential. Bloch theorem ensures that the allowed energy bands are exactly the same of a free electron, but repeated in the \( k \)-space by reciprocal lattice vectors, \( E_n(k) = \frac{\hbar^2}{2m_e} (k - nG)^2 \) where \( n = 0, \pm 1, \pm 2, \ldots \). Note the points of degeneracies: these points can be split to open gaps by a periodic potential.

As shown in Figure 8.13, the NFE bandstructure consists of copies of the free electron bandstructure translated by \( nG \) in the \( k \)-axis, where \( G = \frac{2\pi}{a} \) and \( n = 0, \pm 1, \pm 2, \ldots \). This is a direct consequence of periodicity of the lattice.
Bandgap, band-edge states, effective masses

\[ \langle \psi_k | \frac{\hat{p}}{m_e} | \psi_k \rangle = v(k) = \frac{1}{\hbar} \nabla_k E(k). \]

\[ F = \hbar \frac{d\mathbf{k}}{dt}. \]  
F is an external force, k is the crystal momentum.

Fig. 9.7 Classical vs. Quantum pictures of a particle in a periodic potential. The Bloch state maintains the same velocity in spite of a rapidly varying periodic potential of the crystal - this is impossible in classical mechanics.
Bandgap, band-edge states, effective masses

Fig. 8.14 Mixing of electronic signals produces sum and difference frequencies. The problem of electron wave propagation in a crystal is an analogous problem.

Fig. 8.15 Periodic potentials only scatter states separated by specific $G$ values, and thus open bandgaps at specific $k$ values because they have spectral weight only for specific $k$’s. Non-periodic potentials on the other hand can scatter a state $|k\rangle$ into several states depending on the weight of the potential in the $k$–space.
Bandgap, band-edge states, effective masses

\[ \frac{\hbar^2}{2m_e} (k + G)^2 c_G + \sum_{G'} V_{G-G'} c_{G'} = E_G(k) c_G. \]

→ **Exact Bandstructure**, Chapter \[12\]

\[ E_G(k) = \frac{\hbar^2}{2m_e} (k + G)^2, \text{ and } \psi_G(x) = \frac{1}{\sqrt{L}} e^{i(k+G)x} = e^{ikx} \cdot \left( \frac{1}{\sqrt{L}} e^{igx} \right) \]

→ **Empty lattice bandstructure, Brillouin zones**, this Chapter

\[ \psi_k(x) = \sum_{n=1}^{N} \frac{e^{ika}}{\sqrt{N}} \phi(x - na) \implies \psi_k(x + a) = e^{ika} \psi_k(x). \]

→ **The tight binding model**, Chapter \[10\]

\[ \left[ \frac{\left(\hat{p} + \hbar \hat{k}\right)^2}{2m_e} + V \right] u_k = E(k) u_k. \]

\[ \left[ -\frac{\hbar^2}{2m_e} \nabla^2 + V \right] u_k + \left( \frac{\hbar}{m_e} \hat{k} \cdot \hat{p} \right) u_k = \left[ E(k) - \frac{\hbar^2 |k|^2}{2m_e} \right] u_k. \]

→ **The ‘k · p’ approximation**, Chapter \[11\]
Some consequences of symmetry on $E(k)$

**Fig. 9.14** Properties energy bands must satisfy for Bloch states in crystals.

**Table 9.2** Symmetries of Bloch Eigenvalues.

<table>
<thead>
<tr>
<th>Symmetry Type</th>
<th>Transformation</th>
<th>Eigenvalue Transformation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time Reversal $(t \rightarrow -t)$</td>
<td></td>
<td>$E_{n,\uparrow}(k) \rightarrow E_{n,\downarrow}(-k)$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$E_{n,\downarrow}(k) \rightarrow E_{n,\uparrow}(-k)$</td>
</tr>
<tr>
<td>Inversion $(r \rightarrow -r)$</td>
<td></td>
<td>$E_{n,\uparrow}(k) \rightarrow E_{n,\uparrow}(-k)$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$E_{n,\downarrow}(k) \rightarrow E_{n,\downarrow}(-k)$</td>
</tr>
<tr>
<td>TR &amp; Inversion</td>
<td></td>
<td>$E_n(k) = E_n(-k)$</td>
</tr>
<tr>
<td>Lattice periodicity</td>
<td></td>
<td>$E_n(k + G) = E_n(k)$</td>
</tr>
</tbody>
</table>
Electron group velocity

\[ F = \hbar \frac{dk}{dt} \]

F is an \textbf{external} force, k is the \textbf{crystal momentum}.

\[ \langle \psi_k | \hat{P} | \psi_k \rangle = v(k) = \frac{1}{\hbar} \nabla_k E(k). \]

\[ v(k) = \frac{1}{\hbar} \nabla_k E(k) - \frac{F}{\hbar} \times \Omega_k. \]
Bloch Functions of Electrons in Periodic Potentials

Crystal = Lattice + Basis.

Real Space

\[ \Omega_r = a_1 \cdot a_2 \times a_3 \]

\[ R = n_1 a_1 + n_2 a_2 + n_3 a_3 \]

Wigner-Seitz cell

Reciprocal Space or k-space

\[ e^{ikx} \rightarrow e^{ikx} \left( 1 + \sum_{u_k(x)} c_G(k) e^{iGx} \right) \]

\[ b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3}, \quad b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \cdot a_2 \times a_3}, \quad b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot a_2 \times a_3} \]

\[ G = m_1 b_1 + m_2 b_2 + m_3 b_3 \]

Brillouin Zone

[|\psi_k(r + R)|^2 = |\psi_k(r)|^2 : The Bloch wavefunction squared repeats in every Wigner-Seitz cell]

[|\psi_{k+G}(r)|^2 = |\psi_k(r)|^2 : The Bloch wavefunction squared repeats in every BZ.]

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Crystals in 1D, 2D, and 3D

**Fig. 9.10** Crystal = Lattice + Basis.

**Fig. 9.13** A 2D crystal (top) and its reciprocal lattice points (middle), defining the Brillouin Zones of a 2D square lattice. The bottom figure indicates that the 1st BZ is filled up to the dashed line constant-energy contour for monovalent atoms with $N = 1$, and spills over to the 2nd BZ shown as solid line constant energy contours for divalent atoms with $N = 2$.

**Fig. 9.11** The FCC lattice, a 2-atom basis, and the crystal of Silicon, Diamond, GaAs, InP, and a wide variety of semiconductors. The three arrows from $(0,0,0)$ to the face center lattice sites are the primitive lattice vectors.
2D Bravais Lattices

Fig. 9.21 Bravais Lattices in 2D from Wikipedia.
# 3D Bravais Lattices

<table>
<thead>
<tr>
<th>Crystal Family</th>
<th>Lattice System</th>
<th>Schönflies</th>
<th>14 Bravais Lattices</th>
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</thead>
<tbody>
<tr>
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<td></td>
<td></td>
<td>Primitive (P)</td>
</tr>
<tr>
<td>Triclinic</td>
<td>C1</td>
<td>β ≠ 90°</td>
<td></td>
</tr>
<tr>
<td>Monoclinic</td>
<td>C2h</td>
<td>β ≠ 90°</td>
<td></td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>D2h</td>
<td>a ≠ b = c</td>
<td></td>
</tr>
<tr>
<td>Tetragonal</td>
<td>D4h</td>
<td>a ≠ c</td>
<td></td>
</tr>
<tr>
<td>Rhombohedral</td>
<td>D3d</td>
<td>a ≠ b ≠ c</td>
<td></td>
</tr>
<tr>
<td>Hexagonal</td>
<td>D6h</td>
<td>a ≠ c</td>
<td></td>
</tr>
</tbody>
</table>

**Si, Ge, GaAs**

**GaN, AlN**
The first measured crystal structure: FCC!

Fig. 9.16 The famous ‘Fig 5’, showing the diffraction spots observed by Max von Laue in Munich due to Roentgen’s X-Rays bouncing off a crystal of ZnS, a semiconductor.

Fig. 9.18 Bragg Law for diffraction of X-Rays from a crystal.
TEM images of semiconductor crystals
TEM images of semiconductor crystals

Debdeep Jena (djena@cornell.edu)
Face-Centered Cubic Lattice

1\textsuperscript{st} step in bandstructure calculation: Determine \textbf{primitive lattice vectors, }a_1, a_2, a_3\textbf{.}

primitive lattice vectors for Silicon-like crystals are \(a_1 = a(\frac{1}{2}, \frac{1}{2}, 0),\) \(a_2 = a(0, \frac{1}{2}, \frac{1}{2}),\) and \(a_3 = a(\frac{1}{2}, 0, \frac{1}{2}).\)

\[
\Omega_u = a_1 \cdot a_2 \times a_3 = a(\frac{1}{2}, \frac{1}{2}, 0) \cdot a(0, \frac{1}{2}, \frac{1}{2}) \times a(\frac{1}{2}, 0, \frac{1}{2}) = a^3(\frac{1}{8} + \frac{1}{8}) = \frac{a^3}{4}.
\]

2\textsuperscript{nd} step in bandstructure calculation: Convert real space points to reciprocal space.

Now the greatest importance of the Wigner-Seitz cell is recognized when we move from the real space to the wavevector, or \(k\)-space. Corresponding to the three real space primitive lattice vectors are the three \textbf{primitive reciprocal lattice vectors} given by

\[
\begin{align*}
b_1 &= 2\pi \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3}, & b_2 &= 2\pi \frac{a_3 \times a_1}{a_1 \cdot a_2 \times a_3}, & b_3 &= 2\pi \frac{a_1 \times a_2}{a_1 \cdot a_2 \times a_3}. \\
\end{align*}
\]

With an integer triplet \((m_1, m_2, m_3),\) the vectors

\[
G = m_1 b_1 + m_2 b_2 + m_3 b_3
\]
define the \textbf{reciprocal space lattice}, just as the real-space lattice of the crystal.
The Nearly Free Electron Model for Any FCC Lattice

3rd step in bandstructure calculation: Calculate the Nearly Free Electron Bandstructure for various reciprocal lattice vector bands (typical $G_{\text{max}} < 4$).
The Nearly Free Electron Model for Any HCP Lattice

3rd step in bandstructure calculation: Calculate the Nearly Free Electron Bandstructure for various reciprocal lattice vector bands (typical Gmax<4).

Debdeep Jena (djena@cornell.edu)
Fig. 9.26 Semiconductors, Metals, and Semimetals differ primarily by the density of states at their Fermi level, \( g(E_F) \). The Fermi level is determined by counting the total valence electrons/basis of a crystal and using the rule that each filled band holds \( 2N \) electrons.
**Bloch State: Current with Scattering**

\[
F = \hbar \frac{d}{dt} \frac{\Delta k}{\tau_k}
\]

\[
J = q \frac{g_s g_v}{L} \sum_k v_g(k) f(k) = q \frac{g_s g_v}{L} \sum_k v_g(k) f(k(0)) - \frac{F \tau_k}{\hbar}
\]

\[
f(k(0) - \frac{F \tau_k}{\hbar}) \approx f(k(0)) - \frac{F \tau_k}{\hbar} \cdot \nabla_k f(k(0))
\]

\[
J \approx q \frac{g_s g_v}{L} \sum_k v_g(k) f(k(0)) + q \frac{g_s g_v}{L} \frac{F}{\hbar} \cdot \sum_k v_g(k) \tau_k (-\nabla_k f(k(0))),
\]

\[
n = \frac{g_s g_v}{d} \sum_k f(k)
\]

**Fig. 9.25** The occupation function shifts from the equilibrium Fermi-Dirac value upon the application of an external force. The sketch indicates \( f(k), f(k - \frac{F}{\hbar} \tau), \) and \( \nabla_k f(k) \).

\[
\mathcal{L}_q = \frac{\kappa}{\sigma T} = \frac{g_s g_v \ln(N_k/n) k_b}{T} \int \frac{d^d k}{(2\pi)^d} v^2 E E \frac{df}{dE}
\]

\[
\rightarrow \quad \sim \left( k_b T \right)^2
\]

semi-classical approx.

\[
J \approx \frac{n q^2}{m^*} \left( \frac{2}{d} \frac{\sum k E_k \tau_k (-\frac{df(k)}{dE_k})}{\sum_k f(k)} \right) E = \frac{n q^2 \langle \tau \rangle}{m^*} \underbrace{E}_{\langle \tau \rangle} = \frac{n q \langle \tau \rangle}{m^*} \underbrace{E}_{\mu}
\]

Debdeep Jena (djena@cornell.edu)
Tight-Binding Bandstructure

Energy Bands of Si, Ge, and GaAs for Reference

ECE 4070 / MSE 6050
Energy Bandstructures of the most common Semiconductors

Debdeep Jena (djena@cornell.edu)
The elements that form semiconductors

Some common Semiconductor Families:
- **Group IV:** Diamond, Silicon, Ge, ...
- **Group III-V:** GaAs, InP, InSb, GaN, ...
- **Group II-VI:** ZnO, MgO, CdSe, HgTe...
- **2D Materials:** Graphene, MoS$_2$, GaSe, ...
Metals and the Fermi-Surface Database

The Fermi Surface Database
{click icons}
Semiconductor Orbital Structures

**Group IV**

C: \([1s^2](2s^22p^2) \leftarrow 4\)

Si: \([1s^2][2s^2][2p^6](3s^23p^2) \leftarrow 4\)

Ge: \([1s^2][2s^2][2p^6][3s^2][3p^6][3d_{10}](4s^24p^2) \leftarrow 4\)

**Group III**

B: \([1s^2](2s^22p^1) \leftarrow 3\)

Al: \([1s^2][2s^2][2p^6](3s^23p^1) \leftarrow 3\)

Ga: \([1s^2][2s^2][2p^6][3s^2][3p^6][3d_{10}](4s^24p^1) \leftarrow 3\)

**Group V**

N: \([1s^2](2s^22p^3) \leftarrow 5\)

P: \([1s^2][2s^2][2p^6](3s^23p^3) \leftarrow 5\)

As: \([1s^2][2s^2][2p^6][3s^2][3p^6][3d_{10}](4s^24p^3) \leftarrow 5\)
Which electrons have to be included in band structure calculations?

In principle all, but the inner core electrons are strongly bound and their spatial extension is so small, that no significant overlap of the wavefunctions occur.

In silicon (Si), the 1s, 2s and 2p electrons are inner core electrons.

Si: $[1s^2][2s^2][2p^6]{3s^2,3p^2}$

Most bandstructure calculations only take into account the $\{3s^2,3p^2\}$ valence electrons.

These are 4 electrons per atom, which essentially form the chemical bonds in tetrahedral coordination.

---

The binding energies for the inner core electrons are taken from X-ray photoemission experiments.

- 2p: 99.2 eV
- 2s: 148.7 eV
- 1s: 1838.9 eV

The source is:

Handbook of Chemistry and Physics, E-184
Each band can hold 2 electrons per unit cell.
The factor 2 is the spin-multiplicity.

Valence bands: 4 bands
2 atoms per unit cell   4 electrons per atom
8 electrons in 4 bands
Tight-Binding (or LCAO) Bandstructure

\[ |\psi\rangle = \sum_{m=1}^{N} \frac{e^{ik\cdot R_m}}{\sqrt{N}} |m\rangle \]

\[ \hat{H} \sum_{m=1}^{N} e^{ik\cdot R_m} |m\rangle = E(k) \sum_{m=1}^{N} e^{ik\cdot R_m} |m\rangle \]

\[ E(k) = \frac{\sum_{n,m=1}^{N} e^{i k \cdot (R_m - R_n)} \langle n | \hat{H} | m \rangle}{\sum_{n,m=1}^{N} e^{i k \cdot (R_m - R_n)} \langle n | m \rangle} \]

\[ E(k) = \frac{E_0 - 2t_1 \cos(ka) - 2t_2 \cos(2ka) - 2t_3 \cos(3ka) \ldots}{1 + 2s_1 \cos(ka) + 2s_2 \cos(2ka) + 2s_3 \cos(3ka) \ldots} \approx E_0 - 2t_1 \cos(ka) \]
Tight-Binding Bandstructure

Example: A 1D Crystal with 1 Orbital per Primitive Cell

Consider a 1D lattice of atoms:

Each atom has the energy levels as shown:

- The electrons in the lowest energy level(s) are well localized and do not take part in bonding with neighboring atoms.
- The electrons in the outermost s-orbital participate in bonding.

The crystal has the Hamiltonian: \( \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \sum_{m} V_a (\vec{r} - \vec{R}_m) \)

Potential in a crystal

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Tight-Binding Bandstructure

Tight Binding Approach for a 1D Crystal

\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \sum_m V_a(\vec{r} - \vec{R}_m) \]

Periodic potential

We assume that the solution is of the LCAO form:

\[ \psi(\vec{r}) = \sum_m c_m \phi_s(\vec{r} - \vec{R}_m) \]

And assume that orbitals on different atoms are approx. orthogonal:

\[ \langle \phi_s(\vec{r} - \vec{R}_n) | \phi_s(\vec{r} - \vec{R}_m) \rangle = \delta_{n,m} \]

- If we have \( N \) atoms in the lattice, then our solution is made up of \( N \) different s-orbitals that are sitting on the \( N \) atoms

- In principle one can take the assumed solution, as written above, plug it in the Schrodinger equation, get an \( NxN \) matrix and solve it (just as we did in the case of molecules). But one can do better ...........

We know from Bloch's theorem that the solution must satisfy the following:

\[ |\psi(\vec{r} + \vec{R})|^2 = |\psi(\vec{r})|^2 \]

\[ \psi(\vec{r} + \vec{R}) = e^{i \kappa \cdot \vec{R}} \psi(\vec{r}) \]
Tight-Binding Bandstructure

Consideration 1:
For the solution: \( \psi(\tilde{r}) = \sum_{m} c_m \phi_s(\tilde{r} - \tilde{R}_m) \)
to satisfy:
\[ |\psi(\tilde{r} + \tilde{R})|^2 = |\psi(\tilde{r})|^2 \]
one must have the same value of \( |c_m|^2 \) for all \( m \) (i.e. all coefficients must have the same weight).

So we can write without loosing generality: \( c_m = \frac{e^{i \theta_m}}{\sqrt{N}} \)  \[ \int |\psi(\tilde{r})|^2 d^3\tilde{r} = 1 \]

Consideration 2:
For the solution: \( \psi(\tilde{r}) = \sum_{m} \frac{e^{i \theta_m}}{\sqrt{N}} \phi_s(\tilde{r} - \tilde{R}_m) \)
to satisfy:
\[ \psi(\tilde{r} + \tilde{R}) = e^{i \bar{k} \cdot \tilde{R}} \psi(\tilde{r}) \]
one must have the phase value equal to: \( \theta_m = \bar{k} \cdot \tilde{R}_m \)
Tight-Binding Bandstructure

Consideration 2 (contd...):

Proof:

\[ \psi(\vec{r}) = \sum_m e^{i \theta_m} \frac{1}{\sqrt{N}} \phi_s(\vec{r} - \vec{R}_m) = \sum_m e^{i \vec{k} \cdot \vec{R}_m} \frac{1}{\sqrt{N}} \phi_s(\vec{r} - \vec{R}_m) \]

For the Bloch condition we get:

\[ \psi(\vec{r} + \vec{R}) = \sum_m e^{i \vec{k} \cdot \vec{R}_m} \frac{1}{\sqrt{N}} \phi_s(\vec{r} + \vec{R} - \vec{R}_m) = \sum_m e^{i \vec{k} \cdot \vec{R}_m} \frac{1}{\sqrt{N}} \phi_s(\vec{r} - (\vec{R}_m - \vec{R})) \]

Let:

\[ \vec{R}_m - \vec{R} = \vec{R}_p \]

\[ \Rightarrow \psi(\vec{r} + \vec{R}) = \sum_p e^{i \vec{k} \cdot (\vec{R}_p + \vec{R})} \frac{1}{\sqrt{N}} \phi_s(\vec{r} - \vec{R}_p) = e^{i \vec{k} \cdot \vec{R}} \sum_p e^{i \vec{k} \cdot \vec{R}_p} \frac{1}{\sqrt{N}} \phi_s(\vec{r} - \vec{R}_p) \]

\[ = e^{i \vec{k} \cdot \vec{R}} \psi(\vec{r}) \]
Tight Binding Bandstructure

Tight Binding Approach for a 1D Crystal

\[ \psi_k(\mathbf{r}) = \sum_m \frac{e^{i \mathbf{k} \cdot \mathbf{R}_m}}{\sqrt{N}} \phi_s(\mathbf{r} - \mathbf{R}_m) \]

And we know that it is a Bloch function because:

\[ \psi_k(\mathbf{r} + \mathbf{R}) = e^{i \mathbf{k} \cdot \mathbf{R}} \psi_k(\mathbf{r}) \]

All that remains to be found is the energy of this solution – so we plug it into the Schrodinger equation:

\[ \hat{H} \psi_k(\mathbf{r}) = E(\mathbf{k}) \psi_k(\mathbf{r}) \]

\[ \Rightarrow \sum_m \frac{e^{i \mathbf{k} \cdot \mathbf{R}_m}}{\sqrt{N}} \hat{H} \phi_s(\mathbf{r} - \mathbf{R}_m) = E(\mathbf{k}) \sum_m \frac{e^{i \mathbf{k} \cdot \mathbf{R}_m}}{\sqrt{N}} \phi_s(\mathbf{r} - \mathbf{R}_m) \]
Tight-Binding Bandstructure

\[
\Rightarrow \sum_m \frac{e^{i \mathbf{k} \cdot \mathbf{R}_m}}{\sqrt{N}} \hat{H} \left| \phi_s (\mathbf{r} - \mathbf{R}_m) \right\rangle = E(\mathbf{k}) \sum_m \frac{e^{i \mathbf{k} \cdot \mathbf{R}_m}}{\sqrt{N}} \left| \phi_s (\mathbf{r} - \mathbf{R}_m) \right\rangle
\]

Multiply this equation with \( \langle \phi_s (\mathbf{r}) \rangle \) and:
- keep the energy matrix elements for orbitals that are nearest neighbors and
- assume that the orbitals on different atoms are orthogonal

\[
\frac{e^{i \mathbf{k} \cdot \mathbf{R}_1}}{\sqrt{N}} \langle \phi_s (\mathbf{r}) \rangle \hat{H} \left| \phi_s (\mathbf{r} - \mathbf{R}_1) \right\rangle + \frac{1}{\sqrt{N}} \langle \phi_s (\mathbf{r}) \rangle \hat{H} \left| \phi_s (\mathbf{r}) \right\rangle + \frac{e^{i \mathbf{k} \cdot \mathbf{R}_{-1}}}{\sqrt{N}} \langle \phi_s (\mathbf{r}) \rangle \hat{H} \left| \phi_s (\mathbf{r} - \mathbf{R}_{-1}) \right\rangle
\]

\[
= E(\mathbf{k}) \frac{1}{\sqrt{N}} \langle \phi_s (\mathbf{r}) \rangle \phi_s (\mathbf{r})
\]

\[
\Rightarrow -V_{ss\sigma} \frac{e^{i \mathbf{k} \cdot \mathbf{a}_1}}{\sqrt{N}} + \frac{1}{\sqrt{N}} E_s - \frac{e^{-i \mathbf{k} \cdot \mathbf{a}_1}}{\sqrt{N}} V_{ss\sigma} = E(\mathbf{k}) \frac{1}{\sqrt{N}}
\]

\[
\Rightarrow E(\mathbf{k}) = E_s - 2V_{ss\sigma} \cos (\mathbf{k} \cdot \mathbf{a}_1)
\]
Tight-Binding Bandstructure

\[ E(k) = E_s - 2V_{ss\sigma} \cos(k \cdot \vec{a}_1) \]

Energy levels in an isolated atom

Energy levels in a crystal
Tight-Binding Bandstructure

Tight Binding Approach for a 1D Crystal

\[ E(\vec{k}) = E_s - 2V_{ss}\sigma \cos(\vec{k} \cdot \vec{a}_1) \]

- Number of quantum states at the starting point = 2 x number of orbitals used in the LCAO solution = 2N
- Number of quantum states at the ending point = 2 x energy levels per band for an N atom crystal = 2N
  ⇒ Initial number of quantum states = Final number of quantum states

\[ N : E_s \]

A band of N energy levels
2N quantum states
Atomic Orbitals and their Overlaps

- Wavefunction amplitudes of the atomic s and p orbitals in the angular directions are plotted.
- The s-orbital is spherically symmetric.
- The p-orbitals have +ve and -ve lobes and are oriented along x-axis, y-axis, and z-axis.

\[ p_z \quad p_x \quad p_y \]
Atomic Orbitals and their Overlaps

Orbitals and Bonding

There are two main types of co-valent bonds: sigma bonds (or $\sigma$-bonds) and pi-bonds (or $\pi$-bonds)

1. Sigma bonds (or $\sigma$-bonds):
   - s-s $\sigma$-bond
     (Example: Hydrogen molecule, semiconductors)
     $$\langle \phi_s(\vec{r} - \vec{r}_1) | \hat{H} | \phi_s(\vec{r} - \vec{r}_2) \rangle \approx -V_{ss\sigma}$$
   - p-p $\sigma$-bond
     (Example: Semiconductors)
     $$\langle \phi_p(\vec{r} - \vec{r}_1) | \hat{H} | \phi_p(\vec{r} - \vec{r}_2) \rangle \approx V_{pp\sigma}$$
   - s-p $\sigma$-bond
     (Example: Semiconductors)
     $$\langle \phi_p(\vec{r} - \vec{r}_1) | \hat{H} | \phi_s(\vec{r} - \vec{r}_2) \rangle \approx -V_{sp\sigma}$$
   - s-p $\sigma$-bond
     (Example: Semiconductors)
     $$\langle \phi_p(\vec{r} - \vec{r}_1) | \hat{H} | \phi_s(\vec{r} - \vec{r}_2) \rangle \approx V_{sp\sigma}$$
Atomic Orbitals and their Overlaps

Orbitals and Bonding

What about this situation?

\[ \langle \phi_p (\vec{r} - \vec{r}_1) | \hat{H} | \phi_s (\vec{r} - \vec{r}_2) \rangle \approx 0 \]

The Hamiltonian is up-down symmetric
The s-orbital is up-down symmetric
The p-orbital is up-down anti-symmetric
\[ \Rightarrow \text{The matrix element is zero! No bonding possible} \]

What about this situation? What should be the matrix element?

\[ \langle \phi_p (\vec{r} - \vec{r}_1) | \hat{H} | \phi_s (\vec{r} - \vec{r}_2) \rangle \approx 0 \cdot \sin(\theta) + (-V_{sp\sigma}) \cdot \cos(\theta) \]

\[ = -V_{sp\sigma} \cos(\theta) \]
Atomic Orbitals and their Overlaps

Orbitals and Bonding

(2) Pi bonds (or \( \pi \)-bonds):

\[
\text{p-p } \pi \text{-bond}
\]

(Example: graphene, carbon nanotubes, conjugated conducting molecules)

\[
\langle \phi_p(\vec{r} - \vec{r}_1) | \hat{H} | \phi_p(\vec{r} - \vec{r}_2) \rangle \approx -V_{pp\pi}
\]

What about this situation? What should be the matrix element?

\[
\langle \phi_p(\vec{r} - \vec{r}_1) | \hat{H} | \phi_p(\vec{r} - \vec{r}_2) \rangle \approx (-V_{pp\pi}) \cdot \sin(\theta) + 0 \cdot \cos(\theta)
\]

\[
= -V_{pp\pi} \sin(\theta)
\]
Tight-Binding Bandstructure

LCAO – Tight Binding

\[ E(\vec{k}) = E_s - 2V_{ss\sigma} \cos(\vec{k} \cdot \vec{a}_1) \]

Energy

Would have also obtained the higher energy bands in LCAO if higher energy atomic orbitals were also included in the LCAO solution

Nearly Free Electron Approach (NFEA)

Energy

The energy matrix elements are of the order of:

\[ V_{ss\sigma} \sim \frac{\hbar^2}{2ma^2} \]

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Debdeep Jena (djena@cornell.edu)
Example: A 1D Crystal with 2 Orbitals per Primitive Cell

Each atom now has a s-orbital and a p-orbital that contributes to energy band formation:

\[ \phi_s(\vec{r}) \rightarrow E_s \]
\[ \phi_p(\vec{r}) \rightarrow E_p \]

We write the solution in the form:

\[ \psi_k(\vec{r}) = \sum_m \frac{e^{i \vec{k} \cdot \vec{R}_m}}{\sqrt{N}} [c_s(\vec{k})\phi_s(\vec{r} - \vec{R}_m) + c_p(\vec{k})\phi_p(\vec{r} - \vec{R}_m)] \]

Verify that it satisfies:

\[ \psi_k(\vec{r} + \vec{R}) = e^{i \vec{k} \cdot \vec{R}} \psi_k(\vec{r}) \]

And plug it into the Schrodinger equation:

\[ \hat{H} |\psi_k(\vec{r})\rangle = E(\vec{k}) |\psi_k(\vec{r})\rangle \]
Tight-Binding Bandstructure

Tight Binding Approach for a 1D Crystal

\[ \hat{H} \psi_\bar{k}(\bar{r}) = E(\bar{k}) \psi_\bar{k}(\bar{r}) \]

\[ \bar{R}_m = m \bar{a}_1 \]

Step 1:
Multiply the equation with \( \langle \phi_s(\bar{r}) \rangle \) and:
- keep the energy matrix elements for orbitals that are nearest neighbors and
- assume that the orbitals on different atoms are orthogonal

\[
\left[ E_s - 2V_{ss\sigma} \cos(\bar{k} \cdot \bar{a}_1) \right] c_s(\bar{k}) + 2i V_{sp\sigma} \sin(\bar{k} \cdot \bar{a}_1) c_p(\bar{k}) = E(\bar{k}) c_s(\bar{k})
\]

Step 2:
Multiply the equation with \( \langle \phi_p(\bar{r}) \rangle \) and:
- keep the energy matrix elements for orbitals that are nearest neighbors and
- assume that the orbitals on different atoms are orthogonal

\[
\left[ E_p + 2V_{pp\sigma} \cos(\bar{k} \cdot \bar{a}_1) \right] c_p(\bar{k}) - 2i V_{sp\sigma} \sin(\bar{k} \cdot \bar{a}_1) c_s(\bar{k}) = E(\bar{k}) c_p(\bar{k})
\]
Tight-Binding Bandstructure

Tight Binding Approach for a 1D Crystal

We can write the two equations in matrix form:

\[
\begin{bmatrix}
E_s - 2V_{ss\sigma} \cos(\vec{k} \cdot \vec{a}_1) & 2i V_{sp\sigma} \sin(\vec{k} \cdot \vec{a}_1) \\
-2i V_{sp\sigma} \sin(\vec{k} \cdot \vec{a}_1) & E_p + 2V_{pp\sigma} \cos(\vec{k} \cdot \vec{a}_1)
\end{bmatrix}
\begin{bmatrix}
c_s(\vec{k}) \\
c_p(\vec{k})
\end{bmatrix} = E(\vec{k})
\begin{bmatrix}
c_s(\vec{k}) \\
c_p(\vec{k})
\end{bmatrix}
\]

For each value of wavevector one obtains two eigenvalues – corresponding to two energy bands.

For \( \vec{k} = 0 \) we get:

\[
E(\vec{k} = 0) = E_p + 2V_{pp\sigma}
\]

\[
\begin{bmatrix}
c_s(\vec{k} = 0) \\
c_p(\vec{k} = 0)
\end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}
\]

\[
E(\vec{k} = 0) = E_s - 2V_{ss\sigma}
\]

\[
\begin{bmatrix}
c_s(\vec{k} = 0) \\
c_p(\vec{k} = 0)
\end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}
\]

Bloch function is made of only p-orbitals

Bloch function is made of only s-orbitals

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Tight-Binding Bandstructure

For $\vec{k} = \frac{\pi}{2a} \hat{x}$ we get:

$$E\left(\vec{k} = \frac{\pi}{2a} \hat{x}\right) = ?$$

$$\begin{bmatrix} c_s \left( \vec{k} = \frac{\pi}{2a} \hat{x} \right) \\ c_p \left( \vec{k} = \frac{\pi}{2a} \hat{x} \right) \end{bmatrix} = \begin{bmatrix} ? \\ ? \end{bmatrix}$$

Bloch function is made of both s- and p-orbitals

$$E \left( k = \frac{\pi}{2a} \right) = ?$$

$$\begin{bmatrix} c_s \left( \vec{k} = \frac{\pi}{2a} \hat{x} \right) \\ c_p \left( \vec{k} = \frac{\pi}{2a} \hat{x} \right) \end{bmatrix} = \begin{bmatrix} ? \\ ? \end{bmatrix}$$

Bloch function is made of both s- and p-orbitals
Debdeep Jena (djena@cornell.edu)

Tight-Binding Bandstructure
A Simple Example: 2D Graphene and Boron Nitride

**Sigma-orbitals** hold the atoms together. (3 electrons/carbon atom, one left over)

**Pi-orbitals** are responsible for conduction. (1 electron/carbon atom)

\[
a_{cc} = 1.24 \text{ Angstrom} \\
a = \sqrt{3}a_{cc} = 2.15 \text{ Angstrom} \quad \text{(lattice constant)}
\]

- Sp\(^2\) hybridization
- Orbital figs from Pulfrey

Hopping energy: \(\gamma_0 \approx 3 \text{ eV}\)

- Real-space picture
- Sigma-orbital
- Pi-orbital

Debdeep Jena (djena@cornell.edu)
A Simple Example: 2D Graphene and Boron Nitride

Find the real space lattice vectors

\[ \mathbf{a}_1 = \left( \frac{\sqrt{3}}{2}, \frac{3}{2} \right) \quad \mathbf{a}_2 = \left( -\frac{\sqrt{3}}{2}, \frac{3}{2} \right) \]

Write down the tight-binding Hamiltonian Matrix

\[ \mathcal{H} = \begin{pmatrix} \epsilon_B & h(k) \\ h(k)^* & \epsilon_N \end{pmatrix} \]

hopping energy to each neighbor with phase factor

\[ h(k) = -t \left[ 1 + e^{i\mathbf{k} \cdot \mathbf{a}_1} + e^{i\mathbf{k} \cdot \mathbf{a}_2} \right] \]

on-site energies of each atom in basis

Find the eigenvalues of the Hamiltonian to get the bandstructure

\[ \mathcal{E}_\pm(k_x, k_y) = A \pm \sqrt{B^2 + t^2 \left[ 1 + 4 \cos(3k_x a/2) \cos(\sqrt{3}k_y a/2) + 4 \cos^2(\sqrt{3}k_y a/2) \right]} \]

\[ A = (\epsilon_B + \epsilon_N)/2 \quad B = (\epsilon_B - \epsilon_N)/2 \]
A Simple Example: 2D Graphene and Boron Nitride

- Find the real space lattice vectors
  - $a_1 = (\frac{\sqrt{3}}{2}, \frac{3}{2})$
  - $a_2 = (-\frac{\sqrt{3}}{2}, \frac{3}{2})$

- Write down the tight-binding Hamiltonian Matrix
  - $\mathcal{H} = \begin{pmatrix} \epsilon_B & h(k) \\ h(k)^* & \epsilon_N \end{pmatrix}$

- hopping energy to each neighbor with phase factor
  - $h(k) = -t \left[ 1 + e^{i k \cdot a_1} + e^{i k \cdot a_2} \right]$

- on-site energies of each atom in basis

- Find the eigenvalues of the Hamiltonian to get the bandstructure
  - $\mathcal{E}_\pm(k_x, k_y) = A \pm \sqrt{B^2 + t^2 \left[ 1 + 4 \cos(3k_x a/2) \cos(\sqrt{3}k_y a/2) + 4 \cos^2(\sqrt{3}k_y a/2) \right]}$

- $A = (\epsilon_B + \epsilon_N)/2$
- $B = (\epsilon_B - \epsilon_N)/2$

Debdeep Jena (djena@cornell.edu)
A Simple Example: 2D Graphene and Boron Nitride

Find the eigenvalues of the Hamiltonian to get the band structure

$$\mathcal{E}_\pm(k_x, k_y) = A \pm \sqrt{B^2 + t^2 \left[1 + 4 \cos(3k_x a/2) \cos(\sqrt{3}k_y a/2) + 4 \cos^2(\sqrt{3}k_y a/2)\right]}$$

$$A = (\epsilon_B + \epsilon_N)/2 \quad B = (\epsilon_B - \epsilon_N)/2$$

$$E_g = \mathcal{E}_+ - \mathcal{E}_- = 2B = 5.8 \text{ eV}$$

$$\epsilon_B \sim +2.9 \text{ eV}, \quad \epsilon_N \sim -2.9 \text{ eV}$$

$$E_g = 5.8 \text{ eV}, \quad t = 2.92 \text{ eV}, \quad a \sim 0.15 \text{ nm}$$

Find the conduction and valence band structures and effective masses

$$\mathcal{E}_c(k) = E_g + \frac{\hbar^2 k^2}{2m^*}, \quad \text{(conduction band)}$$

$$\mathcal{E}_v(k) = -\frac{\hbar^2 k^2}{2m^*}, \quad \text{(valence band)}$$

$$m^* = \frac{2\hbar^2 E_g}{9a^2 t^2} \sim 0.6m_0$$
A Simple Example: 2D Graphene Bonds and Bands

For 2D Graphene, because the on-site energies are the SAME, the gap is ZERO!

BN is the compound semiconductor counterpart of Graphene; the broken symmetry opens a very large bandgap.

\[ E(k_x, k_y) = \mathcal{E}_F \pm \gamma_0 \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)} \]

\[ \gamma_0 \approx 3 \text{ eV} \]

\[ E(k_x, k_y) \approx \hbar v_F \sqrt{k_x^2 + k_y^2} \]

\[ v_F \sim 10^8 \text{ cm/s} \]

\[ g_{\text{spin}} = 2 \]

\[ g_{\text{valley}} = 2 \]

\[ \text{Conical! Linear dispersion} \]

• Expand around the Dirac point

• Reviews of Modern Physics, 79 677 (2007).
A Simple Example: 2D Graphene Bonds and Bands

\[ E(k_x, k_y) = E_F \pm \gamma_0 \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)} \]
A Simple Example: 2D Graphene Bonds and Bands

\[ E(k_x, k_y) = E_F \pm \gamma_0 \sqrt{1 + 4 \cos\left(\frac{\sqrt{3} k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)} \]
Comparison of NFE, Tight-Binding, and True Bands

Fig. 2.25. A comparison between the band structure of Ge calculated by (a) the tight-binding method, (b) the empirical pseudopotential method, and (c) the nearly free electron model [Ref. 2.24, p. 79]

From Cardona and Yu

The Tight-Binding (or LCAO) Matrix for FCC Crystals

\[
H = \begin{pmatrix}
\epsilon_{00} & 0 & 0 & 0 & -v_{\text{m}} a_v(k) & v_{\text{m}} a_v(k) & v_{\text{m}} a_v(k) \\
0 & \epsilon_{00} & 0 & 0 & -v_{\text{m}} a_v(k) & v_{\text{m}} a_v(k) & v_{\text{m}} a_v(k) \\
0 & 0 & \epsilon_{00} & 0 & v_{\text{m}} a_v(k) & v_{\text{m}} a_v(k) & v_{\text{m}} a_v(k) \\
0 & 0 & 0 & \epsilon_{00} & v_{\text{m}} a_v(k) & v_{\text{m}} a_v(k) & v_{\text{m}} a_v(k) \\
\end{pmatrix}
\]

\[
\begin{align*}
\epsilon_{00} &= 0 \\
\epsilon_{00} &= 0 \\
\epsilon_{00} &= 0 \\
\epsilon_{00} &= 0 \\
\end{align*}
\]

Hermitean

\[
\begin{align*}
v_1 &= \frac{1}{3} v_{\text{m}} a_v - \frac{2}{3} v_{\text{m}} a_v \\
v_2 &= \frac{1}{3} v_{\text{m}} a_v + \frac{2}{3} v_{\text{m}} a_v \\
\end{align*}
\]
Atoms to Crystals

Quantum Mechanics

Atoms

\[ \begin{align*}
\epsilon_1 \\
\epsilon_2 \\
\epsilon_3
\end{align*} \]

Discrete Energy levels

Atoms in a periodic lattice
CRYSTAL

\[ \text{GAP (FORBIDDEN)} \]
\[ \text{ENERGY BAND} \]
\[ \text{BANDS} \]

Crystal

→

Bandstructure

Direct

Indirect

Conduction Electrons

\[ \text{UPPER VALLEY} \]
\[ \text{LOWER VALLEY} \]

Ge

Si

GOAS

Debdeep Jena (djena@cornell.edu)
Typical 3D semiconductor crystal structures

Due to the covalent bond structure (the bonding orbitals are s-p hybrids), most common semiconductors are found in three distinct structures:

i) The diamond lattice type: e.g. Si, Ge

ii) The zincblende type: e.g. GaAs, InP

iii) The wurtzite type (hexagonal): e.g. GaN, ZnO

Fig. 1.2 Diamond lattice structure.

(a)

(b)

Fig. 1.3 (a) Zincblende lattice structure and (b) Wurtzite lattice structure. (○) A atom, (●) B atom.

(Denninger, Oda)
Nearly free electron bandstructure, k-space points

![FCC Free Electron Energies](rockett.png)
Orbital overlaps and bonds in semiconductors

(a) \[ A_s^\pm \rightarrow B_s \] (b) \[ \sigma \text{(bonding)} \]

\[ \sigma \text{(antibonding)} \]

Fig. 2.17a,b. Overlap of two \( s \) orbitals to form bonding and antibonding \( \sigma \) orbitals

(a) \[ A_{p_x}^\pm \rightarrow B_{p_x} \] (b) \[ \sigma \text{(bonding)} \]

\[ \sigma \text{(antibonding)} \]

Fig. 2.18a,b. Overlap of two \( p_x \) orbitals along the \( x \) axis to form bonding and antibonding \( \sigma \) orbitals

(a) \[ A_{p_y}^\pm \rightarrow B_{p_y} \] (b) \[ \pi \text{(bonding)} \]

\[ \pi \text{(antibonding)} \]

Fig. 2.19a,b. Overlap of two \( p_y \) orbitals to form bonding and antibonding \( \pi \) orbitals

\[ V_{\sigma ss} \]

\[ V_{\sigma pp} \]

\[ V_{\pi pp} \]
Orbital overlaps and bonds in semiconductors

\[ \langle s | H | p_y \rangle = V_{sp\sigma} \cos \Theta + 0 \sin \Theta \]

\[ \langle p_y | H | p_y \rangle = V_{pp\sigma} \cos^2 \Theta + V_{pp\pi} \sin^2 \Theta \]
Tight-Binding Bandstructure Matrix

\[ a_1 = \frac{a}{4}(1,1,1), \quad a_2 = \frac{a}{4}(-1,-1,1), \quad a_3 = \frac{a}{4}(-1,1,-1), \quad a_4 = \frac{a}{4}(1,-1,-1) \]

\[ V_0 = V_{ss\sigma}, \quad V_1 = \frac{1}{\sqrt{3}}V_{sp\sigma}, \]
\[ V_2 = \frac{1}{3}V_{pp\sigma} - \frac{2}{3}V_{pp\pi}, \quad V_3 = \frac{1}{3}V_{pp\sigma} + \frac{1}{3}V_{pp\pi} \]

\[ g_0(k) = e^{i\mathbf{k} \cdot a_1} + e^{i\mathbf{k} \cdot a_2} + e^{i\mathbf{k} \cdot a_3} + e^{i\mathbf{k} \cdot a_4}, \]
\[ g_1(k) = e^{i\mathbf{k} \cdot a_1} - e^{i\mathbf{k} \cdot a_2} - e^{i\mathbf{k} \cdot a_3} + e^{i\mathbf{k} \cdot a_4}, \]
\[ g_2(k) = e^{i\mathbf{k} \cdot a_1} - e^{i\mathbf{k} \cdot a_2} + e^{i\mathbf{k} \cdot a_3} - e^{i\mathbf{k} \cdot a_4}, \]
\[ g_3(k) = e^{i\mathbf{k} \cdot a_1} + e^{i\mathbf{k} \cdot a_2} - e^{i\mathbf{k} \cdot a_3} - e^{i\mathbf{k} \cdot a_4} \]

\[
\begin{pmatrix}
|s^A\rangle & |p_{x}^A\rangle & |p_{y}^A\rangle & |p_{z}^A\rangle \\
\langle s^A| & E_s^A & 0 & 0 & 0 & -V_0 g_0(k) & V_1 g_1(k) & V_1 g_2(k) & V_1 g_3(k) \\
\langle p_{x}^A| & 0 & E_p^A & 0 & 0 & -V_1 g_1(k) & V_2 g_0(k) & V_3 g_3(k) & V_3 g_2(k) \\
\langle p_{y}^A| & 0 & 0 & E_p^A & 0 & -V_1 g_2(k) & V_3 g_3(k) & V_2 g_0(k) & V_3 g_1(k) \\
\langle p_{z}^A| & 0 & 0 & 0 & E_p^A & -V_1 g_3(k) & V_3 g_2(k) & V_3 g_1(k) & V_2 g_0(k) \\
\langle s^B| & c.c. & c.c. & c.c. & c.c. & E_s^B & 0 & 0 & 0 \\
\langle p_{x}^B| & c.c. & c.c. & c.c. & c.c. & 0 & E_p^B & 0 & 0 \\
\langle p_{y}^B| & c.c. & c.c. & c.c. & c.c. & 0 & 0 & E_p^B & 0 \\
\langle p_{z}^B| & c.c. & c.c. & c.c. & c.c. & 0 & 0 & 0 & E_p^B \\
\end{pmatrix}
\]
Tight-Binding Bandstructure

Solid State Table of the Elements

Transition Metals → Covalent Solids → Nonmetals

ECE 4070 / MSE 6050
The Solid-State Table for Elements.
Provides the tight-binding parameters for chemical bonds.

From Harrison
Origin of s and p ‘contents’ in semiconductor bandstructure
Semiconductor Bandstructures

Parameter values for GaAs:

\[ E_{SG} = -11.37 \text{ eV} \]
\[ E_{PG} = -4.90 \text{ eV} \]
\[ V_{ss\sigma} = 1.70 \text{ eV} \]
\[ V_{sp\sigma} = 2.15 \text{ eV} \]
\[ E_{SA} = -17.33 \text{ eV} \]
\[ E_{PA} = -7.91 \text{ eV} \]
\[ V_{pp\sigma} = 3.44 \text{ eV} \]
\[ V_{pp\pi} = 0.89 \text{ eV} \]
Tight Binding Solution for GaAs: States at the Γ-Point

At the Γ-point:

\[ g_0(\vec{k} = 0) = 4 \]
\[ g_1(\vec{k}) = g_2(\vec{k}) = g_3(\vec{k}) = 0 \]

⇒ Energy eigenvalues can be found analytically

Two of the eigenvalues at the Γ-point are:

\[ E_{5,1}(\vec{k} = 0) = \left( \frac{E_{SG} + E_{SA}}{2} \right) \pm \sqrt{\left( \frac{E_{SG} - E_{SGA}}{2} \right)^2 + (4V_{ss\sigma})^2} \]

The Bloch function of the lowest energy band and of the conduction band at Γ-point are made up of ONLY s-orbitals from the Ga and As atoms

\[ \psi_{c,\vec{k}=0}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_m \left[ c_1 | \phi_1(\vec{r} - \vec{R}_m) \rangle + c_5 | \phi_5(\vec{r} - \vec{R}_m - \vec{d}_2) \rangle \right] \]
Tight Binding Solution for GaAs: States at the $\Gamma$-Point

Six remaining eigenvalues at the $\Gamma$-point are:

$$E_{234}^{678}(\vec{k} = 0) = \left( \frac{E_{PG} + E_{PA}}{2} \right) \pm \sqrt{\left( \frac{E_{PG} - E_{PA}}{2} \right)^2 + (4V_1)^2}$$

Each eigenvalue above is triply degenerate

The Bloch function of the highest three energy bands and of the three valence bands at $\Gamma$-point are made up of ONLY p-orbitals from the Ga and As atoms

$$\psi_{v,k=0}(\vec{r}) = \sum_{m}^{8} \left[ \frac{1}{\sqrt{N}} \sum_{j=2}^{4} c_j \phi_j(\vec{r} - \vec{R}_m) + \sum_{j=6}^{8} c_j \phi_j(\vec{r} - \vec{R}_m - \vec{d}_2) \right]$$
Semiconductor Bandstructures

$$\psi_s = \frac{2a_0^{-3/2}}{\sqrt{\pi}} (1 - \frac{r}{2a_0}) e^{-r/2a_0}$$

$$\psi_{px} = \frac{2a_0^{-3/2}}{\sqrt{\pi/3}} (1 - \frac{r}{2a_0}) e^{-r/2a_0} \cos \theta$$

Figure 5.1: Shows the shape of the s and p_x orbitals and the equations that describe them. $a_0$ is the atomic orbital size, $r$ is the radius from the nucleus, and $\theta$ is the angle in the x,y plane.

Wave function amplitudes (probability of finding an electron).

Figure 5.2: Shows the symmetry of the hybridized sp^3 and sp^2 molecular orbitals. The sp^2 orbitals lie in a plane perpendicular to the p_z orbitals and are equal lengths. The sp^3 orbitals are all equivalent to each other and stretch to corners of a tetrahedron.

$V_2 \approx 4.4 \frac{\hbar^2}{md^2} \text{eV}$

Figure 5.3: A schematic diagram illustrating the basis of cohesion in solids resulting from symmetric and antisymmetric combinations of atomic orbitals. The center of electron charge lies between the positive ions for a symmetric bonding orbital and outside of the positive ions for an antisymmetric orbital combination.

Origin of s and p ‘contents’ in semiconductor bandstructure

Debdeep Jena (djena@cornell.edu)
Semiconductor Bandstructures

**Figure 5.4:** A schematic diagram of the evolution of bonding of Si atoms. The filled 3s and partially filled 3p atomic orbitals of two atoms combine to form half-filled sp$^3$ hybrid molecular orbitals. These combine to form bonding and antibonding orbitals. As more atoms collect atoms collect to create a bulk solid, bands form.

**Figure 5.5:** Shows the evolution of atomic orbital energies to form bonds and ultimately bands. The geometries of the atomic and hybrid orbitals are shown schematically as insets.

(Rockett)
Chemical bonding, Lattice Constants, Band edges, and Band Gaps for various Semiconductors

(Rockett)
Semiconductor Bandstructures

Bandstructures of Elemental and Compound Semiconductors

Debdeep Jena (djena@cornell.edu)
Semiconductor Bandstructures

Fig. 2.25. A comparison between the band structure of Ge calculated by (a) the tight-binding method, (b) the empirical pseudopotential method, and (c) the nearly free electron model [Ref. 2.24, p. 79]

Bandstructures and Density of States
Debdeep Jena (djena@cornell.edu)
Electron clouds in semiconductors

Electron wavefunction squared = probability density of finding electrons

(Rockett)
Measurement of Semiconductor Bandstructures

Angle-Resolved Photo-Emission Spectroscopy (ARPES)

Debdeep Jena (djena@cornell.edu)
Semiconductor Bandstructures

Free electron vs. real bandstructure

FIGURE 2.15. (a) Brillouin zone for a face-centred cubic crystal, showing the notation for special points and directions. Solid lines are on the surface with broken lines inside the zone. (b) Band structure in the free-electron model, showing the effect of folding back the parabola into the reduced zone.

FIGURE 2.16. Band structure of four common semiconductors: silicon, germanium, gallium arsenide, and aluminium arsenide. The calculations do not include the spin-orbit coupling. [Results kindly supplied by Prof. G. P. Srivastava, University of Exeter.]
Tight-Binding Bandstructure

Energy Bands of Si, Ge, and GaAs for Reference

ECE 4070 / MSE 6050
Energy Bandstructures of the most common Semiconductors
Semiconductor electronics requires for its foundation primarily wave mechanics and statistics. However, crystallography, thermodynamics, and chemistry also have a share in it and, quite generally, “it is incredible what miserable quantities of thought and mathematics are needed to provide even the simplest tools for daily use in semiconductor physics” (from a conversation of W. Schottky with the author).

**ECE 4070 / MSE 6050**

- If you are finding the course tough at this point, you are in hallowed company.

- That is the nature of the subject - solve problems and think about them (do not let go), you will learn it.

- We have developed a rich range of powerful tools, but the only way to learn their power is to apply them.

- The transition from “no idea” to “completely understand” is very quick in this subject (if you put in the effort) - I am here to help.
Prelim 2 for ECE 4070 / MSE 6050

• Thursday April 11th 2019
• Time: 7:30 – 9:00 pm
• In Phillips Hall 219 (Note: different from class location!)

• No restrictions on books/notes/calculators/computers etc.
• Bring pen/pencil – exam books will be provided.
• The questions will be conceptual, no heavy number crunching will be needed.
• Questions from previous years are fairly representative of what to expect.
• Topics: Chapters 1-9 from the Notes, and suggested Slides.

Exams and Grades:
An assignment every 1.5 weeks. Total of 6-8 homework assignments per semester. Exams: 2 Evening Prelim Exams and 1 Final Exam. Here is the approximate breakup of scores that will go towards your final grade:

35% Assignments
15% Prelim 1 [Tuesday March 5th, 2019]
20% Prelim 2 [Thursday April 11th, 2019]
30% Final [Wednesday May 15th, 2019]
Periodic Table of Elements

Some common Semiconductor Families:
- Group IV: Diamond, Silicon, Ge, ...
- Group III-V: GaAs, InP, InSb, GaN, ...
- Group II-VI: ZnO, MgO, CdSe, HgTe...
- 2D Materials: Graphene, MoS$_2$, GaSe, ...

ECE 4070 / MSE 6050
Fig. 7.6. Bandgap energy and lattice constant of various III-V semiconductors at room temperature (adopted from Tien, 1988).

**ECE 4070 / MSE 6050**

- A wide variety of bandgaps and lattice constant semiconductors are available.
Tight-Binding Bandstructure

Fig. 12.12. Bandgap energy versus lattice constant of III-V nitride semiconductors at room temperature.

**Major HFET families:**

- **GaAs-based** (Al/GaAs/GaAs) (strain-free, or pseudomorphic)
- **InP based** (InGaAs channels)
- 6.1 Angstrom/narrow gap channels (generally grown metamorphically on GaAs)
- **GaN-based** (Al/GaN/GaN and AlN/GaN) (typically pseudomorphic)

ECE 4070 / MSE 6050

- Semiconductors can be grown on top of each other.
Compound Semiconductor Heterostructures: Strain

Lattice-Matching, Strain

\[ \epsilon = \frac{a_S - a_L}{a_L} \]

\[ d_c \approx \frac{a_S}{2|\epsilon|} \]

Critical thickness for coherent strained growth

Figure 1.16: (a) The conceptual exercise in which an overlayer with one lattice constant is placed without distortion on a substrate with a different lattice constant. (b) Dislocations are generated at positions where the interface bonding is lost. (c) The case is shown where the overlayer is distorted so that no dislocation is generated.

Example: AlN on GaN, \(d_c \approx 7\) nm

APPLIED PHYSICS LETTERS 90, 182112 (2007)
Compound semiconductors: Heterostructures

*Semiconductor Heterostructures*

Semiconductor bands line up with each other in 3 ways.

Based on the lineups, one can create
- Barriers
- Wells
- Quasi-Electric fields

For both electrons and holes independently with suitable material choices.
Compound semiconductor heterostructure band offsets

\[ \Delta E_V (A : B) + \Delta E_V (B : C) + \Delta E_V (C : A) = 0. \]

Transitivity of band offsets

**The Common Anion Rule:** When the anion (the electron accepting atom such as As in GaAs and InAs) is in common across a semiconductor heterojunction, the change in the conduction band edge is greater than the change in the valence band edge across the semiconductor heterojunction. Mathematically, \( \Delta E_V < \Delta E_C \).

**The Common Cation Rule:** When the cation (e.g. Ga in GaAs or GaSb) is in common across the junction, the valence band edge energies scale with the anion electronegativities. For example, the valence band edge of phosphide semiconductors will lie below those for arsenides which will lie below those of antimonides. Mathematically, \( E_V (CA_1) < E_V (CA_2) < E_V (CA_3) \), where \( C \) designates a cation, and \( A_1, A_2, \) and \( A_3 \) designate three anions with decreasing electronegativities.
Quasi electric fields in semiconductor heterostructures

Forces different for electrons and holes

Equal force on electrons and holes

FIG. 1. Quasielectric fields: (a) A true electric field simply tilts the bands; (b) quasielectric fields, with no force on electrons, but a force on holes; (c) quasielectric fields forcing electrons and holes in the same direction. From Kroemer, 1957a.
GaN based Visible LEDs and Lasers

The Nobel Prize in Physics 2014
Isamu Akasaki, Hiroshi Amano, Shuji Nakamura

Share this:  

The Nobel Prize in Physics 2014 was awarded jointly to Isamu Akasaki, Hiroshi Amano and Shuji Nakamura "for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources".

Debdeep Jena (djena@cornell.edu)
How to make a Semiconductor Light Emitter

Nobel Lecture: Background story of the invention of efficient blue InGaN light emitting diodes

Shuji Nakamura
University of California, Santa Barbara, California, USA
(published 5 October 2015)

FIG. 2 (color). (a) Image of a blue GaN LED with attached gold wire contacts (size of diode 0.4 × 0.4 mm²) and (b) the same LED packaged as a commercial product. From Nakamura, Mukai, and Senoh, 1994.
How to make white light with semiconductors

\[
\text{IQE} = \frac{\text{Light generated}}{\text{Electrons injected}} = \frac{R_{\text{radiative}}}{R_{\text{radiative}} + R_{\text{nonradiative}}} = \frac{Bn^2}{An + Bn^2 + Cn^3}.
\]
Solid state lighting: The lighting of the future

- White LED (R&D Demo, 2014)
- Fluorescent Compact Fluorescent
- Unfiltered Incandescent
- Thomas Edison's First Bulb
- Oil Lamp

Luminous Efficacy (lm/W)

Year


- GaAsP
- GaP:Zn,O
- GaAsP:N
- AlGaAs/GaAs
- AlGaInP/GaP
- InGaN (green)
- InGaN (blue)

MIS GaN LED Maruska et al.
$p$-$n$ Homojunction GaN LED Akasaki & Amano et al.
InGaN DH LED Nakamura et al.
Effect of Defects and Quantum Wells on Efficiency

Lasers outperform LEDs in efficiency!

FIG. 17 (color). Comparison of external quantum efficiency (EQE) of a commercial LED and laser with increasing current density. From Pourhashemi et al., 2013.
Lasers outperform LEDs in efficiency!
Nobel Lecture: Quasielectric fields and band offsets: teaching electrons new tricks*

Herbert Kroemer
Electrical and Computer Engineering Department, University of California, Santa Barbara, California 93106-9560
(Published 22 October 2001)

I. INTRODUCTION

Heterostructures, as I use the word here, may be defined as heterogeneous semiconductor structures built from two or more different semiconductors, in such a way that the transition region or interface between the different materials plays an essential role in any device action. Often, it may be said that the interface is the device.

The participating semiconductors all involve elements from the central portion of the periodic table of the elements (Table I). In the center is silicon, the backbone of modern electronics. Below Si is germanium. Although Ge is rarely used by itself, Ge-Si alloys with a composition-dependent position play an increasingly important role in today’s heterostructure technology. In fact, historically this was the first heterostructure device system proposed, although it was also the system that took longest to bring to practical maturity, largely because of the 4% mismatch between the lattice constants of Si and Ge.

Silicon plays the same central role in electronic metallurgy that steel plays in structural metallurgy. But just

Similar to the III-V compounds, every element shown in column II may be used together with every element in column VI to create II-VI compounds, and again alloying is possible to create a continuous range of the latter.

II. BAND DIAGRAMS AND QUASIELECTRIC FORCES

Whenever I teach my semiconductor device physics course, one of the central messages I try to get across early is the importance of energy-band diagrams. I often put this in the form of “Kroemer’s Lemma of Proven Ignorance”:

If, in discussing a semiconductor problem, you cannot draw an Energy-Band-Diagram, this shows that you don’t know what you are talking about,
with the corollary
If you can draw one, but don’t, then your audience won’t know what you are talking about.

Nowhere is this more true than in the discussion of heterostructures, and much of the understanding of the latter is based on one’s ability to draw their band diagrams—and knowing what they mean.

• Rev. Mod. Phys., vol 73, pg. 783 (2001)
Effective Mass Approximation

- Effective Mass Approximation MAPS the complicated problem of 
  Electrons in a complicated crystal + heterostructure potential … to … 
  the simplest of all quantum mech problems: The particle in a box

Motion of Electrons and Holes in Perturbed Periodic Fields

J. M. Luttinger* and W. Kohn†
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received October 13, 1954)

A new method of developing an “effective-mass” equation for electrons moving in a perturbed periodic structure is discussed. This method is particularly adapted to such problems as arise in connection with impurity states and cyclotron resonance in semiconductors such as Si and Ge. The resulting theory generalizes the usual effective-mass treatment to the case where a band minimum is not at the center of the Brillouin zone, and also to the case where the band is degenerate. The latter is particularly striking, the usual Wannier equation being replaced by a set of coupled differential equations.

- Developed by Luttinger & Kohn and refined since then…
- Real power of the EMA is exercised in understanding the electronic properties of Quantum Heterostructures.
Effective Mass Approximation

- Effective Mass Approximation MAPS the complicated problem of Electrons in a complicated crystal + heterostructure potential ... to ... the simplest of all quantum mech problems: The particle in a box

\[ \psi(x) = \sum_n \sum_k C(k) \phi_{nk}(x) = \sum_n \int \frac{dk}{2\pi} C(k) \phi_{nk}(x) \]

Wave packet

\[ \psi(x) \approx \phi_{n0}(x) \int \frac{dk}{2\pi} C(k) e^{ikx} = \underbrace{\phi_{n0}}_{\text{Bloch}} \cdot \underbrace{C(x)}_{\text{envelope}} \]
Effective Mass Approximation

\[ \psi(x) \approx \phi_{n0}(x) \int \frac{dk}{2\pi} C(k) e^{ikx} = \phi_{n0} \cdot \underbrace{C(x)}_{\text{Bloch \ envelope}} \]

\[ H_0 \psi(x) = \int \frac{dk}{2\pi} C(k) E_n(k) \phi_{nk}(x) \approx \phi_{n0}(x) \int \frac{dk}{2\pi} C(k) E_n(k) e^{ikx} \]

\[ E_n(k) = \sum a_m k^m \quad \text{Energy “operator”} \]

\[ H \psi(x) \approx \phi_{n0}(x) \sum_m \int \frac{dk}{2\pi} C(k) k^m e^{ikx} \]

\[ \int \frac{dk}{2\pi} k^m C(k)e^{ikx} \leftrightarrow (-i \frac{d}{dx})^m C(x) \]

\[ H \psi(x) \approx \phi_{n0}(x) E_n(-i \nabla) C(x) \]

\[ [E_n(-i\nabla) + V(r)] C(r) = EC(r) \]
Density of States

DOS:
\[ g(\mathcal{E}) = g_s \cdot \sum_{\mathbf{k}} \delta[\mathcal{E} - \mathcal{E}(\mathbf{k})] \]

Valid for electrons, photons, phonons...

Important result:
\[ \sum_{\mathbf{k}} (...) \rightarrow \int \frac{d^d\mathbf{k}}{(2\pi)^d} (...) \]

If we know the energy dispersion \( \mathcal{E}(\mathbf{k}) \), we can find the DOS using this prescription.

Free Electron: \( \mathcal{E}(\mathbf{k}) = \frac{\hbar^2|\mathbf{k}|^2}{2m_0} \)

Free electron in 3D: \( g(\mathcal{E}) = g_s \cdot \frac{1}{(2\pi)^2} \left( \frac{2m_0}{\hbar^2} \right)^{3/2} \sqrt{\mathcal{E}} \)
Effective Mass Approximation

Application: Bulk Semiconductors

- 3D (Bulk)

\[
\left[-\frac{\hbar^2}{2m^*} \nabla^2 + V_{\text{imp}}(r)\right]C(r) = [E - E_c(r)]C(r)
\]

\[
C(r) = \frac{1}{\sqrt{V}} e^{i \mathbf{k} \cdot \mathbf{r}}
\]

\[
E(k) = E_{c0}(r) + \frac{\hbar^2 k^2}{2m^*} = E_{c0}(r) + \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_{xx}^*} + \frac{k_y^2}{m_{yy}^*} + \frac{k_z^2}{m_{zz}^*} \right)
\]

\[
g_{3D}(E) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_{c0}}
\]

\[
n = \int_0^\infty dE f_{FD}(E) g_{3D}(E) = N^3 C F_{1/2} \left( \frac{E_C - E_F}{k_B T} \right) \approx N^3 C e^{-\frac{E_C - E_F}{k_B T}}
\]
Effective Mass Approximation

\[ E_n(k) \approx E_c(r) + \frac{\hbar^2 k^2}{2m^*} \rightarrow E_n(-i\nabla) \approx E_c(r) - \frac{\hbar^2}{2m^*} \nabla^2 \]

Central Result of Effective Mass Approximation

\[ \left[-\frac{\hbar^2}{2m^*} \nabla^2 + V_{\text{imp}}(r)\right]C(r) = \left[E - E_c(r)\right]C(r) \]

“Particle-in-a-box” problem with:
- Real mass -> Effective mass
- Real wavefunction -> Envelope function
- Crystal potential -> Band-edge potential + Impurity potentials, etc

Example: Shallow donor states

\[ E_n = -\frac{m_e q^4}{2(4\pi\varepsilon_0)^2 \hbar^2} \frac{1}{n^2} \]

\[ \left[-\frac{\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{4\pi\varepsilon r}\right]C(r) = (E - E_c)C(r) \]

\[ E - E_c = E_\infty \frac{m^*}{\varepsilon_r^2} \]

\[ a_B^* = a_B \frac{\varepsilon_r}{m^*} \]

\[ C(r) \sim e^{-r/r_0} \]
Semiconductor carrier statistics

Energy distribution of electrons:

\[ f(x) = \frac{1}{1 + \exp \left( \frac{x - \varepsilon_F}{kT} \right)} \]

\( \varepsilon_F \): Fermi energy

Electron density in the conduction band:

\[ n = \int_{E_c}^{\infty} dx \frac{\partial f(x)}{\partial \varepsilon} \]

\[ n = N_C F_\frac{1}{2} (\eta) \]

Effective DOS

\[ N_C = 2 \left( \frac{m^* kT}{2\pi} \right)^{3/2} \]

Fermi-Dirac integral

\[ F_\frac{1}{2}(\eta) = \frac{2}{\sqrt{\pi}} \int_{0}^{\eta} dx \frac{x^{1/2}}{1 + e^{x}} \]

\[ \eta = \frac{E_f - E_c}{kT} \]

For non-degenerate semiconductors, \( \eta \ll -1 \) ⇒ Boltzmann approximation

\[ \Rightarrow F_\frac{1}{2}(\eta) = e^\eta \Rightarrow n = N_C e^{\eta} \exp \left( \frac{E_f - E_c}{kT} \right) \]

Used very often!
Semiconductor carrier statistics

**Carrier Statistics**
(Electrons/Holes)

\[ p = N_v \exp \left( \frac{E_V - E_F}{kT} \right) \]

\[ \Rightarrow \quad n p = n_i^2 = \left( \sqrt{N_c N_v} \exp \left( -\frac{E_g}{2kT} \right) \right)^2 \]

**Semiconductor**

**Intrinsic Carrier Concentration.**

**Where is the Fermi Level** \( E_F \) **?**

**Basic Underlying Principle:** Charge Neutrality

**Will Determine the Fermi Level** \( E_F \) **- More Later.**

**Intrinsic Semiconductor:**

\[ n = p = n_i = \sqrt{N_c N_v} \exp \left( -\frac{E_g}{2kT} \right) \]

\[ E_F = E_i = E_C + E_V + \frac{kT}{2} \ln \left( \frac{N_v}{N_c} \right) \]

**Intrinsic** Fermi Level.
Semiconductor carrier statistics

\[ m_c^* \approx m_v^* = 0.05m_e, \quad E_g = 0.5 \text{ eV} \]

\[ m_c^* \approx m_v^* = 0.1m_e, \quad E_g = 1.0 \text{ eV} \]

\[ m_c^* \approx m_v^* = 0.2m_e, \quad E_g = 3.0 \text{ eV} \]
Semiconductor carrier statistics

**Fig. 14.3** Conduction band minima of Silicon showing the $\gamma$ valleys = 6 valleys along the six $\Gamma - X$ directions, and the origin of the DOS effective mass $(m_L m_T^2)^{\frac{1}{2}}$.

$$E_F = \frac{1}{2}(E_c + E_v) + k_b T \ln\left(\frac{n}{N_c} \cdot \frac{N_v}{p}\right)$$
Semiconductor carrier statistics

**Fig. 14.3** Conduction band minima of Silicon showing the $g_v = 6$ valleys along the six $\Gamma - X$ directions, and the origin of the DOS effective mass $\left( m_L m_T^* \right)^{\frac{1}{2}}$.

\[
E_F = \frac{1}{2} (E_c + E_v) + k_b T \ln \left( \frac{n}{N_c} \cdot \frac{N_v}{p} \right)
\]
Semiconductor doping

**Donor State**

**Acceptor State**

**DOPANT:** Atom that replaces an atom of the intrinsic semiconductor.

** DONOR:** Atom with an extra electron than the atom it replaces; the extra electron can be donated to the conduction band.

** ACCEPTOR:** Atom with one less electron than the atom it replaces; it can accept one electron from the valence band (same as forming a hole in VB).

\[
E_c = E_v + \frac{e^2}{2\epsilon r} < kT \quad \text{to be shallow}
\]

**Effective Bohr radius**

\[
a_B = \frac{\epsilon_0}{\epsilon} \frac{e^2}{\epsilon r} = 0.153 \text{Å, H-atom Bohr radius}
\]

**Typically:**

\[
a_B^+ \gg a_B^0
\]

**EXAMPLE:** $n$-doped semiconductor:

\[
r = p + N_d^+ \quad n_{\text{eq}} = \frac{\sqrt{(N_d^+)^2 + 4N_d^+ N_i}}{2}
\]

If $N_d^+ \gg N_i$, then $n_{\text{eq}} \approx N_d^+$ as many electrons in CB as # of donors.
Semiconductor carrier statistics

\[ \frac{N_D^+}{N_D} = \frac{1}{1 + 2 \cdot e^{\frac{E_F - E_d}{k_bT}}} \quad \frac{N_A^-}{N_A} = \frac{1}{1 + 2 \cdot e^{\frac{E_a - E_F}{k_bT}}} \]

\[ N_p F_{1/2} \left( \frac{E_F - E_F}{k_bT} \right) + \frac{N_D}{1 + 2 \cdot e^{\frac{E_F - E_d}{k_bT}}} = N_c F_{1/2} \left( \frac{E_c - E_F}{k_bT} \right) + \frac{N_A}{1 + 2 \cdot e^{\frac{E_a - E_F}{k_bT}}} \]
Semiconductor doping

**Carrier Statistics in Doped Semiconductors**

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)

- Donor ionization
  \[ N_d^+ = \frac{N_d}{1 + 2 e^{-\frac{(E_d - E_f)}{kT}}} \]

- Acceptor ionization
  \[ N_a^- = \frac{N_a}{1 + 2 e^{-\frac{(E_a - E_f)}{kT}}} \]

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Semiconductor carrier statistics

\[ N_D^+ = \frac{N_D}{1 + 2 \cdot e^{\frac{E_F - E_d}{k_b T}}}, \]

\[ N_A^- = \frac{N_A}{1 + 2 \cdot e^{\frac{E_a - E_F}{k_b T}}}, \]

\[ p = N_v F_\frac{1}{2}\left(\frac{E_v - E_F}{k_b T}\right), \]

\[ n = N_c F_\frac{3}{2}\left(\frac{E_F - E_c}{k_b T}\right), \]

\[ n_i \sim e^{-\frac{E_g}{2k_b T}}, \]

\[ N_D = 10^{15} / \text{cm}^3, \]

\[ N_D = 10^{14} / \text{cm}^3, \]
Graphical Solution for Locating the Fermi Level

Charge Neutrality: \[ n + N_A^- = p + N_D^+ \]

Solve to find the Fermi Level

Example for GaN \((N_A = 10^{18}/\text{cm}^3, \quad N_D = 10^{14}/\text{cm}^3)\)

Temperature dependence of mobile carrier density in doped Silicon
Semiconductor doping

**Controlling resistivity of semiconductors by doping**

**Various methods of “Doping”**

- **Traditional Bulk Semiconductors** -
  - Impurity doping (bulk, uniform)
  - Impurity doping (graded, delta-doping)
    (Since ’50s)

- **Impurity + Heterostructures** -
  - Modulation Doping
    (Since ’80s)

- **Polar Semiconductor Heterostructures** –
  - Polarization-induced doping
    (Since late ’90s)

- **Other “Dynamic” methods** –
  - Electrostatic gating
  - Optical excitation
  - Thermal excitation

*These are the various methods for Creating mobile carriers in the conduction & valence bands*
Fig. 14.7 Location of the Fermi level $E_F$ in Silicon and GaN as a function of temperature for various donor and acceptor doping densities.
Band Diagrams

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Fig. 14.13 Bandgaps vs lattice constants, and band alignments of 3D semiconductors.
Band Alignments: 2D semiconductors

Fig. 14.14 Bandgaps vs lattice constants, and band alignments of 2D semiconductors. From J. Mater. Res. 31, 900 (2016).
The Schottky Diode

**Richardson constant**

\[
J = A^* T^2 e^{\frac{q\phi_b}{k_b T}} (e^{\frac{qV}{k_b T}} - 1)
\]

\[
A^* = \frac{4\pi q k_e^2 m^*}{h^3}
\]

**Metal-Semiconductor Junctions: Current Flow**

**Fig. 16.1** Schottky Diode.

**Fig. 16.2** Walter Schottky was an early investigator of the metal-semiconductor junction. A semiconductor research institute in Munich is named after him.

**Fig. 16.3** Owen Richardson was awarded the 1928 Physics Nobel prize for thermionic emission; the Richardson constant is named after him.

\[
S = \frac{kT}{q} \ln(10)
= 60 \text{ mV/decade at } 300 \text{ K}
\]

This is a **FUNDAMENTAL** limit of voltage control of currents that are limited by **Thermionic Emission** over barriers.

\[q \times \text{Voltage} = \text{Energy of electrons. Therefore, this is also the fundamental limit Of 'energy efficiency' of switching devices That operate using Thermionic Emission currents}\]
The Schottky Diode

Filled states are colored blue

$g_{3dmetal}(E_F)$

$g_{2dsemi}(E)$

$g_{2dsemi}(E_F)$

$E_F$

$E$

$g_{3dmetal}(E)$
The Schottky Diode Rectifier

**Metal-Semiconductor Junctions: Current Flow**

\[ I = I_0 \left[ e^{qV_a/kT} - 1 \right] \]
Various kinds of Metal-Semiconductor Junctions
Energy Band Diagrams

Homojunction Energy Band Diagrams

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Energy Band Diagrams

Heterojunction Energy Band Diagrams

Al$_{0.3}$Ga$_{0.7}$As → GaAs
Energy Band Diagrams

Heterojunction Energy Band Diagrams

(a) GaSb

(b) InAs

\[ \Delta E_C = 0.87 \text{ eV} \]

\[ E_G = 0.72 \text{ eV} \]

\[ E_G = 0.36 \text{ eV} \]
Energy Band Diagrams

Graded Heterojunction
Energy Band Diagrams

\[ E_G = 1.80 \text{ eV} \]

\[ E_G = 1.42 \text{ eV} \]

\[ \Delta E_G = 0.38 \text{ eV} \]

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Band Diagrams for Polar Heterostructures

Fig. 14.15 Energy band diagrams of polar heterostructures such as GaN/AlGaN heterojunctions. Because of the presence of internal electric charges due to spontaneous and piezoelectric polarization, electric fields and band bending happens even in the absence of donor or acceptor doping.
Mobility and Transport

Charge Transport: Drift

**Table 1.6: Effective Mass and Mobility for Various Semiconductors**

<table>
<thead>
<tr>
<th>Material</th>
<th>$m_e^*$</th>
<th>$m_h^*$</th>
<th>$m_j^*$</th>
<th>$\mu_e$</th>
<th>$\mu_h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>IV</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Si</td>
<td>0.26</td>
<td>0.55</td>
<td>0.24</td>
<td>1350</td>
<td>475</td>
</tr>
<tr>
<td>Ge</td>
<td>0.56</td>
<td>0.37</td>
<td>-</td>
<td>3800</td>
<td>1900</td>
</tr>
<tr>
<td>GaP</td>
<td>0.12</td>
<td>0.86</td>
<td>0.14</td>
<td>200</td>
<td>120</td>
</tr>
<tr>
<td>GaAs</td>
<td>0.065</td>
<td>0.45</td>
<td>0.082</td>
<td>8500</td>
<td>420</td>
</tr>
<tr>
<td>III-V</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GaSb</td>
<td>0.049</td>
<td>0.33</td>
<td>0.056</td>
<td>7700</td>
<td>1400</td>
</tr>
<tr>
<td>InP</td>
<td>0.077</td>
<td>0.56</td>
<td>0.12</td>
<td>6000</td>
<td>150</td>
</tr>
<tr>
<td>InAs</td>
<td>0.027</td>
<td>0.41</td>
<td>0.024</td>
<td>33000</td>
<td>460</td>
</tr>
<tr>
<td>InSb</td>
<td>0.0135</td>
<td>0.438</td>
<td>0.016</td>
<td>78000</td>
<td>1700</td>
</tr>
<tr>
<td>II-VI</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ZnSe</td>
<td>0.17</td>
<td>-0.7</td>
<td></td>
<td>530</td>
<td>28</td>
</tr>
<tr>
<td>ZnTe</td>
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<td>0.42</td>
<td>0.17</td>
<td>340</td>
<td>110</td>
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<tr>
<td>CdS</td>
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<td></td>
<td>350</td>
<td>15</td>
</tr>
<tr>
<td>CdSe</td>
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<td>&gt;1.0</td>
<td></td>
<td>650</td>
<td></td>
</tr>
<tr>
<td>CdTe</td>
<td>0.0963</td>
<td>0.62</td>
<td>0.092</td>
<td>1050</td>
<td>80</td>
</tr>
</tbody>
</table>

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High-Field Transport: Electron Velocity Saturation

Hot-electron temperature: models non-equilibrium

Energy balance eqn.

Momentum balance eqn.

Steady state

Ensemble saturation velocity $v_d = v_0 \sqrt{\frac{\tau_m}{\tau_E}}$

$\tau_m = \frac{\hbar \omega_{LO}}{m_e}$

$\tau_E = \frac{1}{1 + \exp \left( \frac{(\varepsilon - \zeta)}{kT_e} \right)}$

$\frac{\partial E}{\partial t} = \frac{eF}{m_e} - \frac{v_d}{\tau_m(T_e)}$

$\frac{\partial v_d}{\partial t} = \frac{eF}{m_e} - \frac{v_d}{\tau_m(T_e)}$

$\frac{1}{1 + \exp \left( \frac{(\varepsilon - \zeta)}{kT_e} \right)}$
Effective Mass Approximation

- **2D (Quantum Wells)**

\[ V(x, y, z) = 0, z < 0 \]
\[ V(x, y, z) = 0, z > W \]
\[ V(x, y, z) = -\Delta E_c, 0 \leq z \leq W. \]

\[ k_{nz} = \frac{\pi}{W} n_z \]

\[ C_{nz}(x, y, z) = \phi(x, y) \chi_{nz}(z) = \left[ \frac{1}{\sqrt{A}} e^{i(k_x x + k_y y)} \right] \cdot [\chi_{nz}(z)] \]

\[ E(k) = E_{c0} + \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_{xx}^*} + \frac{k_y^2}{m_{yy}^*} \right) + \frac{\hbar^2}{2 m_{zz}^*} \left( \frac{\pi n_z}{W} \right)^2 \]

\[ g_{QW}(E) = \frac{m^*}{\pi \hbar^2} \sum_{n_z} \theta(E - E_{n_z}) \]

\[ n_{2D} = \sum_j n_j = N_c^{2D} \sum_j \ln \left( 1 + e^{\frac{E_j - E_{E_j}}{k_B T}} \right) \]

Specific equations and formulas are provided, along with a diagram illustrating a band structure and density of states for realistic heterostructure quantum wells.
Effective Mass Approximation

- 1D (Quantum Wires)

\[ k_{n_x} = \frac{\pi}{L_x} n_x, \]
\[ k_{n_y} = \frac{\pi}{L_y} n_y, \]

\[ C(x, y, z) = \chi_{n_x}(x) \cdot \chi_{n_y}(y) \cdot \left( \frac{1}{\sqrt{L_z}} e^{ik_x x} \right) \]

\[ E(n_x, n_y, k_z) = E(n_x, n_y) + \frac{\hbar^2 k_z^2}{2m^*_z} \]

Figure 3: Bandstructure, and DOS of realistic quantum wires.

\[ C_{n_x, n_y}(x, y, z) = \left[ \sqrt{\frac{2}{L_x}} \sin \left( \frac{\pi n_x}{L_x} x \right) \right] \cdot \left[ \sqrt{\frac{2}{L_y}} \sin \left( \frac{\pi n_y}{L_y} y \right) \right] \cdot \left[ \frac{1}{\sqrt{L_z}} e^{ik_x x} \right] \]

\[ g_{1D}(E) = \frac{1}{\pi} \sqrt{\frac{2m^*}{\hbar^2}} \sqrt{E - E_1} \]

\[ g_{QWire}(E) = \frac{1}{\pi} \sqrt{\frac{2m^*}{\hbar^2}} \sum_{n_x, n_y} \frac{1}{\sqrt{E - E(n_x, n_y)}} \]
Effective Mass Approximation

- 0D (Quantum Dots)

\[ C(x, y, z) = \left[ \sqrt{\frac{2}{L_x}} \sin\left(\frac{\pi n_x}{L_x}\right) \right] \cdot \left[ \sqrt{\frac{2}{L_y}} \sin\left(\frac{\pi n_y}{L_y}\right) \right] \cdot \left[ \sqrt{\frac{2}{L_z}} \sin\left(\frac{\pi n_z}{L_z}\right) \right] \]

\[ E(n_x, n_y, n_z) = \frac{\hbar^2}{2m_{xx}} \left( \frac{\pi n_x}{L_x} \right)^2 + \frac{\hbar^2}{2m_{yy}} \left( \frac{\pi n_y}{L_y} \right)^2 + \frac{\hbar^2}{2m_{zz}} \left( \frac{\pi n_z}{L_z} \right)^2 \]

\[ g_{QDot} = \sum_{n_x, n_y, n_z} \delta(\varepsilon - E_{n_x, n_y, n_z}) \]

Figure 4: Energy levels and DOS of quantum dots.
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Effective Mass Approximation @ Heterojunctions

- Effective Mass Theory works even at sharp heterojunctions, and it works amazingly well! Quantum cascade lasers are designed using this theory.

Proof presented in:
Burt, APL 65 717 (1994)

On the validity and range of applicability of the particle in a box model

M. G. Burt
BT Laboratories, Martlesham Heath, Ipswich IP5 7RE, United Kingdom
(Received 24 February 1994; accepted for publication 27 May 1994)

\[ E_z^A - \frac{\hbar^2}{2m_A m_0} \frac{d^2}{dz^2} \chi(z) = E \chi(z). \]

\[ E_z^B - \frac{\hbar^2}{2m_B m_0} \frac{d^2}{dz^2} \chi(z) = E \chi(z). \]

The difference in the bottoms of the conduction bands behaves like a step potential with material $B$ higher by $\Delta E_z = E_z^B - E_z^A$. If the materials were the same we would simply match the value and derivative of the wave function at the interface, giving the usual conditions

\[ \chi(0_B) = \chi(0_A). \]

\[ \frac{d \chi(z)}{dz} \bigg|_{z=0_A} = \frac{d \chi(z)}{dz} \bigg|_{z=0_B}. \]

where $0_A$ means the side of the interface in material $A$ and so on. This simple condition is not correct for a heterojunction where the two effective masses are different, and we shall see in Section 5.8 that equation (3.18) does not conserve current. A correct set of matching conditions is

\[ \frac{d \chi(z)}{dz} \bigg|_{z=0_A} = \frac{1}{m_A} \frac{d \chi(z)}{dz} \bigg|_{z=0_B}. \]

The condition for matching the derivative now includes the effective mass. Since the derivative is essentially the momentum operator, equation (3.19) requires the velocity to be the same on both sides to conserve current. The envelope function gains a kink at the interface if $m_A \neq m_B$. 

\[ \psi(z) \]

\[ \chi(z) \]
Example: Exciton in an InN Nanowire

\[ |C(r)|^2 \]

envelope function

\[ |\Psi(r)|^2 = |C(r)|^2 \times |u(r)|^2 \]

exciton

Bloch function

Nano Letters (2014)

E. Kioupakis et al. (Michigan)
Infinitely Deep Quantum Wells

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

\( V(x) = 0 \) for \(- L \leq x \leq +L \)

\( V(x) = \infty \) for \(|x| \geq L \)

\[ \psi(x) = Ae^{ikx} + Be^{-ikx} \]

\[ k = \frac{2\pi}{\lambda} = \sqrt{\frac{2m^*(E - V)}{\hbar^2}} \]

\[ \psi(+L) = \psi(-L) = 0 \rightarrow k_n = \frac{n\pi}{2L} \]

\( \psi_{\text{even}}(x) = A_n \cos\left(\frac{n\pi}{2L} x\right) \) for \( n = \pm 1, \pm 2, ... \)

\( \psi_{\text{odd}}(x) = A_n \sin\left(\frac{n\pi}{2L} x\right) \) for \( n = \pm 2, \pm 4, ... \)

\[ E_1^\infty = \frac{\pi^2 \hbar^2}{8m^*L^2} = \frac{\pi^2 \hbar^2}{2m^*L_w^2} \]

\[ E_1^\infty = \frac{3.76}{(m^*/m_0)(L_w/10 \text{ nm})^2} \text{ meV} \]

\[ E_n = n^2 E_1^\infty \]

The particle in a box problem

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Finite Quantum Wells

The particle in a box problem

\[ \frac{d^2 \psi}{dx^2} + \kappa^2 \psi = 0 \]

\[ \kappa^2 = \frac{2mE}{\hbar^2} \]

\[ \psi(x) = Ce^{\kappa x} \quad x < -L \]

\[ \psi(x) = A \cos(kx) + B \sin(kx) \quad -L < x < +L \]

\[ \psi(x) = De^{-\kappa x} \quad x > +L \]

\[ k^2 = -\frac{2m}{\hbar^2} (U_0 + |E|) > 0 \]

Even solutions: \( \tan(kL) \)

Odd solutions: \( -\cot(kL) \)

Density of states for a 1D quantum well

Bound states: Atomic-like

“Continuum” states: Free-electron-like

FIGURE 4.2. Graphical solution of equation (4.12) for a square well in GaAs with depth \( V_0 = 0.3 \) eV and width \( a = 10 \) nm, giving \( \theta_0^2 = 13.2 \). There are three bound states.

FIGURE 4.3. Local density of states \( n(E, x = 0) \) in the middle of a square well in GaAs of width 10 nm and depth 0.3 eV. The result for free electrons, proportional to \( E^{-1/2} \), is shown for comparison.

(Rockett/Davies)
Transitions in Semiconductor Quantum Wells

FIGURE 1.3. Optical absorption in a quantum well formed by a layer of GaAs surrounded by AlGaAs. (a) Potential well in conduction and valence band, showing two bound states in each; the energy gap of GaAs is really much larger than this diagram implies. (b) Transitions between states in the quantum well produce absorption lines between the band gaps of the GaAs well and AlGaAs barrier.

Quasi-2D systems: Quantum Wells

Photoluminescence spectra of quantum wells

(Davies)
Designing the Transitions in Quantum Wells

Rectangular quantum wells

Parabolic quantum wells: Harmonic Oscillator States!
Multiple Coupled Quantum Wells

Interaction energy
1st nearest neighbor wells: ~10 meV

Conduction band edge energy

Position

Number of Coupled Quantum Wells

Quantum State Energies (meV)

States merge into minibands

Note the ‘zero-states’ for odd number of wells

(Rockett)
Designer Quantum Structures

Fig. 3. (a) TEM characterization of a test sample grown by MOCVD. The growth sequence and the structure are shown in (b). The remarkable features are the sharpness of the very narrow GaAs layers (minimum ~25 Å) appearing at the lower right-hand side corner, the interface roughness showing up at the uppermost interface of the AlAs layer, and the subsequent smoothing of this roughness by the multilayer growth (upper left-hand side corner) (after Leys et al.61).

(Weisbuch/Vinter)
Heterostructure Superlattices

Fig. 15. Tight-binding model of superlattices.

FIG. 16. Tight-binding model of GaAs/GaAlAs superlattices: Variation of the fundamental state bandwidth [4t, of Eq. (30)] in the tight-binding model as a function of barrier thickness for three different well thicknesses. $X = 0.2$; $V_0 = 212$ meV (after Bastard).
Heterostructure Superlattices

E = E₁ + S + 2T\cos qd

\[ \varepsilon_n^*(q, k_\perp) = \hbar^2 k_\perp^2 / 2m + \varepsilon_n(q) \]

\[ \rho_n(\varepsilon) = N \frac{m^*}{\pi \hbar^2} \arccos \left( \frac{\varepsilon_i - E_i - S_i}{2t_i} \right) \]

Density of states of a superlattice

DOS of uncoupled 2D wells

Fig. 15. Tight-binding model of superlattices.

Fig. 17. Comparison of the DOS of a superlattice with that of a 2D system (----) and a 3D isotropic system. Note the broadening of the superlattice band with band index as the overlap of wave functions increases with energy E in the tight-binding description, increasing the transfer matrix element tᵢ. (Reprinted with permission from World Scientific Pub. Co., L. Esaki, “Recent Topics in Semiconductor Physics” (H. Kamimura and Y. Toyozawa, eds.), 1983.)
Semiconductor Physics Summary

Fig. 2.24. The valence band structure and density of states (see Sect. 4.3.1 for definition) of Si calculated by the tight-binding method (broken curves) and by the empirical pseudopotential method (solid lines) [225].

Density of States (DOS)

For a semiconductor (bulk, 3D).

Fermi Energy

Strong absorption

Weak absorption

Filled States

Empty states

Energy

Density of States, g(E)

Fig. 1.8. Densities of states for free electrons in one, two, and three dimensions.
**Semiconductor Physics Summary**

Densities of states for free electrons in one, two, and three dimensions.

<table>
<thead>
<tr>
<th>0 Dimension</th>
<th>1 Dimension</th>
<th>2 Dimensions</th>
<th>3 Dimensions</th>
<th>4 Dimensions</th>
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</thead>
<tbody>
<tr>
<td>Conduction Band Structure</td>
<td>$e_i$</td>
<td>$e_i = \frac{\epsilon_0}{2}$</td>
<td>$e_i = \frac{\epsilon_0}{2} (\epsilon_X + \epsilon_y)$</td>
<td>$e_i = \frac{\epsilon_0}{2} (\epsilon_X + \epsilon_y + \epsilon_z)$</td>
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<tr>
<td>Conduction Band DOS $g_c(\epsilon)$</td>
<td>$\delta(\epsilon - E_c)$</td>
<td>$\delta(\epsilon - E_c)$</td>
<td>$\delta(\epsilon - E_c)$</td>
<td>$\delta(\epsilon - E_c)$</td>
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<tr>
<td>Conduction Band-Edge Effective DOS $\Sigma^2$</td>
<td>$\frac{\pi}{2m^2e^2}</td>
<td>\epsilon</td>
<td>^{-3/2}$</td>
<td>$\frac{\pi}{2m^2e^2}</td>
</tr>
<tr>
<td>Electron Density $n_e$</td>
<td>$\frac{1}{\sqrt{\pi}}</td>
<td>\epsilon</td>
<td>^{3/2}$</td>
<td>$\frac{1}{\sqrt{\pi}}</td>
</tr>
<tr>
<td>Source Fermi Level $E_F$ under bias $V$</td>
<td>$n_{so} = \frac{1}{\sqrt{\pi}}</td>
<td>\epsilon</td>
<td>^{3/2}$</td>
<td>$n_{so} = \frac{1}{\sqrt{\pi}}</td>
</tr>
<tr>
<td>Ballistic Electron Current Density $J_0$ at voltage $V$</td>
<td>$\frac{e^2}{2\pi^2}</td>
<td>\epsilon</td>
<td>^{1/2} \frac{\delta(\epsilon - E_c)}{1 - e^{-\frac{\epsilon - E_c}{kT}}}$</td>
<td>$\frac{e^2}{2\pi^2}</td>
</tr>
<tr>
<td>Valence Band Structure</td>
<td>$x_i$</td>
<td>$x_i = \frac{\epsilon_0}{2}$</td>
<td>$x_i = \frac{\epsilon_0}{2} (\epsilon_X + \epsilon_y)$</td>
<td>$x_i = \frac{\epsilon_0}{2} (\epsilon_X + \epsilon_y + \epsilon_z)$</td>
</tr>
<tr>
<td>Valence Band DOS $g_v(\epsilon)$</td>
<td>$\delta(\epsilon - E_v)$</td>
<td>$\delta(\epsilon - E_v)$</td>
<td>$\delta(\epsilon - E_v)$</td>
<td>$\delta(\epsilon - E_v)$</td>
</tr>
<tr>
<td>Valence Band-Edge Effective DOS $\Sigma^2$</td>
<td>$\frac{\pi}{2m^2e^2}</td>
<td>\epsilon</td>
<td>^{-3/2}$</td>
<td>$\frac{\pi}{2m^2e^2}</td>
</tr>
<tr>
<td>Hole Density $p_h$</td>
<td>$\frac{1}{\sqrt{\pi}}</td>
<td>\epsilon</td>
<td>^{3/2}$</td>
<td>$\frac{1}{\sqrt{\pi}}</td>
</tr>
<tr>
<td>Source Fermi Level $E_F$ under bias $V$</td>
<td>$p_{so} = \frac{1}{\sqrt{\pi}}</td>
<td>\epsilon</td>
<td>^{3/2}$</td>
<td>$p_{so} = \frac{1}{\sqrt{\pi}}</td>
</tr>
<tr>
<td>Ballistic Hole Current Density $J_0$</td>
<td>$\frac{e^2}{2\pi^2}</td>
<td>\epsilon</td>
<td>^{1/2} \frac{\delta(\epsilon - E_v)}{1 - e^{-\frac{\epsilon - E_v}{kT}}}$</td>
<td>$\frac{e^2}{2\pi^2}</td>
</tr>
</tbody>
</table>
Physics of Semiconductor Nanostructures Summary

Table 1: Quantum Electronic, Photonic, and Statistical Properties of Conduction and Valence Band Electrons in Semiconductor Nanostructures.

- $E_c$ is the band edge, and $m_e^*$ the effective mass of the conduction band. $E_v$ is the band edge, and $m_v^*$ the effective mass of the valence band.
- For low dimensions, $E_c$ and $E_v$, and the bandgap $E_g = E_v - E_c$ include the quantum confinement energies if present.
- $h$ is Planck's constant, $k_B$ is the Boltzmann constant, and $q$ the electron charge.
- $g_s$ is the spin degeneracy, and $g_v$ the valley degeneracy.
- $F_j(\gamma) = \frac{1}{(\gamma + 1)^{\gamma+1}} \int_{v_{th}}^{\infty} d\nu \frac{\nu^{\gamma}}{e^{\nu/k_BT} - 1}$ is the Fermi-Dirac integral of order $j$, and $\Gamma(\ldots)$ is the Gamma function.
- $E_F$ is the Fermi level at equilibrium. $E_{Fq}$ is the source quasi-Fermi level and $E_{Fd}$ the drain quasi-Fermi level.
- Similarly, $E_c$ is the conduction band quasi-Fermi level and $E_v$ the valence band quasi-Fermi level.
- $I_{ph}$ is the photon energy of frequency $\nu$. $L_x$, $L_y$, $L_z$ are the dimensions of the semiconductor nanostructure.
- $A$ and $B$ are the Einstein $A$ and $B$ coefficients, $\lambda$ is $c/\nu$ the wavelength of the photon in vacuum, and $n$ the refractive index of the semiconductor.
- $f(E) = 1/(1 + e^{E/k_BT})$ is the Fermi-Dirac occupation function of state $E = E_c + \frac{n^2}{2m_e^*}$ in the conduction band.
- $f(E) = 1/(1 + e^{E/k_BT})$ is the Fermi-Dirac occupation function of state $E = E_v - \frac{n^2}{2m_v^*}$ in the valence band.
- $E_2 - E_1 = h\nu = E_g + \frac{n^2}{2m^*}$ is the energy of the photon emitted when the electron transitions from $E_2 \rightarrow E_1$ radiatively.
- The Einstein $A$ and $B$ coefficients are related by $\frac{A}{B} = \frac{k_B^2}{\hbar^4}$.
- The photon density is $\rho_p = I_{ph}/(c/n)$ in eV/cm$^3$, $c$ is the speed of light in a media of refractive index $n$, and $I_{ph} = E_0^2/2\eta$ in W/cm$^2$ is the Poynting energy density with electric field amplitude $E_0$ and wave impedance $\eta$. 

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**Fig. 5.5** Quantum picture of current flow in the 1D k-space due to a difference in the occupation functions of right-going and left-going eigenstates. The left contact is called the source, and the right contact the drain.

**Fig. 5.8** The left plot shows the calculated normalized Fermi level $\eta_F = E_F/k_B T$ at $V = 0$, and the split normalized Fermi levels $\eta_s$ and $\eta_d$ for nonzero normalized voltages $v_d = qV/k_BT$ for two values of 1D electron density at 300 K. The red curves are for $n_{1d} = 5 \times 10^7/cm$, and the blue for $n_{1d} = 10^6/cm$. The right plot shows the resulting quantum mechanical current flowing in response to the voltage for six values of 1D electron densities ranging from $0.1 - 5.0 \times 10^7/cm$. For example, at a 1D electron density of $n_{1d} = 10^7/cm$, the maximum (or saturation) current is $\sim 70 \mu A$. The middle $E(k)$ figures show the changes in the corresponding occupied electron states for $n_{1d} = 5 \times 10^7/cm$ for three different voltages.

\[ \eta_s - \eta_d = v_d, \quad \text{and} \quad n_{1d} = \frac{1}{2} N_c^{1d}(T)[F_{-\frac{1}{2}}(\eta_s) + F_{-\frac{1}{2}}(\eta_d)] \]

\[ J_{1d} = J_R^{1d} - J_L^{1d} = \frac{qg_s g_v}{2\pi \hbar} (k_B T) \ln \left( \frac{1 + e^{\eta_s}}{1 + e^{\eta_d}} \right). \]
Ballistic Transport in 1, 2, and 3 Dimensions

1D

\[ E_{F_1} - E_{F_0} = qV \]

\[ n_{1d} = 1 \times 5 \times 10^6 \text{ cm}^{-1} \]

2D

\[ E_{F_2} - E_{F_1} = qV \]

\[ n_{2d} = 1 \times 5 \times 10^{13} \text{ cm}^{-2} \]

3D

\[ E_{F_3} - E_{F_2} = qV \]

\[ n_{3d} = 1 \times 10^{20} \text{ cm}^{-3} \]

\[ m^*_c = 0.2m_e, g_s = 2, g_v = 1 \]
Ballistic Current in 2 Dimensions

- The physics of a Ballistic FET can be understood by inspecting the carrier distribution in $k$-space at the source-injection Point.

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Ballistic FET

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Ballistic FET

\[ I_d / W = J_0 \left[ F_{1/2}(\eta_s) - F_{1/2}(\eta_d) \right] \]

\[ \eta_s = \ln \left[ \sqrt{1 + e^{V_{ds}}} + 4e^{V_{ds}} \left( e^{2n_s(V_{gs})/n_d} - 1 \right) - (1 + e^{V_{ds}}) \right] - \ln 2 \]

\[ J_0 = \frac{g_s g_v \sqrt{2m^*}}{2\pi^2 h^2} \left( kT \right)^{3/2} \]

\[ F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty du \frac{u^j}{1 + e^{u-\eta}} \]

- \( F_j(\eta) \approx e^{\eta} \) for \( \eta \ll -1 \)
- \( F_j(\eta) \approx \frac{\eta^{j+1}}{\Gamma(j+2)} \) for \( \eta \gg 1 \)

\[ \frac{I_d}{W} \sim J_0 e^{V_{gs} - V_T} \frac{V_{th}}{V_{th}} \]

Subthreshold (off)

On-state
Ballistic FET

\[
\frac{I_d}{W} \sim J_0e^{\frac{V_{gs} - V_T}{V_{th}}}
\]

**Figure 10.4:** Ballistic Silicon FET. The device dimensions are \(t_b = 1\) nm, \(\epsilon_b = 10\epsilon_0\), and for Silicon, \(m^* = 0.2m_0\) and \(g_v = 2.5\) are used.

- Note the on-off ratio, and the sharper switching at low temperatures. The subthreshold slope is \(\sim (kT/q)\ln(10)\).
- This calculation neglects the contact resistance incurred in injecting carriers from 3D source to 2D channel.

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Ballistic FET Limits
Transistor Applications

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Transistor Applications

Communication Devices

- Semiconductor Transistor
- Vacuum tube

Logic Devices

- Digital Switch
- Mechanical Relay

- Charge-based
- Spin-based
- Correlated/Phase transitions

Gain

Speed (Bandwidth)

Quantum Limits?

New Materials with better Transport

Question marks

On - Logic (operation)

Off - Fast (time) / Slow

SRAM Cell (6 Transistors)

DRAM Cell (1 Transistor and one capacitor)

V_{dd}

V_{cc}

V_{ss}

V_{gs}

Charge-based

Spin-based

Correlated/Phase transitions

Flash

Program F-N Tunneling

Off cell (Solid-0)

Erase F-N Tunneling

On cell (Solid-1)

V_{cc} = 18 V

V_{cc} = 0 V

0 V

float

V_{ss} = 0 V

V_{ss} = 20 V

float

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It all began with Light…

• 3 Pillars of Information systems are: “Computation, Memory, and Communication”
The “humble” transistor: Many Avatars...

- The transistor is an electronic switch
- It is also an amplifier: it has gain
- Gain @ high speed: RF electronics
- Switching @ high voltages: Power electronics

\[
I_D \sim e^{\frac{qV_{gs}}{kT}}
\]

\[
\rightarrow SS \sim \frac{kT}{q} \ln 10 \approx 60 \frac{mV}{\text{decade}}
\]
The “humble” transistor: Many Avatars...

- The transistor is an electronic switch
- It is also an amplifier: it has gain
- Gain @ high speed: RF electronics
- Switching @ high voltages: Power electronics

< 60 mV/decade possible
Careful what you wish for: you may get it!

**Implications of Scales in Processing of Information**

The physical form of information processing employing electronics is as a collection of small devices—memories included—beholden to the physics of operation of device and its assembly in achieving desired objectives. This paper reviews and explores these scale connections—of transistors, materials, and the variety of device proposals—internally and in their integration.

By Sandip Tiwari, Fellow IEEE

---

**Fig. 2. Error-energy relationship for an idealized CMOS gate according to (4) for an ensemble of $10^{10}$ $g = -10$ CMOS switches operating at 10% activity factor. For every decade of error improvement, $\approx 15k_BT$ of energy is required in the low error limit.**

- The “fat” in Boolean logic switching buys us robustness against errors.
- Low power switches will have to figure out a way to be robust to fluctuations.
Transistors old and new
Can Transistors beat the Boltzmann Limit?

Tunneling FETs (or TFETs)

Negative Capacitance FETs (NCFETs)
$kT \ln(2) \sim 3 \times 10^{-6}$ fJ

$\frac{\hbar}{kT} \sim 3 \times 10^{-2}$ ps

$\psi(x_1, x_2) = -\psi(x_2, x_1)$

$f(E) = \frac{1}{1 + e^{\frac{E - E_F}{kT}}}$

$F_{mag} \sim F_{el} \cdot \frac{v^2}{c^2}$

$\frac{qV}{e kT}$ vs. $e^{i\phi}$ logic

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New Devices Promise to Do Better

\[ kT \ln(2) \sim 3 \times 10^{-6} \text{ fJ} \]

\[ \frac{\hbar}{kT} \sim 3 \times 10^{-2} \text{ ps} \]

\[ \psi(x_1, x_2) = -\psi(x_2, x_1) \]

\[ f(E) = \frac{1}{1 + e^{\frac{E-E_F}{kT}}} \]

\[ F_{mag} \sim F_{el} \cdot \frac{v^2}{c^2} \]

\[ \frac{qV}{e kT} \text{ vs. } e^{i\phi} \text{ logic} \]

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TABLE 1: Landmarks in the Science of Tunneling

<table>
<thead>
<tr>
<th>No.</th>
<th>Phenomena</th>
<th>Investigators</th>
<th>Year</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>Observation of field-emission from metals</td>
<td>Lilienfeld</td>
<td>1922</td>
</tr>
<tr>
<td>2</td>
<td>Ionization of hydrogen atoms by electron tunnelling</td>
<td>Oppenheimer</td>
<td>1928</td>
</tr>
<tr>
<td>3</td>
<td>Explanation of field-emission</td>
<td>Fowler and Nordheim</td>
<td>1928</td>
</tr>
<tr>
<td>4</td>
<td>Alpha-decay Theory</td>
<td>Glanze, Gurney and Condon</td>
<td>1928</td>
</tr>
<tr>
<td>5</td>
<td>Theory of Interband Tunneling in solids</td>
<td>Zener</td>
<td>1934</td>
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<tr>
<td>6</td>
<td>Field Emission Microscope (FEM)</td>
<td>Muller</td>
<td>1937</td>
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<tr>
<td>7</td>
<td>Observation of Zener Breakdown</td>
<td>Chyrowitz and Mclay</td>
<td>1957</td>
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<td>8</td>
<td>Tunneling in Degenerate pn Junctions</td>
<td>Esaki</td>
<td>1958</td>
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<tr>
<td>9</td>
<td>Extension of Zener’s Theory to Tunnel Diodes</td>
<td>Kalliny, Rowe and Price</td>
<td>1958-1961</td>
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<tr>
<td>10</td>
<td>Measurement of energy gap of superconductors</td>
<td>Giaever</td>
<td>1960</td>
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<td>11</td>
<td>Perturbation Treatment of Tunneling</td>
<td>Bardeen</td>
<td>1961</td>
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<td>12</td>
<td>Tunneling of Cooper Particles</td>
<td>Josephson</td>
<td>1962</td>
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<tr>
<td>13</td>
<td>Experimental Verification of Josephson Effect</td>
<td>Anderson et al.</td>
<td>1963-1964</td>
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<td>14</td>
<td>Isotopic Tunneling Spectroscopy (ITS)</td>
<td>Jaklevic and Lamb are</td>
<td>1966</td>
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<td>15</td>
<td>Observation of Tunneling Tails</td>
<td>Lee and Gomer</td>
<td>1970-1971</td>
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<td>16</td>
<td>Development of Scanning Tunneling Microscope (STM)</td>
<td>Binnig</td>
<td>1981</td>
</tr>
</tbody>
</table>

Applications:
- SEMs
- TEMs
- STMs
- Tunnel diodes
- Ohmic contacts
- RTDs
- Quantum Cascade Lasers
- TFETs...
Why can electrons tunnel through barriers?

---

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Why can electrons tunnel through barriers?

Total internal reflection

photons
Why can electrons tunnel through barriers?

Total internal reflection

"tunneling of photons"
Why can electrons tunnel through barriers?

De Broglie

\[ \lambda = \frac{\hbar}{mv} \]

Total internal reflection

“tunneling of photons”
Why can electrons tunnel through barriers?

De Broglie:
\[ \lambda = \frac{\hbar}{mv} \]

Total internal reflection

"tunneling of photons"

Electrons

Reflection of electron wave

"tunneling of electrons"

Total internal reflection

"tunneling of photons"
Tunneling in Semiconductors

\[ V(x) \]

Energy levels:
- \( E_L \)
- \( E_H \)

Potential energy barrier at position \( x \) within the semiconductor material.
Tunneling in Semiconductors

\[ T(E) = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)} \sin^2(k_b a)} \]

\[ k_b = \sqrt{\frac{2m_e}{h^2} (E - V_0)} \]

\[ E = \frac{\hbar^2 k^2}{2m_e} + V_0. \]

\[ \sin(iy) = i \sinh(y) \]

\[ T(E) \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2k_b a} \]

\[ T_{wkb} \approx e^{-\left(\frac{k_b}{0.1 \text{ nm}}\right)\sqrt{\left(\frac{m_e^*}{m_e}\right)\left(\frac{V_0}{1 \text{ eV}}\right)}} \]

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Classical Quantum

\[ a = 1 \text{ nm} \]
\[ V_0 = 1 \text{ eV} \]

\[ a = 3 \text{ nm} \]
\[ V_0 = 1 \text{ eV} \]
Electron Quantum Transport in Smooth Potentials

Effective Mass Equation for Electron Wavepackets

\[ [E_n(-i\nabla)]C(x) = [E - E_c(x)]C(x) \implies \frac{d^2}{dx^2}C(x) = \frac{-2m_c^*}{\hbar^2} [E - E_c(x)]C(x) \]

The Effective Mass Approximation For Bands in Semiconductors

The WKB approximation

\[ C(x) \approx \frac{K}{Q(x)^{1/4}} e^{\pm \int_a^x du \sqrt{Q(u)}}. \]

\[ E > E_c(x), \quad Q(x) < 0 \]

\[ k(x) = \sqrt{\frac{2m_c^*}{\hbar^2} (E - E_c(x))} \]

\[ C(x) \approx \frac{K'}{\sqrt{k(x)}} e^{\pm i \int_a^x du k(u)} , \]

\[ |C(x)|^2 \propto \frac{1}{k(x)} \]

Fig. 18.3 Electron transport and approximate wavefunction in smoothly varying potentials.
Electron Quantum Transport in Smooth Potentials

\[ \left[ -\frac{\hbar^2}{2m_e} \frac{d^2}{dx^2} + V(x) \right] \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t) \implies j = \frac{\psi^* \hat{p} \psi - \psi \hat{p} \psi^*}{2m_e} \]

\[ \left[ -\frac{\hbar^2}{2m_c^*} \frac{d^2}{dx^2} + E_c(x) \right] C(x, t) = i\hbar \frac{\partial}{\partial t} C(x, t) \implies j = -\frac{i\hbar}{2m_c^*} \left[ C^* \frac{\partial C}{\partial x} - C \frac{\partial C^*}{\partial x} \right] \]

\[ C(x) \approx \frac{K'}{\sqrt{k(x)}} e^{i \int_{x_0}^x du k(u)} \quad \|C(x)\|^2 \propto \frac{1}{k(x)} \]

\[ n(x) = C^*(x) C(x) = \frac{|K|^2}{k(x)} \]

\[ J = \sum_k j_k = q g_s g_v \sum_k v_g(k) |C(x)|^2 \]

\[ E_c(k) = E_c(x) + \frac{\hbar^2 k(x)^2}{2m_c^*}, \quad v_g(k) = \frac{1}{\hbar} \frac{\partial E_c(k)}{\partial k} = \frac{\hbar k(x)}{m_c^*} \]

\[ J = q g_s g_v \frac{\hbar k(x)}{m_c^*} \frac{|C(x)|^2}{v(x) n(x)} = q g_s g_v \frac{\hbar k(x)}{m_c^*} \frac{|K|^2}{k(x)} = q g_s g_v \frac{\hbar |K|^2}{m_c^*} \]

Fig. 18.4 Transport of an effective mass electron wavepacket in the conduction band in a smoothly varying potential. The group velocity \( v(x) \sim k(x) \) increases as the kinetic energy increases, but the carrier density \( n(x) = |C(x)|^2 \sim 1/k(x) \) decreases, keeping the net current \( J(x) \sim n(x) v(x) \) constant.

Quantum Current carried by an electron wavepacket in arbitrary potentials
Tunneling of Electrons Through Arbitrary Barriers

\[ C(x) = \frac{Ke^{\int_a^x k(u)du}}{\sqrt{k(x)}} \]

\[ C(x) = \frac{K'e^{\int_a^x \kappa(u)du}}{\sqrt{\kappa(x)}} \]

\[ k(x) = \sqrt{\frac{2m^*_c}{\hbar^2} (E - E_c(x))} \]

\[ \kappa(x) = -\frac{2m^*_c}{\hbar^2} (E - E_c(x)) > 0 \]

\[ C(x) \approx \frac{K}{\sqrt{\kappa(x)}} e^{\pm \int_a^x \kappa(u)du} \]

\[ \frac{C(x_2)}{C(x_1)} \approx \frac{e^{-\int_a^{x_2} \kappa(u)du}}{e^{-\int_a^{x_1} \kappa(u)du}} \approx e^{i\phi} e^{-\int_a^{x_2} \kappa(u)du} \]

\[ |\frac{C(x_2)}{C(x_1)}|^2 \approx e^{-2 \int_{x_1}^{x_2} \kappa(u)du} \]

\[ T_{wkb} \approx e^{-2 \int_{x_1}^{x_2} dx \sqrt{\frac{2m^*_c}{\hbar^2} [E_c(x) - E]}} \]

\[ T_{wkb} \approx e^{-\left( \frac{t_h}{0.1 \text{nm}} \right) \sqrt{\frac{m^*_c}{m_e} \cdot \frac{V_0}{1 \text{eV}}}} \]

The WKB Tunneling Probability for tunneling in semiconductors
Tunneling in Homojunctions

Reverse-bias tunneling current

If \( qV >> 2\bar{E}_\parallel \),

\[
T \approx \frac{q^2 m^* T_0 \bar{E}_\parallel}{2\pi^2 \hbar^3} V
\]

\[\implies \sim \text{linear } I - V.\]

\[
T_0 = \exp\left[-\frac{\pi \sqrt{m^* E_g^{3/2}}}{2\sqrt{2} q F \hbar}\right]
\]

\[
\bar{E}_\parallel = \frac{\sqrt{2} q F \hbar}{2\pi \sqrt{m^* \sqrt{E_g}}}
\]

Tunneling current depends exponentially on the
- Bandgap
- Effective mass
- Electric field
Tunneling in Homojunctions

A back-of-the-envelope evaluation of interband tunneling current in semiconductors

\[ T_{WKKB} \sim e^{-2S} \]

\[ S = \int_{x_1}^{x_2} \sqrt{\frac{2m^*}{\hbar^2}} (E_g - eFx) \, dx \]

\[ x_1 = 0, \quad x_2 = E_g/eF \]

\[ \Rightarrow T_{WKKB} \sim \exp\left[-\frac{2^\frac{5}{2}}{3eFt^h} E_g^\frac{3}{2}\right] = \exp\left[-F_0/F\right] \]

\[ \hbar \frac{dk}{dt} = eF \Rightarrow k(t) = k(0) + \frac{eF}{\hbar} t \]

\[ \Rightarrow \text{Bloch Osc. period: } T = \frac{\hbar G}{eF} \]

Rate of incidence on band-edge:

\[ \gamma_{inc} = \frac{1}{T} = \frac{eF}{\hbar G} = \frac{a_0 eF}{\hbar} \]

where \( G = 2\pi/a_0 \) is the reciprocal lattice vector.

Frequency of electron escape:

\[ f_{esc} \sim \gamma_{inc} T_{WKKB} = \frac{a_0 eF}{\hbar} \times \exp\left[-\frac{2^\frac{5}{2}}{3eFt^h} E_g^\frac{3}{2}\right] \]

Tunneling current density:

\[ J_T \sim eN_s f_{esc} = eN_v x_{win} f_{esc} = eN_v (eV/F)f_{esc} \]

\[ \Rightarrow J_T \sim \frac{e^2}{h} \cdot \left[a_0 N_v \exp\left[-\frac{2^\frac{5}{2}}{3eFt^h} E_g^\frac{3}{2}\right]\right] \cdot V \]

Very rough estimates! (V=0.2 Volt)

Debdeep Jena (djena@cornell.edu)
Tunneling in Semiconductor Homojunctions

Increasing doping in the pn junction

Doping: $10^{19}$, $5 \times 10^{19}$, $10^{20}$/cm$^3$

Peak electric field increases

@0.3 V
Tunneling in Semiconductor Homojunctions

Increasing doping in the pn junction

Doping: $10^{19}$, $5 \times 10^{19}$, $10^{20}$/cm$^3$

Peak electric field increases

Current density (A/cm$^2$)

@0.3 V

Solar cells
Tunneling in Semiconductor Homojunctions

Increasing doping in the pn junction

Doping: $10^{19}$, $5 \times 10^{19}$, $10^{20}$/cm$^3$

Peak electric field increases

@0.3 V

Solar cells

LEDs

Si

GaN

InN

Ge

Current density (A/cm$^2$)
Tunneling in Semiconductor Homojunctions

Increasing doping in the pn junction

Doping: $10^{19}$, $5 \times 10^{19}$, $10^{20}$/cm$^3$

Peak electric field increases

Solar cells

LEDs

Lasers

Ge

InN

Si

GaN

@0.3 V
Tunneling in Semiconductor Homojunctions

Increasing doping in the pn junction

Doping: $10^{19}$, $5 \times 10^{19}$, $10^{20}$/cm$^3$

Peak electric field increases

Increasing doping in the pn junction

Peak electric field increases

@0.3 V

Solar cells

LEDs

Lasers

TFETs

Si

Ge

GaN

Doping: $10^{19}$, $5 \times 10^{19}$, $10^{20}$/cm$^3$
Increasing doping in the pn junction

Doping: $10^{19}$, $5 \times 10^{19}$, $10^{20}$/cm$^3$

$3 \times 10^{20}$/cm$^3$ + Donor delta spikes

Peak electric field increases
Tunneling in Semiconductors

Zener (Interband) Tunneling

bulk semiconductor  \hspace{1cm} p-n junctions  \hspace{1cm} heterojunctions

ECE 4070 / MSE 6050

* "Interband" Zener Tunneling Currents
Resonant Tunneling in Semiconductor Nanostructures

Debdeep Jena (djena@cornell.edu)
The idea behind “Scattering”

Discrete, specific frequencies

Continuous, all weights

“Bands” and “Gaps”

States mixed; extended states may not be allowed → localization, but gaps still possible
How to find $f(k)$ in the presence of scattering

The Boltzmann Transport Equation

$$\frac{\partial f_k}{\partial t} + v_k \cdot \nabla_r f_k + \frac{F}{\hbar} \cdot \nabla_k f_k = \sum_{k'} [S(k' \to k) f_{k'}(1 - f_k) - S(k \to k') f_k(1 - f_{k'})].$$

scattering term, $\hat{C} f_k$

$$S(k \to k') = \frac{2\pi}{\hbar} |W_{k,k'}|^2 \delta(E_k - E_{k'} \pm \hbar\omega)$$

Fermi's Golden Rule for Scattering Rates
How to find the quantum current with scattering

$$g_d(\varepsilon) = \frac{1}{2^{d-1} \pi^{\frac{d}{2}} \Gamma(\frac{d}{2}) \left(\frac{2m^*}{\hbar^2}\right)^{\frac{d}{2}} \varepsilon^{\frac{d}{2}-1}}$$

$$n = \int \frac{d^dk}{(2\pi)^d} f(k) = \int d\varepsilon f(\varepsilon) g_d(\varepsilon)$$

$$J = 2e \int \frac{d^dk}{(2\pi)^d} v f(k).$$

$$J_i = en \left( \frac{2e}{dm^*} \int d\varepsilon \tau_m \varepsilon^{\frac{d}{2}} \frac{\partial f_0(\varepsilon)}{\partial \varepsilon} \right) F_i$$

Mobility definition for any dimension

$$f(k) = f_0(k) + e F_i \tau(k) v_i \frac{\partial f_0}{\partial \varepsilon}$$

The Boltzmann Transport Equation

Water

River Bed

Water

River Bed

River bed fluctuations 'screened' by water

Insufficient water fails to screen fluctuations

$$U_{sc}(q) = \frac{e^2}{4\pi \varepsilon^2 K} \int r^2 \sin(\theta) dr d\theta d\phi \frac{e^{-\frac{r}{\lambda_D}}}{r} e^{iqr \cos(\theta)}$$

Example of scattering matrix element

$$\mu_I = \frac{2^7 (4\pi \varepsilon) \sqrt{2\pi}}{\pi^{\frac{3}{2}} Z^2 e^3 \sqrt{m^* N_D F(\beta)}} \sim \frac{T^{\frac{3}{2}}}{N_D}$$
The Boltzmann Transport Equation gives $f(k)$

The Boltzmann transport equation gives a full-blown treatment of transport properties, and can be solved in several levels of approximation.

The Boltzmann Transport Equation

$$ f_0(\varepsilon) = \frac{1}{1 + e^{\frac{\varepsilon - \mu}{k_B T}}} $$

$df \over dt = \frac{F_t}{\hbar} \cdot \nabla_k f(k) + v \cdot \nabla_r f(k) + \frac{\partial f}{\partial t}$

Particle number conserved

$$ \frac{\partial f}{\partial t} = \frac{\partial f}{\partial t}_{\text{coll}} - \frac{F_t}{\hbar} \cdot \nabla_k f(k) - v \cdot \nabla_r f(k) $$

Relaxation time approximation

$$ \frac{\partial f}{\partial t} \bigg|_{c} = -\frac{(f - f_0)}{\tau_m} $$

**equilibrium**

$\Rightarrow$

**perturbation**

$\Rightarrow$

**scattering**

**equilibrium**

$\Rightarrow$

**bandstructure**

$\Rightarrow$

**applied forces**

$\Rightarrow$

**conc. gradients**
Formalism for diffusive charge transport

- Find the perturbation potential due to the defect.
- Use Fermi’s Golden rule to evaluate the single-particle scattering rate
- Add up for all allowed states
- Use the solution of Boltzmann equation to find the mobility/conductivity.

\[
\mathbf{E}_c(\mathbf{r}) = \mathbf{E}_c^0 + \mathbf{W}(\mathbf{r})
\]

\[
V(q) = \langle k' | W(\mathbf{r}) | k \rangle
\]

\[
\frac{1}{\tau_{kk'}} = \frac{2\pi}{\hbar} |V(q)|^2 \delta[E_{k'} - (E_k \pm \hbar \omega)]
\]

\[
f(k) = f_0(k) + eFz\tau(k)\frac{\partial f_0}{\partial \epsilon}
\]

\[
\mathbf{J} = 2e \int \frac{d^d k}{(2\pi)^d} \mathbf{v} f(k)
\]

Distribution function: Solution of Boltzmann Transport Equation

Current density: Sum over all group velocities \(\mathbf{v}\) in k-space
The Boltzmann Transport Equation

Boltzmann equation →

\[ f(k) = f_0(k) + e \tau_m(k)(\mathbf{F} \cdot \mathbf{v}) \frac{\partial f_0(k)}{\partial \varepsilon} \]

\[ \frac{1}{\tau_m(k)} = \sum_k S(k, k')(1 - \cos \theta) - \text{Momentum scattering time} \quad (\mu = \frac{e\langle \tau_m(k) \rangle}{m^*}) \]

\[ \frac{1}{\tau_q(k)} = \sum_k S(k, k') - \text{Quantum scattering time} \]

Most general expression for ‘Current Density’ in ‘d’ dimensions:

\[ J_d = q \times \frac{g_s g_v}{L^d} \sum_k \mathbf{v}_g(k) f(k) \]

where \( \mathbf{v}_g(k) \) is the group velocity, \( f(k) \) is the Fermi-Dirac function.

\( qv_g \) may be replaced by other physical quantities:

\( qv_g \rightarrow \) charge current density (electrical cond.)

1 \( \rightarrow \) carrier density

E \( (k) \rightarrow \) heat current density (thermal cond.)

…
Time-dependent perturbation theory

If the system was in an eigenstate $|\Psi_{t_0}\rangle = |0\rangle$ of energy $E_0$ at time $t_0$, then the state at a future time differs from the initial state by a phase factor $e^{-i\frac{E_0}{\hbar}(t-t_0)}$.

$H_0$ is the Hamiltonian operator.

$\Psi(t)$ evolves in the interaction picture.

If $W=0$, the state vector does not rotate in time in the interaction picture.

$\Psi(t)$ evolves in the Schrodinger picture.

Starting point for time-dependent perturbation theory.
The probability of the state making a transition from $|0\rangle$ to $|n\rangle$ at time $t$ is

$$|\langle n|\Psi(t)\rangle|^2 = |\langle n|W|0\rangle|^2 \approx |\langle n|W|0\rangle|^2 \frac{e^{2\eta t}}{(E_0 - E_n)^2 + (\eta)^2}.$$ 

The rate of transitions from state $|0\rangle \rightarrow |n\rangle$ is

$$\frac{1}{\tau_{|0\rangle \rightarrow |n\rangle}} = \frac{d}{dt}|\langle n|\Psi(t)\rangle|^2 \approx |\langle n|W|0\rangle|^2 \frac{2\eta}{(E_0 - E_n)^2 + (\eta)^2} e^{2\eta t}.$$ 

$$\lim_{\eta \to 0^+} \frac{2\eta}{x^2 + \eta^2} = \lim_{\eta \to 0^+} \frac{1}{i} \left[ \frac{1}{x - i\eta} - \frac{1}{x + i\eta} \right] = 2\pi \delta(x)$$

$$\delta(ax) = \delta(x)/|a|$$

$$\frac{1}{\tau_{|0\rangle \rightarrow |n\rangle}} \approx \frac{2\pi}{\hbar} |\langle n|W|0\rangle|^2 \delta(E_0 - E_n),$$

Fermi's golden rule for time-varying potentials

Two useful results to be used extensively later!

\[ \theta(\omega) = \int_0^\infty dt e^{i\omega t} = \lim_{\eta \to 0^+} \int_0^\infty dt e^{-\eta t} e^{i\omega t} = \lim_{\eta \to 0^+} \frac{i}{\omega + i\eta} = \frac{i}{\omega^+} \]

\[ \frac{1}{\omega^+} = P[\frac{1}{\omega}] - i\pi \delta(\omega) \rightarrow \int_{-\infty}^{+\infty} d\omega \frac{f(\omega)}{\omega^+} = P[\int_{-\infty}^{+\infty} d\omega \frac{f(\omega)}{\omega}] - i\pi f(0) \]

Here $P[...]$ is the "principal part" of a function

Fermi’s golden rule for oscillating potentials

Perturbations oscillating in time

\[ W_t = 2We^{nt} \cos(\omega t) = e^{nt}W(e^{i\omega t} + e^{-i\omega t}) \]

\[ \langle n|\Psi(t)\rangle \approx \frac{\langle n|W|0\rangle}{i\hbar} \left( \int_{t_0}^t dt' e^{i\left(\frac{E_n - E_0 + i\hbar\omega}{\hbar}\right)t'} e^{nt'} + \int_{t_0}^t dt' e^{i\left(\frac{E_n - E_0 - i\hbar\omega}{\hbar}\right)t'} e^{nt'} \right) \]

\[ \frac{1}{\tau_{|0\rangle \rightarrow |n\rangle}} \approx \frac{2\pi}{\hbar} \times |\langle n|W|0\rangle|^2 \times \left[ \delta(E_0 - E_n + \hbar\omega) + \delta(E_0 - E_n - \hbar\omega) \right]. \]

absorption

emission
Scattering rate due to point scatterers

\[ W(r) = V_0 \delta(r) \]

\[ \langle k'|V_0 \delta(r)|k \rangle = \int d^3r \left( \frac{e^{-ik' \cdot r}}{\sqrt{V}} \right) V_0 \delta(r) \left( \frac{e^{+ik \cdot r}}{\sqrt{V}} \right) = \frac{V_0}{V} \]

\[ \frac{1}{\tau(|k\rangle \to |k'\rangle)} = \frac{2\pi}{\hbar} \left( \frac{V_0}{V} \right)^2 \delta(E_k - E_{k'}) \]

\[ \frac{1}{\tau(|k\rangle)} = \sum_{k'} \frac{1}{\tau(|k\rangle \to |k'\rangle)} = \frac{2\pi}{\hbar} \left( \frac{V_0}{V} \right)^2 \sum_{k'} \delta(E_k - E_{k'}) \]

\[ \frac{1}{\tau(E_k)} = \frac{2\pi}{\hbar} \left( \frac{V_0}{V} \right)^2 n_{sc} V \int \frac{d^3k'}{(2\pi)^3} \delta(E_k - E_{k'}) = \frac{2\pi}{\hbar} V_0^2 n_{sc} g(E_k) \]
Fermi’s Golden Rule tells us that the scattering potential is the SUM of ALL the scatterers in the macroscopic crystal.

How do multiple scattering centers add up and contribute to the total scattering rate?

\[
\frac{1}{\tau_{kk'}} = \frac{2\pi}{\hbar} |V(q)|^2 \delta[E_{k'} - (E_k \pm \hbar \omega)]
\]

\[
q = k - k'
\]

\[
V(q) = \langle k' | W(r) | k \rangle
\]

\[
= \int_V \left[ \frac{e^{-i k' \cdot r}}{\sqrt{V}} u^*_K(r) \right] \times W(r) \times \left[ \frac{e^{+i k \cdot r}}{\sqrt{V}} u_K(r) \right] d^3r
\]

\[
= \int_V \left[ \frac{e^{i(k-k') \cdot r}}{V} \right] W(r) \times [u^*_K(r) u_K(r)] d^3r
\]

\[
\approx \left( \int_V e^{i q \cdot r} W(r) \frac{d^3r}{V} \right) \times \left( \int_{\Omega} u^*_K(r) u_K(r) \frac{d^3r}{\Omega} \right)
\]

\[
\approx \left( \int_{\text{crystal}} e^{i q \cdot r} W(r) \frac{d^3r}{V} \right) \times \left( \int_{\Omega} u^*_K(r) u_K(r) \frac{d^3r}{\Omega} \right)
\]

\[
= 1
\]

\[
V(q) \approx \int_V e^{i q \cdot r} W(r) \frac{d^3r}{V}
\]
Scattering by many impurities

\[ W_{\text{total}}(r) = W(r) + W(r - R_1) + W(r - R_2) + \ldots \]

\[ V_0(q) \approx \int_V e^{i\mathbf{q} \cdot \mathbf{r}} W(r) \frac{d^3r}{V} \]

\[ V_{\text{total}}(q) = V_0(q) + \int_V e^{i\mathbf{q} \cdot \mathbf{r}} W(r - R_1) \frac{d^3r}{V} + \ldots \]

\[ V_{\text{total}}(q) = V_0(q) + V_0(q)e^{i\mathbf{q} \cdot \mathbf{R}_1} + V_0(q)e^{i\mathbf{q} \cdot \mathbf{R}_2} \ldots \]

|\[ V_{\text{total}}(q) \]²| = |V_0(q)|²[(1 + e^{i\mathbf{q} \cdot \mathbf{R}_1} + e^{i\mathbf{q} \cdot \mathbf{R}_2} \ldots) \times (1 + e^{-i\mathbf{q} \cdot \mathbf{R}_1} + e^{-i\mathbf{q} \cdot \mathbf{R}_2} \ldots)]

\[ \approx 0(RPA) \]

\[ |V_{\text{total}}(q)|^2 = N_{\text{imp}} |V_0(q)|^2 \]

\[ \frac{1}{\tau_{kk'}^{(\text{total})}} = \frac{2\pi}{\hbar} N_{\text{imp}} \times |V_0(q)|^2 \delta[E_{k'} - (E_k \pm \hbar\omega)] \]

Scattering rate is linearly proportional to impurity density in the dilute uncorrelated limit!
Scattering events in semiconductors

A static periodic potential causes no scattering → every other potential causes scattering!

Periodic ‘non-static’ potentials: Phonons.
Static non-periodic potentials: Defects & Impurities.
General Nature of Scattering Rates

Scattering rates are typically proportional to the density of states

From Lundstrom: Fundamentals of Carrier Transport
Scattering by each type of impurity affects the net electron mobility.

- Mobility in a ultra-clean (defect-free) semiconductor is limited by phonon (optical+acoustic) scattering.
- If the scattering rate of defects/impurities exceed that of phonons, then they determine the mobility.
- Method: find the scattering rate due to each type of defect. The total scattering rate is the sum of all.
Scattering by a neutral impurity

\[ \mathcal{E}_c(r) = \mathcal{E}_c^0 + W(r) \]

\[ W(r) = W_0 \Theta(r - r_0) \]

\[ V(q) = \langle k' | W(r) | k \rangle \]

\[ \frac{1}{\tau_{kk'}} = \frac{2\pi}{\hbar} |V(q)|^2 \delta[E_{k'} - (E_k \pm \hbar \omega)] \]

\[ (\tau_m) = \frac{2}{3} \frac{\int_0^\infty \tau_m (-\partial \rho_0/\partial x) x^{3/2} dx}{\int_0^\infty \rho_0 x^{1/2} dx} \]

\[ \mu = \frac{e}{20 a_B \hbar} \frac{m/m_0}{\kappa N^x} \]

which is independent of temperature.

\[ \mu = \frac{1.44 \times 10^{22} \text{ cm}^{-3}}{N^x} \frac{m/m_0}{\kappa} \]

For example, for electrons in Ge, where \( m/m_0 = 0.12 \) and \( \kappa = 16 \), a mobility of \( 1.1 \times 10^3 \text{ cm}^2/\text{V s} \) is obtained assuming, e.g., \( 10^{17} \text{ cm}^{-3} \) neutral impurities.
Scattering by charged impurities

Screened coulomb scattering potential

\[ V(r) = -(Z \frac{|e|}{4\pi \varepsilon_0 r}) \exp(-r/L_D) \]

\[ |k - k'| \approx 2k \sin(\theta/2) \]

\[ \beta_{BH} = 2 \frac{m}{\hbar} \left( \frac{2}{3} k_B T \right)^{1/2} L_D \]

Brooks-Herring dimensionless factor

The mobility \( \mu \) is given by

\[ \mu = \frac{2^{7/2} (4\pi \varepsilon_0)^2 (k_B T)^{3/2}}{\pi^{3/2} Z^2 e^3 m^{1/2} N_1 \left[ \ln (1 + \beta_{BH}^2) - \beta_{BH}^2 / (1 + \beta_{BH}^2) \right]} \]

which in units of \( \text{cm}^2/\text{Vs} \) is

\[ \mu = \frac{3.68 \times 10^{20} \text{ cm}^{-3} \frac{1}{Z^2} \left( \frac{x}{16} \right)^2 \left( \frac{T}{100 \text{ K}} \right)^{1.5}}{m/m_0^{1/2} \left[ \ln (1 + \beta_{BH}^2) - 0.434 \beta_{BH}^2 / (1 + \beta_{BH}^2) \right]} \]

and the log is to the base 10.
Phonons in Semiconductors

Newton's law for mass-spring chain

\[ F = M \frac{d^2 u_s}{dt^2} = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) \]

Vibrations form a wave

\[ u_s = u_0 e^{i(qsa - \omega t)} \]

Acoustic phonon dispersion

\[ \omega^2(q) = \frac{2C}{M} (1 - \cos qa) \]
Phonons in Semiconductors

Acoustic and optical phonon dispersion

$$\omega^2(k) = \frac{C}{M_r} \left[ 1 \pm \sqrt{1 - \frac{2M_r}{M_1 + M_2} (1 - \cos ka)} \right]$$
Phonons in Semiconductors

Typical phonon spectra of semiconductors

Difference in energies of longitudinal and optical acoustic phonons
Electron-Def. Pot. Acoustic Phonon interaction

Deformation Potential Acoustic Phonon Scattering Potential

\[ u(r, t) = au(r, t) \]  

(6.4)

where

\[ u(r, t) = u \exp [i(q_s \cdot r - \omega_s t)] \]  

(6.5)

In these equations \( a \) is the displacement direction, and \( u \) is the amplitude. The strain associated with the displacement is

\[ \nabla \cdot u(r, t) = a \cdot \nabla u(r, t) \]  

(6.6)

\[ \nabla \cdot u(r, t) = iq_s \cdot au(r, t) \]  

(6.7)

Equation (6.7) indicates that for the transverse components of a phonon where the displacement and the wavevector are orthogonal, \( q_s \cdot a = 0 \), and no strain is produced. The scattering potential for the longitudinal component is, therefore,

\[ \Delta U(r, t) = \xi_A \nabla \cdot u(r, t) \]  

(6.8)

where the deformation potential, \( \xi_A \), in units of energy, is defined as the proportionality constant between the scattering potential (units of energy) and the strain.
Electron-Piezoelectric Acoustic Phonon interaction

Piezoelectric Acoustic Phonon Scattering Potential

\[ \Delta U(r, t) = -q \psi(r, t) \]

\[ \psi(r, t) = -\int E(r, t) \cdot dr \]

\[ D(\omega) = \epsilon(\omega)E = \epsilon_0E + P(\omega) \]

\[ D(0) = \epsilon(0)E = \epsilon_0E + P(0) \]

\[ E(r, t) = -\frac{\epsilon_{pe}}{\epsilon(0)} \nabla u(r, t) \]

\[ \Delta U(r, t) = \frac{q\epsilon_{pe}}{\epsilon(0)} \nabla \cdot u(r, t) \]

Piezo charge

Figure 6.2: Displacements of a diatomic chain for LA and TA phonons at (a) the center and (b) the edge of the Brillouin zone. The lighter mass atoms are indicated by open circles. For zone edge acoustic phonons only the heavier atoms are displaced.
Electron-Def. Pot. Optical Phonon interaction

Typical phonon spectra of semiconductors

Optical Deformation Potential scattering potential $D \sim 10^8$ eV/cm
Electron-Polar Optical Phonon interaction

\[ D(0) = \varepsilon(0) E = \varepsilon_0 E + P(0) \]

\[ D(x) = \varepsilon(x) E = \varepsilon_0 E + P(x) \]

\[ P(0) = P(x) = P_0 \]

Using (6.22) in (6.20) and subtracting (6.21), we obtain

\[ \varepsilon(0) E = \varepsilon(x) E + P_0 \]

or

\[ D(0) = \varepsilon(x) E + P_0 \]

From (6.24) we can determine the internal fields induced by the optical phonon polarization of the unit cell.

The polarization of a unit cell, \( P_0(x, r) \), is determined by the relative displacement of the ions in a unit cell, \( u(x, r) \), and the effective ionic charge, \( \varepsilon^* \), such that

\[ P_0(x, r) = \frac{\varepsilon^*}{\Omega} \delta u(x, r) \]

In this equation \( \Omega = V/N \) is the volume of the \( N \) primitive or Wigner-Seitz unit cells and \( \varepsilon^* \) is the Born effective charge given by

\[ \varepsilon^* = \Omega \varepsilon_0 \varepsilon(x) \rho \left[ \frac{1}{\varepsilon(x)} - \frac{1}{\varepsilon(0)} \right]^{1/2} \]

where \( \rho \) is the mass density. This equation is derived in Chapter 7. Assuming no space or surface charges, (6.24) and (6.25) give an internal field,

\[ E(x, r) = -\frac{\varepsilon^*}{\Omega \varepsilon(x)} \delta u(x, r) \]

Optical phonon absorption and emission processes

\[ \frac{\varepsilon_s(0)}{\varepsilon_s(\infty)} = \left( \frac{\omega_{LO}}{\omega_{TO}} \right)^2 \]

as the Lyddane–Sachs–Teller relation

Polar optical phonon scattering potential

Frohlich interaction
Amplitude of Phonon Vibrations

\[ u_s(x, t) = u_0 e^{i(\beta x - \omega t)} + u_0 e^{-i(\beta x - \omega t)} \]
\[ |u_s|^2 = 4u_0^2 \cos(\beta x - \omega t) \]

\[ \text{KE} = \frac{1}{2} M \left( \frac{du_s}{dt} \right)^2 = 2M \omega^2 u_0^2 \sin^2(\beta x - \omega t) \]
\[ \text{PE} = \frac{1}{2} Ku_s^2 = 2K u_0^2 \cos^2(\beta x - \omega t) \]

but... \( \omega^2 = \frac{K}{M} \rightarrow \)
\[ \text{KE} + \text{PE} = 2M \omega^2 u_0^2 = N_\omega \cdot \hbar \omega \rightarrow \]

since... \( M = \rho V, \)

\[ u_0^2 = \frac{\hbar}{2\omega \rho V} \cdot N_\omega \]

\[ N_\omega(T) = \frac{1}{e^{\frac{\hbar \omega}{kT}} - 1} \]

Typical phonon spectra of semiconductors

Vibration amplitude as a function of the temperature: Quantum-Classical connection of the phonon harmonic oscillator
Electron-Phonon Scattering Rates

Polar optical phonon

\[ D = \epsilon_0 E + \frac{q^* u}{\Omega} \]

\[ E(x, t) = -\frac{q^* u}{\epsilon_0 \Omega} \]

\[ W(r, t) = -q \int dx E(x, t) = \frac{q}{i\beta \epsilon_0} \cdot \frac{q^*}{\Omega} \cdot u_0 e^{i(\beta r - \omega t)} \]

\[ \left( \frac{q^*}{\Omega} \right)^2 = \rho \epsilon_0 \omega_0^2 \left( \frac{1}{\epsilon_s} - \frac{1}{\epsilon_0} \right) \]

\[ W(r, t) = -q \int dx E(x, t) = \frac{q \omega_0 \sqrt{\rho}}{i\beta} \sqrt{\frac{1}{\epsilon_s^0} - \frac{1}{\epsilon_s^0}} \cdot u_0 e^{i(\beta r - \omega t)} \]

Piezoelectric acoustic phonon

\[ D = \epsilon_0 \epsilon_s e + \frac{e_{pz} \partial u}{\partial x} \]

\[ E(x, t) = -\frac{e_{pz}}{\epsilon_0 \epsilon_s} \cdot \frac{\partial u}{\partial x} \]

\[ W(r, t) = -q \int dx E(x, t) = \frac{q e_{pz}}{\epsilon_0 \epsilon_s} u_0 e^{i(\beta r - \omega t)} \]

\[ K^2 = \frac{e_{pz}^2}{\epsilon_0 \epsilon_s v_s} \]

\[ \frac{1 - K^2}{1 - K^2} = \frac{e_{pz}^2}{\epsilon_0 \epsilon_s v_s} \]

\[ S(k \rightarrow k') = \frac{2\pi}{\hbar} |W(q_s)|^2 \frac{\hbar}{2\rho \Omega \omega_q} \left[ N(\omega_q) + \frac{1}{2} \mp \frac{1}{2} \delta[ \pm \cos(\theta) + \frac{q_s}{2k} \mp \frac{\omega_q}{v_{qs}}] \right] \]

Deformation potential acoustic phonon

\[ W(x, t) = D_{ac} \frac{\partial u}{\partial x} \]

\[ W(r, t) = D_{ac} (\nabla \cdot \mathbf{u}) = iD_{ac} \beta u_0 e^{i(\beta r - \omega t)} \]

Deformation potential optical phonon

\[ W(r, t) = D_{op} u = D_{op} u_0 e^{i(\beta r - \omega t)} \]

Momentum conservation

\[ \hbar k' = \hbar k + \hbar \beta \]

Energy conservation

\[ E_{k'} = E_k \pm \hbar \omega_\beta \]

\[ k'^2 = k^2 + \beta^2 \pm 2k \beta \cos \theta \]

\[ \beta^2 \pm 2\beta k \cos \theta \mp \frac{2m^* \hbar \omega_\beta}{\hbar^2} = 0 \]

For acoustic phonons, \( \hbar \omega_\beta = \hbar v_\beta \), and we get

\[ \beta = 2k \mp \hbar \cos \theta \pm \frac{m^* v_s}{\hbar k} = 2k \mp \frac{v_s}{v_k} \]

Allowed angles for acoustic phonon scattering events

For optical phonons, we get

\[ \beta = \mp k \cos \theta \pm \sqrt{k^2 \cos^2 \theta \pm \frac{2m^* \hbar \omega_\beta}{\hbar^2}} \]

Allowed angles for optical phonon scattering events

Debdeep Jena (djena@cornell.edu)
Electron-Acoustic Phonon interaction: Mobility

\[ \delta r = A_{i} \exp \left[ \pm \frac{1}{2} \left( \frac{q_{i}}{r} \right) \right], \]

\[ |H_{i\kappa}| = \frac{\varepsilon_{ac} q_{i} A_{i}}{V} |\exp \left[ \pm \frac{1}{2} \left( \frac{k - k' \pm q_{i}}{r} \right) \right]|. \]

\[ K' = k \pm q_{i} \]

\[ |H_{k'k}| = \varepsilon_{ac} q_{i} A_{i}. \]

\[ 2M\omega^{2}u_{0}^{2} \approx N_{ph} \times \hbar \omega \]

Acoustic phonon scattering

Deformation potential

\[ A_{i} \rightarrow |\exp (i\varepsilon_{i}/k_{B} T) - 1| \]

\[ |H_{k'k}| = \varepsilon_{ac} q_{i}((N_{i} + 1/2) \pm 1/2) \varepsilon_{ac} V_{\omega}^{2} |^{1/2}. \]

\[ |H_{k'k}|' = \varepsilon_{ac} q_{i}[(k_{B}/2 V_{\omega})^{2}]^{1/2} = \varepsilon_{ac} [(k_{B}/2 V_{\omega})^{2}]^{1/2} \]

SHO: |amplitude|\(^{2} \sim \) number of phonons

absorption\(\sim\)emission

Piezoelectric

Coupling \(K \sim 10^{-3}\)

\[ \Delta U(r, t) = \varepsilon_{A} \nabla \cdot \mathbf{u}(r, t) \]

\[ \mu = \frac{2}{3} \frac{e h^{4} c_{l}}{m^{5/2}(k_{B})^{3/2} e_{ac}^{2}} T^{-3/2} \]

which in units of \(\text{cm}^{2}/\text{V s}\) is given by

\[ \mu = 3.06 \times 10^{4} \frac{c_{l}10^{12} \text{ dyn cm}^{-2}}{(m/m_{0})^{5/2}(T/100 \text{ K})^{3/2}(e_{ac}/e)^{2}} \propto T^{-3/2}. \]

Piezoelectric

\[ \Delta U(r, t) = \frac{B_{ps} c_{l}}{e(0)q_{s}} \nabla \cdot \mathbf{u}(r, t) \]

\[ K^{2} = \frac{e_{ps}^{2} c_{l}}{\tau \kappa_{0} + e_{ps}^{2} c_{l}} \]

\[ \mu = 16 \frac{\sqrt{2}}{3} \frac{m^{5/2} e^{2} K^{2}(k_{B} T)^{1/2}}{e^{2} K^{2}(k_{B} T)^{1/2}} \alpha T^{-1/2} \]

and in units of \(\text{cm}^{2}/\text{V s}\)

\[ \mu = 2.6 \frac{\mathcal{X}}{(m/m_{0})^{5/2} K^{2}(T/100 \text{ K})^{1/2}}. \]
Deformation potential Optical Phonon

\[ \hbar \omega_0 = k_B \Theta. \]

\( \Theta \) is known as the Debye temperature

Polar Optical Phonon Scattering

\[ \mu = \frac{4 \sqrt{2 \pi} e \hbar^2 q (k_B \Theta)^{1/2}}{3 m^{5/2} D^2} f(T/\Theta). \]

The function \( f(T/\Theta) \) is given by

\[ f(T/\Theta) = \left(2z\right)^{3/2} \left(e^{2z} - 1\right) \int_0^\infty \frac{y^{3/2} e^{-2y} dy}{\sqrt{y + 1 + e^{2z}} \text{Re}\{\sqrt{y - 1}\}}. \]

where \( z = \Theta/2T \) and \( y = \epsilon/k_B \Theta \). The function is shown

Its numerical value in units of \( \text{cm}^2/\text{V} \text{s} \) is given by

\[ \mu = 2.04 \times 10^3 \frac{(\rho/ \text{g cm}^{-3}) (\Theta/400 \text{ K})^{1/2}}{(m/m_0)^{5/2} (D/10^8 \text{ eV cm}^{-1})^2} f(T/\Theta). \]


The mobility is simply \((e/m) \tau_m:\)

\[ \mu = \left[|e|/(2m \alpha \omega_0)\right] \exp(\Theta/T) \]

which in units of \( \text{cm}^2/\text{V} \text{s} \) is given by

\[ \mu = 2.6 \times 10^5 \frac{\exp(\Theta/T)}{\alpha(m/m_0) (\Theta/K)} \text{ for } T \ll \Theta \]

For example, in n-type GaAs where \( \Theta = 417 \text{ K}, m/m_0 = 0.072, \alpha = 0.067 \), we calculate a mobility at 100 K of \( 2.2 \times 10^5 \text{ cm}^2/\text{V} \text{s} \). This is of the order of magnitude of the highest mobilities observed in this material. At this and
Electron-Photon Interactions

Major III-V Semiconductor families:

- GaAs-based (Al/GaAs/GaAs)
  (strain-free, or pseudomorphic)
- InP based (InGaAs channels)
- 6.1 Angstrom/narrow gap channels
  (generally grown metamorphically on GaAs)
- GaN-based (InGaN/GaN and Al/GaN/GaN)
  (typically pseudomorphic)
Electron-Photon Interactions

Fig. 12.12. Bandgap energy versus lattice constant of III-V nitride semiconductors at room temperature.

Major III-V Semiconductor families:
- GaAs-based (AlGaAs/GaAs)
  (strain-free, or pseudomorphic)
- InP based (InGaAs channels)
- 6.1 Angstrom/narrow gap channels
  (generally grown metamorphically on GaAs)
- GaN-based (InGaN/GaN and AlGaN/GaN)
  (typically pseudomorphic)
How to make white light with semiconductors

\[
IQE = \frac{\text{Light generated}}{\text{Electrons injected}} = \frac{R_{\text{radiative}}}{R_{\text{radiative}} + R_{\text{nonradiative}}} = \frac{Bn^2}{An + Bn^2 + Cn^3}.
\]
Electron-Photon Interactions

Figure 26.1: Schematic absorption spectrum $\alpha(\hbar\omega)$ of bulk semiconductors. The insets depict various state transitions upon absorption of photons.

- Absorption power is Quantified by “Absorption Coefficient”
- A negative absorption coefficient is equivalent to optical gain!

Adapted from: Wolfe/Holonyak/Stillman, Physical Properties of Semiconductors

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Absorption Coefficient of Compound Semiconductors

\[ \alpha(\hbar\omega) = \frac{\text{Number of photons absorbed per unit volume per second}}{\text{Number of photons incident per unit area per second}} \]

\[ \alpha(\hbar\omega) = \frac{R}{S/\hbar\omega} \]

Number of photons incident per unit area per second:

- Vector potential: \( A(r, t) = \hat{e}A_0 \cos(k_{\text{op}} \cdot r - \omega t) \)
- Electric Field: \( E(r, t) = -\frac{\partial}{\partial t} A(r, t) = -\hat{e}\omega A_0 \sin(k_{\text{op}} \cdot r - \omega t) \)
- Magnetic Field: \( H(r, t) = \frac{1}{\mu} \nabla \times A(r, t) = -\frac{1}{\mu} k_{\text{op}} \times \hat{e}A_0 \sin(k_{\text{op}} \cdot r - \omega t) \)

Poynting Vector:

\[ S(r, t) = E(r, t) \times H(r, t) = k_{\text{op}} \frac{\omega A_0^2}{\mu} \sin^2(k_{\text{op}} \cdot r - \omega t) \]

\[ \langle S(r, t) \rangle = \frac{\omega A_0^2}{2\mu} k_{\text{op}} \]

Incident energy per unit area per second:

\[ S = |\langle S(r, t) \rangle| = \frac{\omega A_0^2}{2\mu} k_{\text{op}} = \frac{n_r c \epsilon_0 \omega^2 A_0^2}{2} \]

- Incident photon number per unit area per second: \(|\text{Poynting vector}|/\text{photon energy}
- Goes as square of the amplitude of vector potential (or electric field, or magnetic field)
Absorption Spectra of Compound Semiconductors

Optical absorption coeff. of bulk semiconductor (general form applicable to quantum wells, etc...)

\[ \alpha_0(\hbar\omega) = C_0 \left| \hat{e} \cdot \mathbf{p}_{cv} \right|^2 \cdot \rho_T(\hbar\omega - E_g) \]

\[ \rho_T(u) = g_sg_v \cdot \frac{1}{(2\pi)^2} \cdot \left( \frac{2m_r^*}{\hbar^2} \right)^{3/2} \cdot \sqrt{u} \]

\[ C_0 = \frac{\pi e^2}{n_r \epsilon_0 m_0^2 \omega} \]

first assume \( f_v(k) = 1 \), \( f_c(k) = 0 \)

Fermi’s Golden Rule

\[ \gamma_{abs} = \frac{2\pi}{\hbar} |\langle b|W(r)|a\rangle|^2 \delta[E_b - (E_a + \hbar\omega)] \]

\[ \gamma_{em} = \frac{2\pi}{\hbar} |\langle a|W(r)|b\rangle|^2 \delta[E_a - (E_b - \hbar\omega)] \]
Electron-Photon Interactions

Loss Coefficient of Semiconductors

\[ \alpha (\text{cm}^{-1}) \]

\[ \lambda_{\text{abs}} (\mu\text{m}) \]

\[ \text{WAVELENGTH } \lambda \text{ (nm)} \]

\[ \ln \gamma (\text{eV}) \]

\[ \text{InSb} \]
\[ \text{InAs} \]
\[ \text{GaAs} \]
\[ \text{GaP} \]
\[ \text{InP} \]
\[ \text{ZnS} \]
\[ \text{SiC} \]
\[ \text{PbO} \]
\[ \text{Si} \]
Optical Matrix Elements for Transitions

\[
\alpha_0(\hbar \omega) = \frac{2.64 \times 10^5}{\eta_r} \cdot \frac{2|\hat{e} \cdot \mathbf{P}_{cv}|^2/m_0}{\hbar \omega} \cdot \left(\frac{2m_r^*}{m_0}\right)^{3/2} \cdot \sqrt{\hbar \omega - E_g} \quad \text{cm}^{-1}
\]

'oscillator strength' \(\propto\) reduced DOS

Absorption spectrum of a general III-V semiconductor at equilibrium

Momentum matrix elements for bulk & quantum well structures

\[
M_b^2 = \frac{1}{3} P_x^2 = \frac{m_0^2}{3\hbar^2} P^2
\]

\[
= \left(\frac{m_0}{m_e^*} - 1\right) \frac{m_0 E_g (E_g + \Delta)}{6(E_g + \frac{2}{3}\Delta)}
\]

Table 9.1 Summary of the Momentum Matrix Elements in Parabolic Band Model (\(|\hat{e} \cdot \mathbf{p}_{cv}|^2 = |\hat{e} \cdot \mathbf{M}|^2\))

| Bulk | | Quantum Well |
|------|-----------------|
| \(|\hat{e} \cdot \mathbf{p}_{cv}|^2 = |\hat{y} \cdot \mathbf{p}_{cv}|^2 = |\hat{z} \cdot \mathbf{p}_{cv}|^2 = M^2_b = \frac{m_0}{6} E_p\) | \(|\hat{e} \cdot \mathbf{M}_{c-\Delta h}|^2 = \frac{3}{4}(1 + \cos^2 \theta)M^2_b\) & \(|\hat{e} \cdot \mathbf{M}_{c-\Delta h}|^2 = \frac{3}{4}\sin^2 \theta M^2_b\) |
| \(|\hat{e} \cdot \mathbf{M}_{c-\Delta h}|^2 = \left(\frac{3}{4} - \frac{3}{2}\cos^2 \theta\right)M^2_b\) & \(|\hat{e} \cdot \mathbf{M}_{c-\Delta h}|^2 = \frac{3}{4}(1 + 3 \cos^2 \theta)M^2_b\) |
| Conservation Rule | \(|\hat{e} \cdot \mathbf{M}_{c-\Delta h}|^2 + \langle|\hat{y} \cdot \mathbf{M}_{c-\Delta h}|^2\rangle + \langle|\hat{z} \cdot \mathbf{M}_{c-\Delta h}|^2\rangle = 3M^2_b, (h = hh \text{ or } lh)\) & \(|\hat{e} \cdot \mathbf{M}_{c-\Delta h}|^2 + \langle|\hat{z} \cdot \mathbf{M}_{c-\Delta h}|^2\rangle = 2M^2_b\) |

Debdeep Jena (djena@cornell.edu)
Optical Gain in Semiconductors

- We have looked at light absorption by a semiconductor (useful for photodetectors & solar cells)
- But LEDs and LASERs are electrically injected light emitters
- The same theory that explains absorption explains emission under electrical injection as well

Non-equilibrium Fermi-Dirac functions with electron quasi-Fermi levels (note: not necessary to talk about holes here)

- $F_c$: Conduction Band quasi-Fermi level
- $F_v$: Valence Band quasi-Fermi level

Fundamental result for understanding LEDs and LASERs
Optical Gain in Non-Equilibrium Conditions

The inversion conditions can be achieved by
- Optical pumping (gas lasers), or
- Electrical pumping (semiconductor LEDs & Lasers)

A laser requires a light emitter to be placed in a high-finesse (hi-Q) optical cavity to amplify a specific mode.

Bernard-Duraffouerg inversion condition
Absorption Coefficient/Optical Gain in Quantum Wells

\[ \psi_v(r) = u_v(r) \times \left[ \frac{1}{\sqrt{A}} e^{ik_t \cdot \rho} \right] \times V(n_v, z) \]

\[ \psi_c(r) = u_c(r) \times \left[ \frac{1}{\sqrt{A}} e^{ik'_t \cdot \rho} \right] \times C(n_c, z) \]

\[ pba = \langle \psi_c | p | \psi_v \rangle \approx \langle u_c | p | u_v \rangle \times \delta_{k_t, k'_t} \times I_{v,n_v}^{c,n_c} \]

\[ I_{hm}^{en} = \int_{-\infty}^{+\infty} dz C^*(n_c, z)V(n_v, z) \]

General form of absorption coefficient:

\[ \alpha_0(\hbar\omega) = C_0 |\hat{e} \cdot \hat{p}_{cv}|^2 \cdot \rho_r (\hbar\omega - E_g) \]

\[ C_0 = \frac{\pi e^2}{n_c \varepsilon_0 m_0^2 \omega} \]

\[ \rho_r^{2D} = \frac{m_r}{\pi \hbar^2 L_z} \]

\[ \alpha_0(\hbar\omega) = \begin{cases} \frac{m_r}{\pi \hbar^2 L_z} & \text{for } E_{n1}^r < \hbar\omega < E_{n2}^r \\ \frac{2 m_r}{\pi \hbar^2 L_z} & \text{for } E_{n2}^r < \hbar\omega < E_{n3}^r \\ \frac{3 m_r}{\pi \hbar^2 L_z} & \text{for } E_{n3}^r < \hbar\omega < E_{n4}^r \\ \text{etc.} \end{cases} \]
Using effective-mass theory, optical matrix elements in quantum wells:

For INTERBAND transitions:

\[ M_{\text{interband}} \sim a_0, \text{ dipole length } \sim \text{lattice constant} \]

For INTERSUBBAND (intra-band) transitions:

\[ M_{\text{intersubband}} \sim L_{\text{well}}, \text{ dipole length } \sim \text{Quantum Well Width} \text{ (giant dipole effect!!)} \]
Equilibrium absorption coefficient in QW is proportional to the joint DOS and has 2D subband features.
Compound Semiconductor Heterojunction LEDs

\[ R_{\text{radiative}} = \frac{np\nu_{th}S_R}{2\eta^2} \]

\[ S_R \approx 5 \times 10^{-25} \eta^2 E_{\text{gap}}^2 \alpha \left( \frac{m_e m_h}{m^*} \right)^{3/2} \left( \frac{300}{T} \right)^{5/2} \text{cm}^2 \]

(Rockett)
Gain spectrum in QWs follows the equilibrium JDOS modulated by the Fermi Dirac functions in accordance with the Bernard-Duraffourg condition.
Compound Semiconductor Heterojunction Devices

- 3d: bulk material ($\alpha E^{1/2}$)
- 2d: quantum wells (constant)
- 1d: quantum wires ($\alpha E^{1/2}$)
- 0d: quantum dots (delta function)

Conventional edge-emitting laser

Current injection region

- Optical confinement layers
- Quantum-well emitter layer

Active area

- p-semiconductor
- n-semiconductor

Upper distributed Bragg reflector (99% reflection)

Optical confinement layer

- Quantum-well
- Optical confinement layer

Lower distributed Bragg reflector (99.9% reflection)

Vertical-cavity surface-emitting laser
Compound Semiconductor Heterojunction Devices

(Rockett)
Applications: The Double-Heterostructure Laser
Fig. 91. Schematics of the gain formation in DH lasers (top) and QW lasers (bottom).

Fig. 96. Schematics of GRIN–SCH and SCH structures, and corresponding density-of-states and occupied states.
When $L \gg a_B$, (but still well-separated, confined energy levels), a “giant” oscillator strength situation develops, which yields a transition matrix element,

$$f = f_{at} \left( \frac{V_{box}}{V_{exc}} \right)$$

where $V_{box}$ and $V_{exc}$ are the QB and exciton volume, respectively. The enhancement of the oscillator strength originates in the coherent excitation of the QB volume (somewhat analogous to the intersubband giant dipole matrix element of Eq. (54e)), which yields an increased dipole moment.

Fig. 100a. Schematics of band-filling for conduction and valence band states for equal numbers of injected electrons and holes in unstrained (left) and strained (right) QW active layers.

Fig. 113. Schematics of gain curves in 2D, 1D, and 0D structures. Similar numbers of electrons and holes are being injected above transparency, yielding equal integrated gain. (From Nagle and Weisbuch,

Fig. 114. Schematics of quantum box structure and gain curves 3D, 2D, 1D, 0D lasers, with optimized optical confinement in each case. (Adapted from M. Asada, Y. Miyamoto, and Y. Suematsu, IEEE J. Quantum Electron. QE-22, 1915, © 1986 IEEE)
Reduction of lasing threshold current density

Alferov Nobel Lecture 2000
Intersubband Optical Transitions

Optical transitions for intersubband processes

\[ \psi_a(r) = u_c(r) \times \left[ \frac{1}{\sqrt{A}} e^{ik_t \cdot \rho} \right] \times \phi_1(z) \]

\[ \psi_b(r) = u_c(r) \times \left[ \frac{1}{\sqrt{A}} e^{ik'_t \cdot \rho} \right] \times \phi_2(z) \]

\[ \mu_{ba} = \langle \psi_b | e \mathbf{e} | \psi_a \rangle \approx \langle u_c | u_c \rangle \times \langle \frac{1}{\sqrt{A}} e^{ik_t \cdot \rho} | e \mathbf{r} | \frac{1}{\sqrt{A}} e^{ik'_t \cdot \rho} \rangle \]

\[ \approx \delta_{k_t,k'_t} \langle \phi_2 | ez | \phi_1 \rangle \hat{z} \approx \delta_{k_t,k'_t} \times e\mathbf{z}_{12} \]

For INTERSUBBAND (intra-band) transitions:

\[ M \sim \int_{\text{crystal}} \chi_e(z) \mathbf{r} \cdot \chi'_e(z) d\mathbf{r} \int_{\text{cell}} u_{cke}(\mathbf{r})u_{cke}^*(\mathbf{r}) d^3r \]

\[ M_{\text{intersubband}} \sim L_{\text{well}}, \text{ dipole length} \sim \text{Quantum Well Width} \]

(giant dipole effect!!)
Intersubband Optical Transitions

\[ \alpha(h\omega) = \left( \frac{\omega}{n_r c \varepsilon_0} \right) \frac{|\mu_2|^2 (\Gamma/2)}{(E_2 - E_1 - h\omega)^2 + (\Gamma/2)^2} \left( \frac{m^* k_B T}{\pi h^2 L} \right) \ln \left( \frac{1 + e^{(E_F - E_i)/k_B T}}{1 + e^{(E_i - E_F)/k_B T}} \right) \]

Figure 9.15. A period of a quantum cascade laser [27] using intersubband transition between \( E_1 \) and \( E_2 \). The barriers are \( \text{Al}_{0.33} \text{In}_{0.67} \text{As} \) and the wells are \( \text{In}_{0.25} \text{Ga}_{0.75} \text{As} \) materials. The calculated values are \( E_1 - E_2 = 295 \text{ meV} \) and \( E_2 - E_3 = 30 \text{ meV} \).

Applications of ISB transitions: In Quantum Cascade Lasers
Electron-Photon Interactions

Fig. 12.12. Bandgap energy versus lattice constant of III–V nitride semiconductors at room temperature.

ECE 4070 / MSE 6050

- Design of a quantum well blue laser diode
Electron-Photon Interactions

Quantum well Heterostructures grown by MBE (Henryk Turski)

ECE 4070 / MSE 6050
- Demonstration of a GaN/InGaN/GaN Quantum Well Laser Diode

Debdeep Jena (djena@cornell.edu)
Electron-Photon Interactions

ECE 4070 / MSE 6050
- Demonstration of a GaN/InGaN/GaN Quantum Well Laser Diode

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Electron-Photon Interactions

- InGaN Quantum Well LASER
- Beam Splitter
- Spectrometer

Diagram showing current density vs. bias voltage with QW LED and QW LASER.

Graphs at 0 V, 3 V, and 3.5 V showing bandgap, Fermi level, and population inversion.

Equations:
- $E_{fn} < E_C$
- $E_{fp} > E_V$
- $E_{fn} > E_C$
- $E_{fp} > E_V$
- $E_{fn} > E_C$
- $E_{fp} < E_V$

ECE 4070 / MSE 6050
- Demonstration of a GaN/InGaN/GaN Quantum Well Laser Diode

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End