Plan for Lecture 24 (Chapter 43):

Some topics in the physics of molecules and solids

1. Physics of atoms
2. Physics of molecules
3. Physics of solids
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In the Davisson-Germer experiment, 54.0 eV electrons were diffracted from a nickel lattice. If the first maximum in the diffraction pattern was observed at \( \phi = 50.0^\circ \), what was the spacing \( d \) between the planes of atoms causing this diffraction?
Webassign hint -- continued:

Bragg condition: \[ 2d \sin \theta = \lambda \]
Webassign hint -- continued:

Bragg condition: \(2d \sin \theta = \lambda\)

\[\delta_1 + \delta_2 = 2d \sin \theta = m \lambda\]
Some ideas of quantum theory discussed last time:

Matter wave equation – Schrödinger equation:

\[
\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + U(r)\right] \Psi(r, t) = -i\hbar \frac{\partial}{\partial t} \Psi(r, t)
\]

Stationary-state wavefunctions: \( \Psi(r, t) = \psi(r)e^{-iEt/\hbar} \)

In this case, the Schrödinger equation becomes:

\[
\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + U(r)\right] \Psi(r, t) = E\Psi(r, t)
\]

Here Planck's constant: \( h = 6.63 \times 10^{-34} \text{ J} \)

\( \hbar \equiv \frac{h}{2\pi} = 1.05 \times 10^{-34} \text{ J} \)
Example - free particle -- $U(r) = 0$: \[ \Psi(r, t) = \psi(r) e^{-iEt/\hbar} \]

\[ \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right] \Psi(x, t) = E\Psi(x, t) \]

\[ \Psi(x, t) = \Psi_0 \sin(kx)e^{-iEt/\hbar} \]

\[ E = \frac{\hbar^2 k^2}{2m} \text{ Note: This is consistent with de Broglie's } \lambda = \frac{\hbar}{p} \]

\[ k = \frac{2\pi}{\lambda} \implies \lambda = \frac{\hbar}{\sqrt{2mE}} \text{ or } E = \frac{\hbar^2}{2m\lambda^2} \]

Example: Suppose we want to create a beam of electrons ($m = 9.1 \times 10^{-31} \text{kg}$) for diffraction with $\lambda = 1 \times 10^{-10} \text{m}$. What is the energy $E$ of the beam?

\[ E = \frac{\hbar^2}{2m\lambda^2} = \frac{\left(6.6 \times 10^{-34}\text{ J} \right)^2}{2 \cdot 9.1 \times 10^{-31}\text{ kg} \cdot \left(10^{-10}\text{ m} \right)^2} = 2.4 \times 10^{-17}\text{ J} = 150\text{ eV} \]
Recall de Broglie’s relation between wavelength and momentum:

\[ \lambda = \frac{h}{p} \quad h = 6.6 \times 10^{-34} J \]

Which has the larger de Broglie wavelength:

A. An electron with a velocity of 100 m/s (mass = 9.1x10^{-31} kg)
B. A baseball with a velocity of 100 m/s (mass = 1 kg)
Another example -- electron bound to a proton:

(H atom) \[ U(r) = -\frac{Z e^2}{4\pi \varepsilon_0 r} \]

\[
\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + U(r)\right] \Psi(r, t) = -i\hbar \frac{\partial}{\partial t} \Psi(r, t)
\]

Stationary-state wavefunctions: \[ \Psi(r, t) = \psi(r)e^{-iEt/\hbar} \]

Solutions: \[ E_n = -\frac{Z^2 e^2}{8\pi \varepsilon_0 a_0 n^2} \frac{1}{n^2} = -13.6 \frac{Z^2}{n^2} \text{eV} \quad n = 1, 2, 3, \ldots \]

\[ a_0 = \frac{4\pi \varepsilon_0 \hbar^2}{m e^2} = 0.0529 \text{ nm} \]
Quantum theory for electromagnetic radiation
The transition between bound quantum states can correspond to the emission (production) or absorption (consumption) of electromagnetic quanta:

Coupling of states of matter with EM radiation:

\[ hf^{\text{photon}} = \frac{hc}{\lambda^{\text{photon}}} = |E_{\text{final}} - E_{\text{initial}}| = |\Delta E| \]

\[ \lambda^{\text{photon}} = \frac{hc}{\Delta E} \approx \frac{1234}{\Delta E_{12}(eV)} \text{ nm} \]
Energy level diagram for H atom

The colored arrows for the Balmer series indicate that this series results in the emission of visible light.

\[
E_n = -\frac{Z^2 e^2}{8\pi\varepsilon_0 a_0} \frac{1}{n^2}
\]

\[
= -13.6 \frac{Z^2}{n^2} \text{ eV} \quad n = 1, 2, 3, \ldots
\]

Radiation produced by "emission" or the transition from \( n_1 \rightarrow n_2 \)

Examples (for \( Z = 1 \)):

\[ E_2 - E_1 = (-3.401) - (-13.606) = 10.205 \text{ eV} \]

\[ \lambda_{12}^{\text{photon}} = \frac{hc}{\Delta E_{12}} \approx \frac{1234}{\Delta E_{12} (\text{eV})} \text{ nm} = 120 \text{ nm} \]

\[ E_3 - E_1 = (-1.512) - (-13.606) = 12.094 \text{ eV} \]

\[ \lambda_{13}^{\text{photon}} = \frac{hc}{\Delta E_{13}} \approx \frac{1234}{\Delta E_{13} (\text{eV})} \text{ nm} = 100 \text{ nm} \]

\[ E_\infty - E_1 = (-0.000) - (-13.606) = 13.606 \text{ eV} \]

\[ \lambda_{1\infty}^{\text{photon}} = \frac{hc}{\Delta E_{1\infty}} \approx \frac{1234}{\Delta E_{1\infty} (\text{eV})} \text{ nm} = 90 \text{ nm} \]
Physics of molecules – H₂
Recall for H atom:

\[
\begin{bmatrix}
- \frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \frac{Ze^2}{4\pi\varepsilon_0 r}
\end{bmatrix} \psi (r) = E \psi (r)
\]

For ground state: \( E_1 = -\frac{Z^2 e^2}{8\pi\varepsilon_0 a_0} \)

\[
\psi_1 (r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}
\]
Physics of molecules – H₂ -- continued

\[
\psi(r) = E\psi(r)
\]

Approximate solutions:

\[
\psi_{\text{approx}}(r) = C \left( \frac{1}{\sqrt{\pi a_0^3}} e^{-|r-R_1|/a_0} \pm \frac{1}{\sqrt{\pi a_0^3}} e^{-|r-R_2|/a_0} \right)
\]
Physics of molecules – H₂ -- continued

\[ \psi_{\text{approx}}(r) = C \left( \frac{1}{\sqrt{\pi a_0^3}} e^{-|r-R_1|/a_0} \pm \frac{1}{\sqrt{\pi a_0^3}} e^{-|r-R_2|/a_0} \right) \]

http://farside.ph.utexas.edu/teaching/qmech/lectures/node129.html
Physics of molecules – continued

Energy diagram for NaCl molecule as a function of ion separation

Stable equilibrium
Physics of molecules – continued

Vibration about equilibrium point

The distance $r_0$ is the equilibrium separation distance of the atoms.

$$U(r) \approx U(r_0) + \frac{1}{2} k(r - r_0)^2$$

The vibration of the molecule is along the molecular axis.

Schrodinger equation for vibrating nuclei

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} kx^2 \right] \psi(r) = E \psi(r)$$

Here

$$m = \frac{m_1 m_2}{m_1 + m_2} \quad x = r - r_0$$
Physics of molecules – continued
Vibration about equilibrium point

Solution to Schrödinger equation for vibrating nuclei

\[
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} kx^2 \right] \psi(r) = E \psi(r)
\]

\[
E_v = \hbar f_0 \left( \frac{1}{2} + \nu \right) \quad f_0 \equiv \frac{1}{2\pi} \sqrt{\frac{k}{m}}
\]

Given that \( f_0 = 6 \times 10^{13} \) cycle/s for a vibrating CO molecule, if this vibration were to couple to EM radiation, what would be the wavelength of light?

A. \( 5 \times 10^{-6} \) m
B. \( 2 \times 10^5 \) m
C. \( 1 \times 10^{-47} \) m
Physics of molecules and solids

\[ E\psi(r) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + U(r) \right] \psi(r) \]

Example: electron density associated with

H\(_2\) molecule: 

CH\(_4\) molecule:
Molecular binding of nuclei due to electron “glue”:

\[ V(R) = \frac{1}{R} \]

ionic interaction

Dissociation energy
Physics of solids

\[ E\psi(\mathbf{r}) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + U(\mathbf{r}) \right] \psi(\mathbf{r}) \]

\[ U(\mathbf{r}) = \sum_i u(|\mathbf{r} - \mathbf{R}_i|) \]

Energy spectrum of atom or molecule:

- highest filled state for insulator
- highest filled state for metal
Insulator

The available states in the conduction band are separated from the valence band by a large energy gap.

Metal

The states in the gold region of the band are available to account for electron motion.
Example: 2 materials made of pure carbon:

- **diamond (insulator)**
  - $E_g = 5.5$ eV

- **graphite (semi-metal)**
  - $E_g = 0.0$ eV
Which photo is diamond?

A. left  
B. right
Some energy band gaps:

- C (diamond) \(5.5\) eV
- \(\text{SiO}_2\) (quartz) \(8.9\)
- NaCl (rock salt) \(8.5\)

Two images of quartz:
Semi-conductor materials; $E_g < 5$ eV or so

The small energy gap allows electrons to be thermally excited into the conduction band.

### TABLE 43.3

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<th>Crystal</th>
<th>$E_g$ (eV)</th>
<th>$E_g$ (eV)</th>
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<td>Si</td>
<td>1.17</td>
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<tr>
<td>Ge</td>
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<tr>
<td>InP</td>
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<td>GaP</td>
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<tr>
<td>CdS</td>
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<td>ZnO</td>
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<td>3.6</td>
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Electron conductivity in metals and semiconductors:

\[
\sigma = \frac{ne^2\tau}{m^*} = ne^2\tau \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k^2}
\]

\( n \equiv \text{# carriers/volume} \)

\( \tau \equiv \text{scattering time} \)

\[
\frac{1}{m^*} \equiv \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k^2} \quad \text{"effective mass"}
\]

In a perfect semiconductor at \( T=0K \) \( n=0 \). To control conduction, impurities are introduced.
Electron doping

Each double line between atoms represents a covalent bond in which two electrons are shared.

- Gray = Semiconductor atoms
- Yellow = Impurity atom with five outer-shell electrons
- Blue = Extra electron from impurity atom

A small amount of energy $E_d$ can excite the electron into the conduction band.

“Hole” doping

The single line between the impurity atom and the semiconductor atom below it represents that there is only one electron shared in this bond.

- Gray = Semiconductor atoms
- Yellow = Impurity atom with three outer-shell electrons
- Red = Hole, or electron deficiency in a bond

A small amount of energy $E_a$ excites an electron into the energy level of the acceptor atom, leaving a hole in the valence band.
Semiconductor devices; combining electron doped and hole doped materials to control the flow of mobile carriers.
Photovoltaic devices

When an electron falls from the conduction band to the valence band, a photon of light is emitted.

When a photon is absorbed, an electron is raised from the valence band to the conduction band.
Laser technology:

- System with ground and excited state at desired $\lambda$ ($E_{ex} - E_g = hc/\lambda$).
- Standing EM wave
- Mechanism for “population inversion”

The Helium–Neon Gas Laser

Figure 41-21 shows a type of laser commonly found in student laboratories. It was developed in 1961 by Ali Javan and his coworkers. The glass discharge tube is filled with a 20:80 mixture of helium and neon gases, neon being the medium in which laser action occurs.

**Fig. 41-21** The elements of a helium–neon gas laser. An applied potential $V_{dc}$ sends electrons through a discharge tube containing a mixture of helium gas and neon gas. Electrons collide with helium atoms, which then collide with neon atoms, which emit light along the length of the tube. The light passes through transparent windows $W$ and reflects back and forth through the tube from mirrors $M_1$ and $M_2$ to cause more neon atom emissions. Some of the light leaks through mirror $M_2$ to form the laser beam.
Figure 41-22 shows simplified energy-level diagrams for the two atoms. An electric current passed through the helium–neon gas mixture serves—through collisions between helium atoms and electrons of the current—to raise many helium atoms to state $E_3$, which is metastable.