# *4B5: Nanotechnology & Quantum Phenomena*

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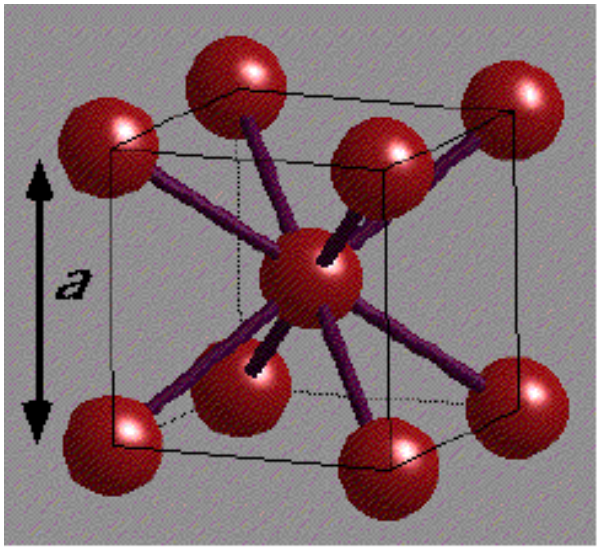
# *Lecture 5* *(23 & 26/10/2012)*

## *The Quantum Harmonic Oscillator and the origins of electrical resistance*

*In this lecture, we are going to examine the problem of the quantum harmonic oscillator (i.e. the simple harmonic oscillator treated quantum mechanically), and see it's relevance to the electrical and thermal properties of crystalline materials.*

*Consider a solid, crystalline material, e.g. a metal, as shown below. The atoms are bound together by chemical bonds. To a first approximation, we can represent these bonds by springs, i.e. if we try to move the atoms closer together, they will resist and likewise if we try to separate them. Therefore, any vibrations of the atoms about their mean positions will be similar to a simple harmonic oscillator. In reality this is a surprisingly good approximation: the forces holding atoms together are linear for small movements of the atoms. When we heat up a material, all that happens is that the atoms inside start jiggling around. Because the atoms are all bound together by springs, the motion of all the atoms will be correlated, i.e. the whole lattice will vibrate somehow. These lattice vibrations are called "phonons", and are waves (like sound waves). They are responsible for thermal conduction, and play a major role in determining the electrical resistance (see at the end), and are responsible for the observed variation of resistance with temperature.*




Crystal structure of a metal

# *The 1-Dimensional Quantum Harmonic Oscillator*

Relevant for explanation of :

Vibration energies of molecules

Specific heat of gasses & solids

Electrical resistance

Consider a particle suspended by a spring of Stiffness k:

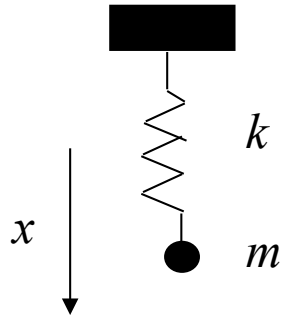
Classically, this will oscillate at the natural frequency

$\omega_c = (k/m)^{1/2}$

The force on the particle, $F = - kx$

The potential energy of the system is V, where

$V = \frac{1}{2} kx^2 = \frac{1}{2} m\omega_c^2 x^2$




Schrödinger's equation for this system =

$$-\hbar^2/2m d^2\psi/dx^2 + \frac{1}{2} m\omega_c^2 x^2\psi = E\psi$$

To make the maths simpler, employ a change of variables from $x$ to $y$, where

$y = (m\omega_c/\hbar)^{1/2}x$, and define $\alpha = 2E/\hbar\omega_c$

Schrödinger's equation is now:

$$d^2\psi/dy^2 + (\alpha - y^2)\,\psi = 0 \qquad (1)$$

Try a trial solution $\psi(y) = F(y)\exp(-y^2/2)$

*To see where this comes from, look at the asymptotic solution when y>>a, and it turns out to be of the form* $y = y^n \exp(-y^2/2)$

Substituting into (1) gives:

$$F'' - 2yF' + (\alpha - 1)F = 0 \qquad (2)$$

We now assume a power series solution for *F(y)*, i.e.

$$F = \sum_{p=0}^{\infty} a_p y^p$$

now, $F' = \sum_{p=0}^{\infty} p a_p y^{p-1}$ and $F'' = \sum_{p=0}^{\infty} p(p-1) a_p y^{p-2}$

Important point, $y$ can never have a negative power, as that would lead to an infinity at $y = 0$. The first two terms of F`` therefore must equal 0, so we can put $p = p+2$ without changing anything.

$$\Rightarrow \qquad \sum_{p=0}^{\infty}\left[(p+2)(p+1)a_{p+2}-(2p+1-\alpha)a_p\right]y^p = 0$$

Now, for a non-trivial solution, the coefficient of each power of $y$ must vanish, which leads us to the recursion relation:

$$\boxed{\frac{a_{p+2}}{a_p} = \frac{(2p+1-\alpha)}{\left[(p+1)(p+2)\right]}}$$

This power series will tend to infinity with increasing $y$. Therefore, the sum must be truncated. Where?
Well, sum can be re-written as two power series, each containing all even or odd powers of $y$.
Using the recursion relation, all coefficients can be expressed in terms of either $a_0$ or $a_1$

Choose α such that for some value of $p$, say $n$, then $2p+1-\alpha = 0$, or $a = 2n+1$. That series will terminate there.

Terminate other series by setting it's coefficient = 0.

The combination of these two conditions leads to:

$\alpha = 2n+1$ for $n$ = 0,1,2…..

$a_1 = 0$ for n even, $a_0 = 0$ for n odd

From definition of $\alpha( = 2E/\hbar\,\omega_c)$ we have the energy eigenstates of the quantum simple harmonic oscillator as:

$$E_n = (n + ½)\hbar\omega_c$$

i.e. Discrete equally spaced energy levels, with a ground state or ***Zero-Point Energy*** of $½\,\hbar\omega_c$

*What is the consequence of the Zero-point Energy? It means that according to quantum mechanics, a harmonic oscillator can never be completely at rest, because then we would know it's momentum (zero) and position precisely, which goes against Heisenberg's Uncertainty principle. It means that even at absolute zero, the atoms in a material will still be moving around by a very small amount.*

What are the wave functions like?
Well, using our recursion relation, i.e.

$$\frac{a_p}{a_{p-2}} = \frac{(2(p-2)-2n)}{[p(p-1)]}$$

we get for the first 3 levels that:

$$F_0 = a_0$$
$$F_1 = a_1 y$$
$$F_2 = a_0 - 2a_0 y^2$$

$$\psi_0(x) = \frac{m\omega_c}{4\pi\hbar} e^{-\frac{m\omega_c}{\hbar}x^2}$$

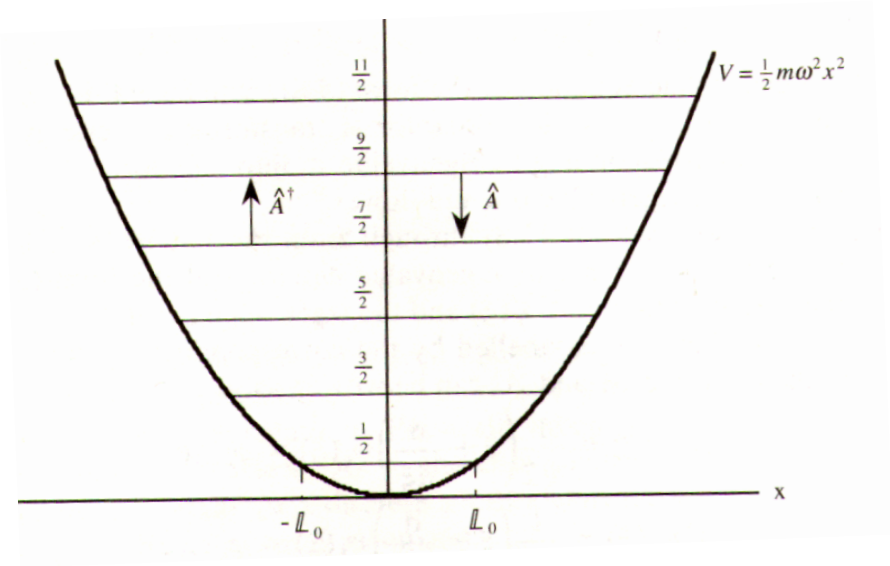
$$\psi_1(x) = \frac{3m\omega_c}{4\pi^2\hbar} x e^{-\frac{m\omega_c}{\hbar}x^2}$$

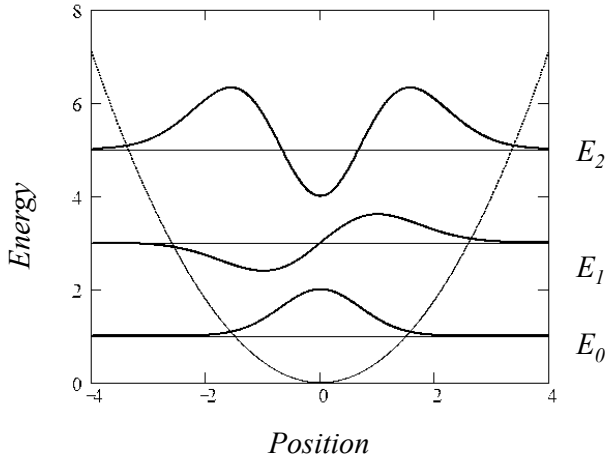
$$\psi_2(x) = \frac{m\omega_c}{16\pi\hbar}\left(\frac{2m\omega_c}{\hbar}x^2 - 1\right) e^{-\frac{m\omega_c}{\hbar}x^2}$$

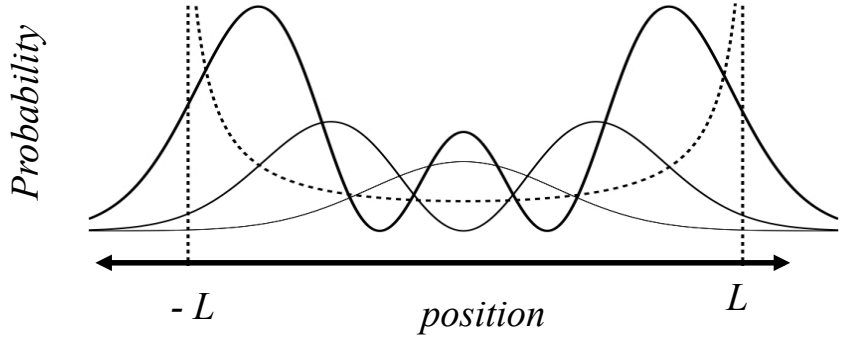
**In the ground state, the most probable position is in the centre, whereas for higher levels, the probability oscillates quickly.**

**Compare to the conventional simple harmonic oscillator: the most probable position is always at the extrema (the velocity is lowest there).**

What do the wave-functions and energy levels look like?



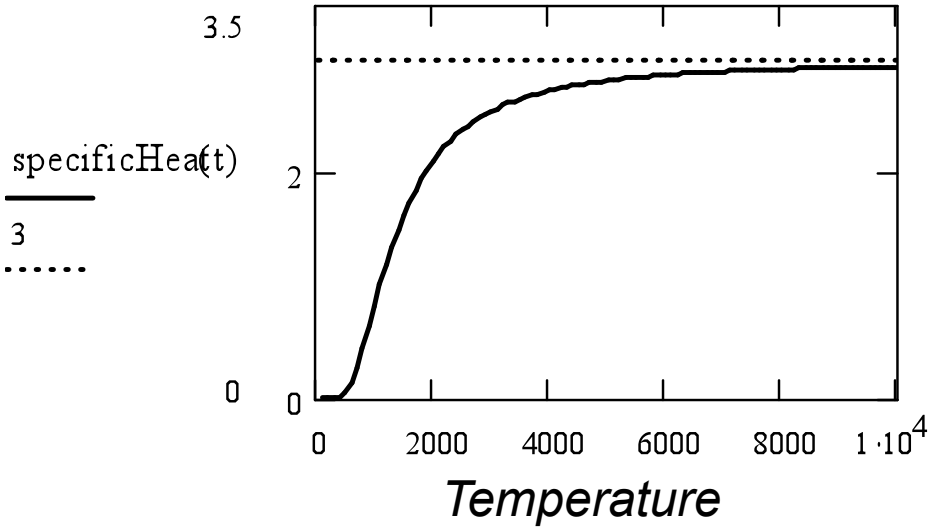



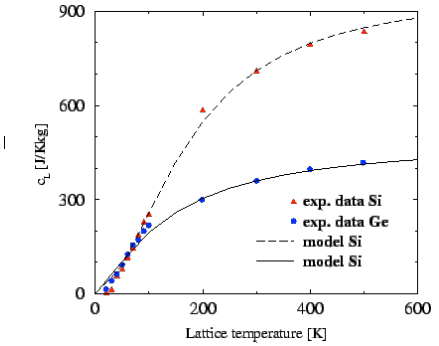
For specific heat of a solid, if we use Planck's expression for <*E*>, i.e. we assume that lattice vibrations are quantised rather than continuous, we get the following:

$$\langle E \rangle = \frac{h\upsilon}{e^{\frac{h\upsilon}{k_B T}} - 1}$$

Remember that Specific heat = *dE/dT*, where *E* is the internal energy, which in this case is <*E*>. Non-Quantum approach leads to the result that Specific heat should be a constant for all materials, and independent of temperature, which we know isn't actually true!

By finding *d*<*E*>*/dT*, we get the following curve:




Agrees very well with experiment!

# *The origins of electrical resistance*

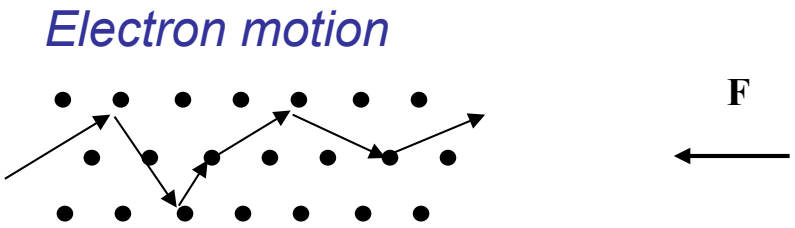
From solutions to Schrödinger's equation for weak periodic potential, we will see that electrons in lattice are travelling waves, i.e. not localised or decaying, i.e. no resistance.

What is the origin of resistance then? – any deviation from perfect periodicity, and a reason for dissipation of energy.

Scattering

## How do conductors conduct electricity?

Under influence of electric field, F from applied bias, electrons experience a force = eF. They accelerate until a scattering event stops them, and then they accelerate again. *Only the average motion is along the direction of the applied field.* The distance and time between collisions are called the mean free path, l and time, t respectively. The mean velocity along the field direction is called the *drift velocity.*



The effect of the scattering events is to slow down electrons, and therefore reduce the electric current. This is the origin of resistance. Typical values for $\lambda$ in a metal ~ 40 nm at Room Temperature.

What causes scattering? -> deviations from perfect periodicity, i.e., lattice vibrations, impurities, defects, electron-electron coupling…

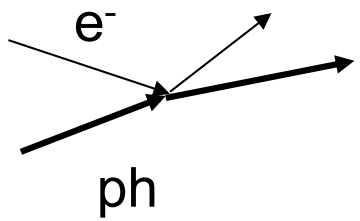
As the dimensions of conductors decreases below the mean-free path, their *resistivity* starts increasing rapidly.

## Scattering by Lattice vibrations

Atomic cores in lattice are coupled together. Interatomic potential can be approximated as harmonic to 1$^{st}$ order.

Recap Quantum harmonic oscillator : quantised energy levels. Lattice essentially consists of QHOs, so lattice vibrations are quantised. Quantum is called a *Phonon, in direct analogy to a photon.*

**electron-phonon scattering:**



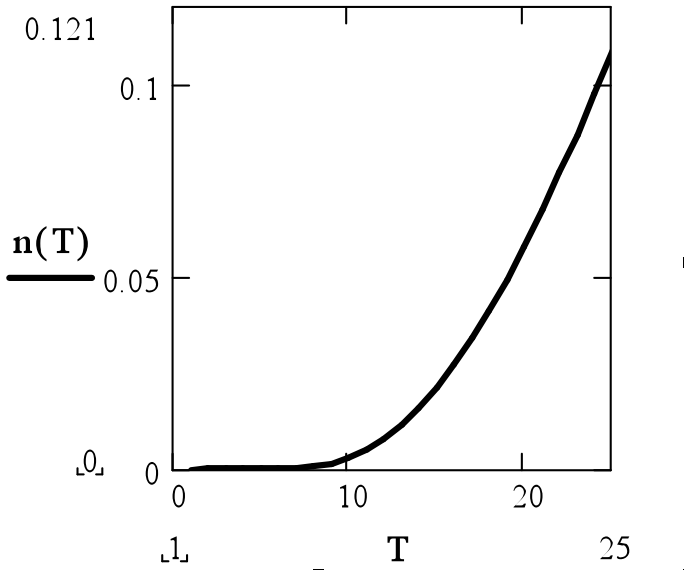
How many phonons are present in a lattice? i.e. if we assume a constant electron-phonon coupling strength and probability, then the temperature dependence of this contribution to resistance can be calculated by knowing the number of phonons. The probability of occupation of the $n^{th}$ energy level due to thermal excitation is

$e^{-E_n/k_BT}$ . *(cf. Boltzmann factor)*

Therefore, average energy = $$\langle E \rangle = \frac{\sum_{n=0}^{\infty} E_n e^{-E_n/k_BT}}{\sum_{n=0}^{\infty} e^{-E_n/k_BT}}$$

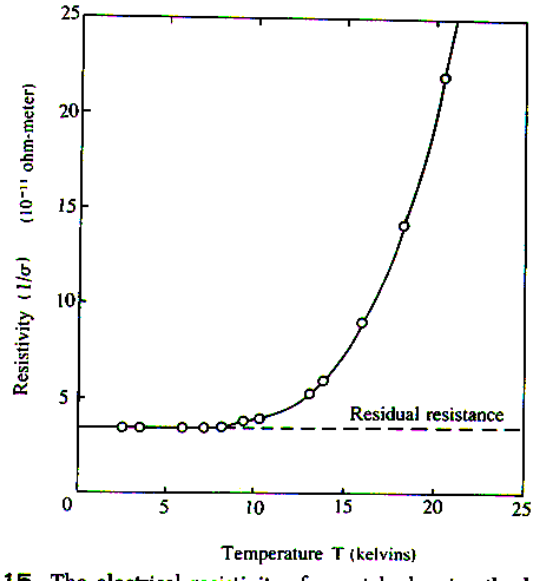
given that the spacing between energy levels is $\hbar\omega$, and the energy per oscillator is also $\hbar\omega$, we can write the phonon occupation number $\langle n \rangle$ as $\langle E \rangle / \hbar\omega$
i.e.
$\langle n \rangle = 1/[\, e^{(\hbar w / k_B T)} - 1]$

As a function of temperature, this looks like:




Using our simple approximations, we would expect the resistance to follow this curve.

Experimentally:

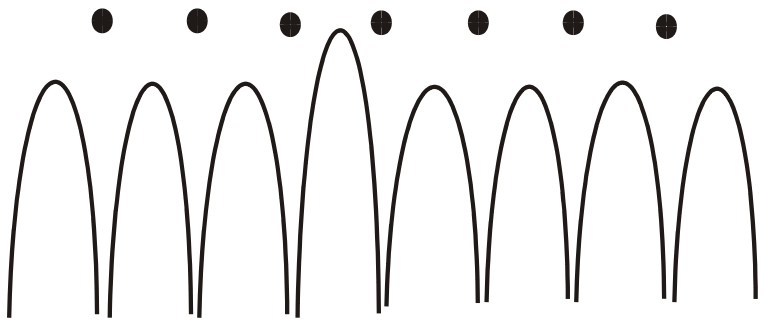



generally very good agreement!

One main difference: residual resistance. This is due to scattering from lattice imperfections and impurities.
What is effect of lattice imperfections, i.e. how do they cause resistance?

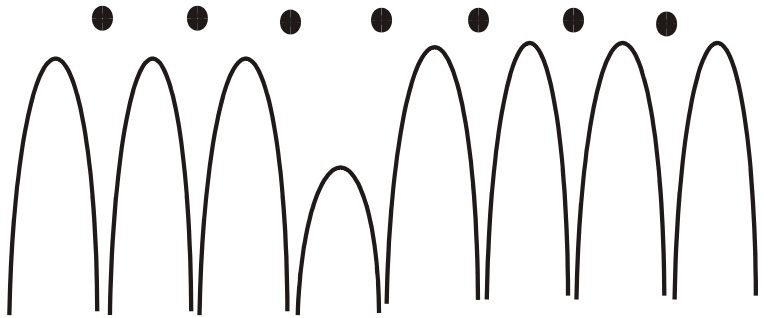
## Scattering by Lattice imperfections

First, consider the case when the imperfection has a higher energy than the surrounding atoms, i.e.:



This is similar to the case we studied earlier, i.e. scattering by a potential barrier. An electron encountering this barrier will be partly reflected, hence the current will be reduced and we have resistance!

Now consider the case where the imperfection has a lower energy than the surrounding atoms, i.e.:



This time, an electron encountering this potential well may become trapped into one of its bound states. This process also reduces the current flow and causes resistance.

These two mechanisms are the primary cause of the residual resistance we saw earlier. Sample treatment, e.g. annealing can reduce the number of imperfections in a lattice and reduce the residual resistance.

What is meant by a lattice imperfection?

- anything breaking the lattice symmetry, -> missing atom, substituted atom, dopant, any lattice defect, ….