Lecture 11: Periodic systems and Phonons

Mainly: Vibrations in a periodic solid

- **Aims:**
  - Complete the discussion of the electron-gas
    - Astrophysical electrons
    - Degeneracy pressure
    - White dwarf stars
    - Compressibility/bulk modulus of metals
  - Introduction to periodic systems:
    - Waves in periodic systems
    - Electron bands (not for examination)
  - Lattice vibrations
    - Modes of a 1-dimensional, harmonic chain
      - Monatomic chain with nearest neighbour forces

![Diagram of a 1-dimensional, harmonic chain with wavevector and frequencies](image)
**Astrophysical electrons**

♦ **Typical star**
  - Mainly composed of ionised hydrogen
    
    \[
    M \sim 3 \times 10^{30} \text{ Kg}, \\
    R \sim 3 \times 10^7 \text{ m} \\
    T \sim 10^7 \text{ K}
    \]

  - Electrons form a degenerate gas.
  - Nuclear energy keeps the star hot and inflated.

♦ **White dwarf stars**
  - What happens when the nuclear reaction of hydrogen stops? The star is then mainly helium.
  - Star contracts under gravity until balanced by a "degeneracy pressure" due to the electrons
  - Recall the energies of electrons in box side \( a \)
    
    \[
    \varepsilon = \left( \frac{\hbar^2}{2m} \right) k^2 = \frac{\hbar^2}{2m} \left( \frac{\pi}{a} \right)^2 (l^2 + m^2 + n^2)
    \]
  - It takes energy to compress the box, in order that the single-particles energies rise. Hence there is an outwards pressure.

\[ T_F \sim 3 \times 10^8 \text{K} \]

\[ T < T_F \]
Degeneracy pressure

Pressure due to a Fermi gas at $T=0$.

- Compressing the gas, we have $\Delta U = -P \Delta V$ and hence
  \[ P = -\frac{\partial U}{\partial V} \]

- First, calculate $\langle U \rangle$, the mean energy of a Fermi electron

\[ \langle U \rangle = \int_0^{\varepsilon_F} \varepsilon g(\varepsilon) \, d\varepsilon \]
\[ = \int_0^{\varepsilon_F} \varepsilon \, d\varepsilon = \frac{\varepsilon_F^3}{3} - \frac{\varepsilon_F^3}{3} = \frac{2}{5} \varepsilon_F^{5/2} \]
\[ = \frac{2}{5} \varepsilon_F^{5/2} \left( \frac{2}{3} \varepsilon_F^{3/2} \right) = \frac{3}{5} \varepsilon_F \]

- For $N$ electrons
  \[ U = N \langle U \rangle = 3N \varepsilon_F^2 / 5 \]

\[ P = \frac{\partial U}{\partial \varepsilon_F} \frac{\partial \varepsilon_F}{\partial V} = \frac{3}{5} N \left( -\frac{2}{3} \varepsilon_F \right) \]

\[ P = \frac{2n \varepsilon_F}{5} \propto \left( \frac{N}{V} \right)^{5/3} \propto M^{5/3} / R^5 \]
White dwarf stars

- Gravitational forces: In equilibrium the degeneracy pressure balances gravitational attraction. Taking $P$ to depend only on $G$, $M$ and $R$

$$P \propto G^\alpha M^\beta R^\gamma$$

$$M L^{-1} T^{-2} = L^{3\alpha} M^{-\alpha} T^{-2\alpha} M^\beta L^\gamma$$

$$\Rightarrow 1 = -\alpha + \beta; \quad -1 = 3\alpha + \gamma; \quad -2 = -2\alpha$$

$$\Rightarrow P \propto GM^2 / R^4$$

- Equating gravitation and degeneracy pressures

$$M^{5/3} / R^5 \propto GM^2 / R^4$$

$$M^{1/3} R = \text{const}$$

- Result derived by Fowler in the late 1920’s is correct in the non-relativistic limit.

- Best known white dwarf is Sirius B:
  radius $5.6 \times 10^6$ m (< earth); mass, $2 \times 10^{30}$ Kg.

$$N = 2 \times 10^{30} / 1.67 \times 10^{-27} \approx 1.2 \times 10^{57}$$

$$N/V = 1.2 \times 10^{57} (3/4 \pi^2 5.6 \times 10^6) \approx 1.6 \times 10^{36} \text{ m}^{-3}$$

$$k_F = (3\pi^2 n)^{1/3} = 3.8 \times 10^{-22} \text{ m}^{-1}$$

$$v_F = \hbar k_F / m_e = 4.2 \times 10^8 \text{ ms}^{-1}$$

- A relativistic analysis is needed ($\epsilon_F \approx 500$ keV)
Chandrasekhar mass limit

- Chandrasekhar ~1930
  - Re-analysed the problem relativistically.
    \[ \varepsilon(k) = \left( \frac{\hbar c k}{2m_e^2 c^4} \right)^{1/2} - m_e c^2 \approx \hbar c k \]
  - \( g(\varepsilon) \) is affected (see problem sheet 1); however, other steps in the analysis are the same as before. The key result is that the degeneracy pressure~\( R^{-4} \) (rather than \( R^{-5} \))
  - It follows that the final radius is independent of the mass i.e. no white dwarfs above a limiting mass (1.45 x mass of sun)

More massive stars contract to neutron stars, and ultimately to black-holes.
  - Won 1983 Nobel prize
**Degeneracy pressure in metals**

- The pressure of the degenerate electron gas also contributes to the mechanical properties of metals.

- Isothermal bulk modulus, $K_T$ is defined as

  \[ K_T = -V \frac{\partial p}{\partial V} \mid_T \]

  \[ P = \frac{2}{5} \frac{N}{V} \varepsilon_F \Rightarrow \frac{\partial p}{\partial V} = -\frac{2}{3} \frac{N\varepsilon_F}{V^2} \]

  \[ K_T = \frac{2}{3} \frac{N\varepsilon_F}{V} \]

  
  Calculated values are of the right magnitude. We have neglected the attractive forces, due to the ion cores. Attractive forces make the metal more compressible (Experimental bulk modulus, $K_{exp}$, is usually smaller than $K_T$, above).

<table>
<thead>
<tr>
<th>Metal</th>
<th>$n=(N/V)/\text{m}^{-3}$</th>
<th>$E_F/\text{eV}$</th>
<th>$K_{exp}/K_T$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>4.6E+28</td>
<td>4.7</td>
<td>0.63</td>
</tr>
<tr>
<td>Na</td>
<td>2.5E+28</td>
<td>3.1</td>
<td>0.83</td>
</tr>
<tr>
<td>K</td>
<td>1.3E+28</td>
<td>2.0</td>
<td>1.03</td>
</tr>
</tbody>
</table>
Waves in crystals

So far we have neglected the periodicity (symmetry) of typical, crystalline solids.

The periodicity influences the way in which a wave propagates through the medium.

A key concept is that the periodicity in real space introduces a periodicity in momentum space, \( k \)-space, as we shall see.

Start from a familiar example (IB Waves course): Light passing through a periodic structure (e.g. a diffraction grating)
Waves in crystals

Periodic structures

- We can think of the process as an “input” wavevector, \( k_i \), being converted to many “output” wavevectors defined by \( k_f(y) = k_i(y) + nG(y) \) (in general, a vector equation); \( n \) is an integer.
- The lattice symmetry (periodicity) induces a symmetry (periodicity) in any wave propagating through the lattice.
- \( G \) is a reciprocal lattice vector (see later in the section on phonons).
- In a crystal any \( k \)-dependent property (such as energy) must be periodic.

Electrons

- E versus \( k \) relation (dispersion relation) in the free-electron case is

\[
E(k) = \frac{\hbar^2 k^2}{2m}
\]
Origin of electron bands
(Not for examination)

Electrons in a periodic solid. (A quantitative treatment appears in Part II)

Consider a solid with periodicity in 1-D. If the periodicity is “weak”, it only introduces tiny changes to the $E(k)$ dispersion curve.

Using the argument that $E(k)$ must be periodic, with period $G$, we can construct multiple copies of the free electron curve.

All the information is in the central section – known as the First Brillouin zone (right).

Bands are labelled accordingly (separate colours).

Note also the potential for band gaps (at crossings) and, hence, insulating behaviour. (For gaps to appear we need some modification of the free electron curves, i.e. “scattering from the lattice”)

Lattice vibrations

♦ 1-D harmonic chain

- The effects of diffraction in a periodic structure are similar for all waves. These effects emerge naturally from a discussion of any one system. We will discuss lattice vibrations.

- Take identical masses, $m$, connected by springs (spring constant, $\alpha$)

This is a model limited to “nearest-neighbour” interactions. Equation of motion for the $n$th atom is

$$m\ddot{u}_n = \alpha\left\{(u_{n+1} - u_n) - (u_n - u_{n-1})\right\}$$

$$m\ddot{u}_n = \alpha(u_{n+1} + u_{n-1} - 2u_n)$$

- We have N coupled equations (for N atoms)
Normal modes

Look for travelling wave solutions

- Wave of angular frequency, $\omega$, and wavevector, $q$ ($q$ is the conventional choice for phonons)
  \[ u_n = u_0 \exp\{i(nqa - \omega t)\} \]

- Substitute into equation of motion
  \[
  -m\omega^2 u_0 \exp\{i(nqa - \omega t)\} = \alpha(e^{-ina} + e^{ina} - 2)u_0 \exp\{i(nqa - \omega t)\}
  \]
  \[
  m\omega^2 = \alpha(2 - 2\cos qa) = 4\alpha \sin^2 \left(\frac{qa}{2}\right)
  \]

\[
\omega(q) = \sqrt{\frac{4\alpha}{m}} \sin \left(\frac{qa}{2}\right)
\]

These are the normal modes for the system of coupled atoms.

Note: the continuum model for compressive waves (1B Physics, Oscillations, waves and optics course) gave dispersionless solutions, which are the same as the above in the limit of $q \to 0$, (i.e. the long wavelength limit).
Phonon dispersion

♦ Dispersion curves

- $\omega$ versus $q$ gives the wave dispersion

![Dispersion curves diagram](image)

Key points

- The periodicity in $q$ (reciprocal space) is a consequence of the periodicity of the lattice in real space (c.f. diffraction on slide 2). Thus the phonon at some wavevector, say, $q_1$ is the same as that at $q_1 + nG$, for all integers $n$, where $G = \frac{2\pi}{a}$ (a reciprocal lattice vector).

- In the long wavelength limit ($q \to 0$) we expect the “atomic character” of the chain to be unimportant.
Limiting behaviour

- **Long wavelength limit**
  - dispersion formula (p. 4)
    \[ \omega = \sqrt{\frac{4\alpha}{m}} \sin\left(\frac{qa}{2}\right) \]
  - leads to the continuum result (see IB waves course)
    \[ \omega \to q \sqrt{\frac{\alpha a}{m/a}} \quad \text{and} \quad \frac{\omega}{q} = \sqrt{\frac{Y}{\rho}} \]
  - These are conventional sound-waves.

- **Short wavelength limit**
  - “Atomic character” is evident as the wavelength approaches atomic dimensions \( q \to \pi/a \). \( \lambda = 2a \) is the shortest, possible wavelength
  - Here we have a standing wave \( \partial \omega / \partial q = 0 \)

Continuum result
- \( Y \) - Young’s modulus
- \( \rho \) - density

\[ \omega_{\text{max}} = \sqrt{\frac{4\alpha}{m}} \]
Periodicity: All the physically distinguishable modes lie within a single span of $2\pi a$.

First Brillouin zone (BZ)

- choose the range of $q$ to lie within $|q| < \pi a$. This is the 1st BZ.

Number of modes (must equal the number of atoms, $N$, in the chain)
- the allowed $q$ values are discrete.

Each mode (at particular $q$) is a quantised, simple-harmonic oscillator

\[
E = \left(n + \frac{1}{2}\right)\hbar\omega; \quad \langle n \rangle = \frac{1}{\exp(\hbar\omega/kT)-1}
\]

- with a particulate character (bosons).
  - Energy=$\hbar\omega$, Moment.$=\hbar q$, Velocity=$v_g=\partial\omega/\partial q$. 

1st Brillouin zone (shaded)

Wavevector, $q$