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Paper No. : Physics at Nanoscale - I

Module : **Examples of Changes in Properties at Nanoscale And Introduction to Mesoscopic Physics**

Development Team

Principal Investigator	
Paper Coordinator	Prof. Subhasis Ghosh, School of Physical Sciences Jawaharlal Nehru University, New Delhi
Content Writer	Prof. Subhasis Ghosh, School of Physical Sciences Jawaharlal Nehru University, New Delhi
Content Reviewer	

Table of Contents of Chapter 1

MODULE III

1.2.4 Examples of Changes in Properties at Nanoscale

1.2.4.1 Quantum Confinement and Electrical properties

The electrical properties of a material depend on its electronic configuration. Based on the energy gap between the valence and the conduction bands, the materials can be classified as conductors, semiconductors or insulators as shown in the figure.

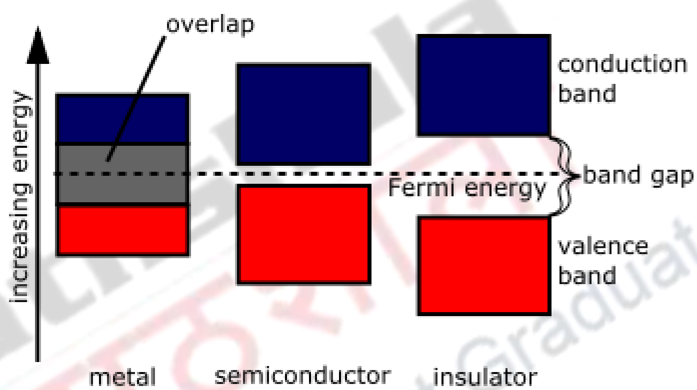

Fig 2. *The electron band structure of materials at T = 0K. The image has been taken from:* https://en.wikibooks.org/wiki/Semiconductors/What_is_a_Semiconductor

The electrons associated with conductors and semiconductors are either tightly bound to the nucleus of the atoms or are free to roam about in the bulk of the material. It is these free electrons that can be confined by means of the effect called quantum confinement. In the bulk materials, with large number of atoms the energy levels are so closely spaced that they resemble bands, the spacing between the levels being inversely proportional to the number of atoms. Having very few atoms in material, however, causes the energy states to spread out and widens the band gap. The expression for energy difference shows that as the size of the sample is reduced the spacing between the energy levels increases, and the discreteness of these levels becomes more pronounced. It is possible to create 'islands' of conductor and semiconductor structures in the interior of insulators to confine the electrons. To reduce the volume of three dimensional structures we have to reduce the samples to a size in which at least of the dimensions falls to less than 100nm. Constraining electrons inside a region of minimal width creates a quantum well which can be realized and fabricated from alternating layers of different semiconductors, or by deposition of very thin metal films. By further constraining the depth of the electron's domain, a quantum wire can be created from quantum well. Carbon nanotubes and other nanoscale wires, and for that matter DNA are natural quantum wires. And all the three dimensions are minimized, or when quantum wires are chopped into small pieces we get quantum dot. The dot can be a particle located inside a larger structure or on its surface. It can also be a place where electrons have been trapped using electric fields. Whether they are confined to a quantum wells, quantum wires or quantum dots, quantum mechanics dictates that the wavefunction of the electron must drop down to zero at the boundaries of the confining structure. The dimension of the material for confinement is reached when the size of the material becomes comparable to the wavelength of the electron.

In metals, particles with diameters 1-10 nm can behave as quantum dots and in semiconducting particles quantum confinement is seen for sizes up to a few hundred nanometers. The conducting nature of the metals can be transformed to insulators, as the size is reduced, because of the increase in the spacing between energy levels. The fact that metals have overlapping valence and conduction bands changes at the smaller dimensions and it is seen that the metals exhibit a band gap and are converted into semiconductors or insulators, if the band gap at a particular temperature exceeds the thermal energy available to the electrons at that temperature. Carbon nanotubes, for example, can behave as conductors or semiconductors depending on their nanostructure.

1.2.4.2 Optical properties

In general, light incident on a material is transmitted, absorbed or reflected. The color of a material is determined by the wavelengths of light reflected by it. A material absorbs light of certain wavelengths, depending on its energy levels. It is a molecular phenomenon which depends on the chemical constituents and structure of the substance, and also on the electronic, rotational and vibrational transitions. An observer will not see the colors whose wavelengths have been absorbed, and will only see colors associated with the reflected light. For example leaves appear green because chlorophyll, which is a pigment, absorbs the blue and red colors of the spectrum reflecting only the green color.

Another phenomenon that is important in determining the color or transparency of a material is scattering. It is the phenomenon that occurs when light is incident on a structure with dimensions comparable to its wavelength. It is a physical process which is different from the phenomena discussed earlier and depends on size of the sample and in case of suspension, it alos depends on the index of refraction of the cluster and the index of refraction of the suspension medium. The wavelength of the incoming light and outgoing light are the same. It can be shown that the maximum scattering occurs for wavelengths twice as large as the cluster size. Thus for structures with sizes in the nanoscale, the scattering of light plays an important role in determining the color and transparency.

Nanomaterials in general can have varied optical properties as a result of the way light either absorbed, or scattered from nanostructure. For example, the color of butterfly wings is the result of the constructive interference of the light wavelengths as they interact with the photonic crystals (which is a nanomaterial) embedded on the wings of butterfly.

1.3 Introduction to Mesoscopic Physics

1.3.1 Quantum Coherence

A mesoscopic system is one whose size is in between a microscopic and macroscopic system. It could be much larger than a few atoms or molecules or nanoparticles, but it is small enough that the degrees-of-freedom are to be regarded as quantum mechanical. A mesoscopic system has a size l that is larger than a microscopic length scale a (for example the Bohr radius or de Broglie wavelength), yet typically smaller than a length scale, known as phase-coherence length l_{φ}, which is the characteristic length beyond which the wave function represents the system loses phase coherence. l_{φ} generally depends on the dimension, microscopic details and the temperature of the system. Therefore, a mesoscopic system in which quantum mechanics is fully manifested, is one that is larger than microscopic or nanoscopic system.

1.3.2 Quantum Transport

Let us try to understand the different length scales defining the motion of electrons through a conductor. The most obvious is the geometrical size of the conductor. The size may be different for the three dimensions x, y and z and we can assume a characteristic dimension l, whose comparison with one of the other length scales determines the behavior of the system. The next length scale comes from the fact that in a mesoscopic system, the electron is considered to behave as a wave that, depending on the energy, has a characteristic wavelength associated with it. For electron transport, nearly always only those electrons become important whose energy is equal to or close to the Fermi energy. Thus the Fermi wavelength is a relevant length scale in a variety of quantum effects, in particular those depending on wave-interference.

As opposed to ideal conductors with regular lattices, conductors in the real world may have lattice irregularities or defects, and thus do not show translational invariance. The electron waves will interact with these irregularities, leading to a scattering of the wave. The mean free path or the average distance travelled by the electron between two successive scattering events is finite. If the electrons are scattered by static faults in the crystals (such as dislocations, impurities or walls) where the size of the scattering center is much greater than the mass of the electron, the result is a change in the direction of the wave propagation with virtually no change in the electron energy. Such events are called elastic scattering and the distance associated is the elastic mean free path, l_e. Other causes of electron scattering may be time-dependent in nature. For example, an electron travelling in the crystal may respond through electron-phonon interaction. In this case, the energy of the scattering electron will change, and may end up absorbing energy in quanta of the characteristic phonon energy, which at a temperature T, would be of the order kT, where k is Boltzmann constant. Thus this is an example of inelastic scattering and the associated mean free path is l_i. This interaction is dependent on the temperature, since the phonon momentum decreases with temperature. Other causes of inelastic scattering include the Coulomb interaction among electrons.

The final length scale of significance in the case of electron transport is the phase coherence length. The phase of the electron wave is changed whenever it undergoes scattering. The distance an electron can travel before its phase is randomized, being influenced by mechanisms that vary with space and time, is called the phase coherence or the phase breaking length. The finite value of l_φ arises from the residual Coulomb interaction which is responsible for the quasiparticle lifetime, as well as from other inelastic phase-breaking events, such as coupling to the degrees of freedom of external environment, electron-phonon scattering and any other inelastic scattering.

Summary of characteristic lengths

Geometrical dimension: l, size of conductor

Phase coherence length: l_φ, distance an electron travels before suffering a phase change of 2π.

Elastic scattering length: l_e, mean free path between elastic scattering events

Inelastic scattering length: l_{in}, distance an electron travels before losing an energy kT

Macroscopic conductor: $l_e \le l_\varphi \le l_{in} \le l$

Mesoscopic conductor: $l_e \le l \le l_\varphi \le l_{in}$

Electrons in a mesoscopic conductor i.e. a conductor with length smaller than l_φ move as a wave, not as a particle, similar to an electromagnetic wave propagating inside a wave guide and wave-like nature of the electron is mesoscopic conductors leads to many unusual physical properties which are revealed only after 1988 by two seminal papers. Perhaps the most profound is the origin of the resistance of smaller system, which could be as small as single hydrogen molecule. Resistance is generally caused by inelastic scattering of the electrons with disorder (impurities and other imperfections), other electrons, and with phonons (lattice vibrations). In a mesoscopic conductor, however, an electron typically travels the entire length of the system without undergoing phase-breaking inelastic collisions. Apparently, this seems that there would be no resistance at all of a conductor whose length less than l_φ. However, to determine experimentally what is the actual resistance one has to attach electrical leads, which are ought to be macroscopic contact pads. Then in a mesoscopic conductor, the resistance is caused by a combination of elastic scattering of electron waves from disorder and coupling with the macroscopic leads. In this scenario, Rolf Landauer in 1957 proposed that the magnitude of the resistance is determined exclusively by the contact pads in a mesoscopic conductor. Landauer proposed that R is proportional to h/e^2t, where t is the quantum transmission probability for an electron injected on one end of the conductor to propagate through the conductor to the other end. The ratio h/e^2 of the fundamental constants has dimensions of resistance and is about 26 kΩ. The Landauer formula shows that the resistance (conductance) of a mesoscopic conductor is inversely (directly) related to the quantum mechanical probability that an electron can propagate through the system without scattering inelastically. Landauer's formula is unusually successful in determining the resistance of a mesoscopic conductor.

1.3.3 Weak localization

Weak localization is another important consequence of the phase-coherent nature of electron transport in a mesoscopic system. To understand weak localization it is first necessary to understand Anderson localization, also known as strong localization, is the absence of diffusion of waves in a *disordered* medium. This means that the eigenstates of an electron in a disordered environment become spatially localized around impurities, causing the system to behave as an insulator instead of a conductor. Whereas weak localization is a very different process that also increases the resistance of a disordered conductor and is resulted due to quantum interference effect that occurs in systems with time-reversal symmetry. The probability P for an electron to propagate from point **r** to point **r′** is the sum of quantum amplitudes A_i for the electron to take all possible paths i, and then calculate the modulus squared, $P = \left| \sum_i A_i \right|^2$. This can be viewed as a generalization of the double-slit interference with infinite number of "slits". The cross-terms in this expression are responsible for interference. In a normal conductor, when different paths from **r** to **r′** considered, the randomness due to inelastic scattering quantum interference effects are washed out. However, in a mesoscopic conductor, there is a special class of paths, closed paths with **r = r′,** where interference effects can be important. In systems with time-reversal symmetry, i.e., in absence of any magnetic field, there will always be pairs of closed paths and their time-reversed counterparts in the above summation that have the same amplitude resulting the probability to go from **r** to **r,** is enhanced by quantum interference effects between different scatterers, and this leads to an increase in resistance which can be measured experimentally at low temperature.

1.3.4. Dephasing by electron-electron interaction

As explained above**,** the effects of weak localization is significant when the electron motion is sufficiently phase-coherent. This fact can be exploited to measure the phase-coherence length l_φ or phase coherence-time τ_φ, the characteristic time beyond which the electron becomes decoherent. l_φ and τ_φ are simply related to each other. The increase in resistance due to weak localization depends on the number of closed paths that contribute to the summation in $P = |\sum_i A_i|^2$, for a closed path in a length of the sample so that $L < l_\varphi$ otherwise if $L > l_\varphi$ the electron would not have the phase coherence necessary to exhibit interference. In case of $L < l_\varphi$, it possible to turn on and off the weak localization effect by applying a magnetic field and can be used to determine the value of l_φ or τ_φ. At low temperatures, electron-electron scattering is responsible for phase breaking and the fluctuating electric field produced by the other electrons scrambles the phase of electron after some time τ_φ. It is predicted that the dephasing rate vanishes at low temperature as $\tau_\varphi^{-1} \alpha T^\beta$, where β is a positive exponent, but recently it has been shown experimentally that there is a saturation of τ_φ^{-1} in the T→0 limit. This issue requires further investigation and is currently a problem of great interest.

1.3.5 Thouless Energy

The extensive research on mesoscopic physics in different nanosystems has led to a profound new discoveries and new insight into quantum systems. In particular, several new aspects of quantum transport in mesoscopic systems have been revealed in recent past. In the 1970's David Thouless showed that any quantum system possesses an important fundamental energy scale, now called the Thouless energy E_T which is essentially a measure of how sensitive the eigenstates in a quantum system due to change in boundary conditions. Specifically, E_T is defined as the energy change of a state at the Fermi energy when boundary conditions change from periodic to antiperiodic. E_T would be zero in an insulator-with localized eigenstates, because if the wave functions do not extend to the boundaries their energies will be independent of boundary conditions. Thouless showed that the dimensionless ratio $g \equiv E_T/\Delta\varepsilon$ of E_T with the energy level spacing at the Fermi energy, $\Delta\varepsilon$ can be used to determine whether the system is a conductor (g > 1) on an insulator(g < 1). In fact, g is can be scaled with the conductance of the system.