ELECTRON LOCALIZATION IN LOW DIMENSIONAL SYSTEMS

A thesis submitted for the degree of

DOCTOR OF PHILOSOPHY

by

RAISHMA KRISHNAN

School of Physics
University of Hyderabad
Hyderabad 500 046
INDIA

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Dedicated to

Papa and Mataji
whose blessings i have experienced
throughout.....

DECLARATION

I hereby declare that the research work embodied in this thesis entitled **Electron Localization in Low Dimensional Systems** has been carried out by me in the School of Physics, University of Hyderabad, Hyderabad, India, under the supervision of **Professor Vipin Srivastava**.

29 May 2002

(Raishma Krishnan)

CERTIFICATE

This is to certify that the thesis entitled **Electron Localization in Low Dimensional Systems** submitted by **Raishma Krishnan** to the University of Hyderabad is a bonafide work carried out by her under my supervision. The matter embodied in this thesis has not been submitted to any other University or Institute for the award of any degree or diploma.

29/5/02

(Professor Vipin Srivastava)
Thesis Supervisor

29/05/2002

Professor S. N. KAUL
Dean
School of Physics

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LIST OF SYMBOLS

Symbol	Meaning
ξ, l	Localization length
$g_c(L)$	Dimensionless conductance or Thouless number
α	Inverse localization length
l_{in}	Inelastic scattering length
l_e	Elastic scattering length
D	Diffusion constant
$\Delta R/R_0$	Incremental resistance ratio
ρ_e	Impurity resistivity
τ_{in}	Inelastic scattering time
l_r, &, L_r	Short and long-steps
L_ϕ	Dephasing length
τ_ϕ	Phase-decoherence time
λ	Tunneling parameter
Δ_0	Overlap between wave functions in the TS or coupling energy
J	Interaction energy between TLS
μ	Dimensionless parameter, mobility
n_s	Concentration of electrons
n_c	Critical concentration
r_s	Dimensionless parameter
a_B	Bohr radius

Symbol	Meaning
J_{ij}	Transfer integral
Δ_{ij}	Difference between energies on site i and j
r_m	Length associated with the largest resistance R_m in the current carrying network
ν_{ph}	Typical phonon frequency
q_{TF}	Thomas-Fermi screening vector
r_d	Dimensionless measure of disorder
σ_{min}	Minimum metallic conductivity
$P_a(t)$	Stay-put probability
Σ_0	Self energy

PREAMBLE

The electrical properties of crystalline systems are fairly well understood with the firm base of the Bloch-Floquet theorem. But most of the materials we deal with in nature do not possess a strictly ordered character and imperfections are inevitably present in them. The complexity involved due to the lack of periodicity makes it necessary to study the effect of disorder in these systems.

Much of the work in this area was initiated by the seminal work of Anderson in 1958. His results revealed that the electronic states in disordered systems are spatially localized. Later Mott and Cohen, Fritzsche and Ovshinsky put forth what is known as the Mott-CFO model, which conjectured that depending on the extent of disorder present in the system there can be both extended as well as localized states and that they should be separated by a critical energy E_c, called the mobility edge. Economou and Cohen subsequently gave a simple criterion to find the mobility edge E_c.

Mott and Tworse's result on complete localization in one dimensional (1D) system for any extent of disorder emphasized the importance of dimensionality in the phenomenon of localization. It was believed for some time that 1D was the marginal dimension for localization. But the simulation work done by Thouless and coworkers showed that in 2D also all states could be localized at any disorder. This view was consolidated by the scaling theory of Abrahams et al. and also the subsequent experiments that followed it.

Also, Thouless's criterion as to when a given wire of small cross-section would behave one dimensionally sparkled a lot of experimental activity in this area. But the experimental results did not show complete agreement with his results based on the localization theory.

In this thesis we have studied electron localization and metal-insulator transition (MIT) in low-dimensional disordered systems. To begin with we investigate the resistance of thin-wires (quasi 1-dimensional). We develop the problem initiated by Thouless and study in detail the dependence of the resistance on temperature, area of cross-section and bulk resistivity. The dependence of the ratio of the increase in resistance ΔR to the metallic resistance R_0, $\Delta R/R_0$, on the bulk resistivity ρ_e is studied within the framework of localization theory. By considering the diffusion of an electron as a wave packet made up of broad localized states, we distinguish between two regimes defined in terms of step lengths travelled by the wavepackets on the scale of localization length. We calculate $\Delta R/R_0$ from the exponential length dependence of R given by the scaling theory of localization. What we have focussed on is that it is the tunneling states (TS) or the two level systems (TLS) that play a pivotal role in deciding the inelastic scattering rate. Thouless' result is retrieved in our approach under a special condition. Also, the order of magnitude of $\Delta R/R_0$ that comes from our expression is in good agreement with the experimental value.

Next we study the effect of the influence of the environment in dephasing an electron system of mesoscopic dimensions. Theoretically it has been believed that $\tau_\phi(T)$, the time over which the phase memory is retained should increase with the decrease in inelastic events and should become infinite at $T = 0$ in very large systems. However recent experiments contradict this belief. Alternatively, the decoherence time saturates with the lowering of temperature. A proper theoretical consensus regarding the saturation of $\tau_\phi(T)$ is still in debate. We propose here that inelastic scattering from TLS is important in this connection. The coherent oscillation of the tunneling entity between the wells of a TLS gets affected and become incoherent when the TLS start to interact with one another. This happens at lower T and a dense concentration of TLS, and shows up in the scattering

of electrons from them. It is this incoherent oscillation, we argue in this chapter, that eventually leads to the saturation of $\tau_\phi(T)$.

After studying the quasi-1D and mesoscopic systems we moved on to 2D systems. It is the unexpected experimental result of Kravchenko et al. that caused a revival of work in this area by showing that at very low electron concentrations, n_s, and low disorder, a metallic state could be produced and a MIT could occur as a function of n_s. This and the following experimental results led to a drastic change in the localization scenario in 2D systems as described by the scaling theory. The new experimental results revealed the existence of an anomalous metallic phase contrary to the widely accepted view based on scaling theory. We have critically examined experimental results and the theories that attempt to explain them in the light of the old results where complete localization was found. We are of the view that one cannot look at the new results independently of the old ones because one should either prove that the old results are wrong or show that the new results are due to new conditions under which the experiments are performed. Even in the latter approach one should ensure that the old results are obtained in appropriate limits.

We have attempted to explain this MIT by taking into account various factors like electron-electron interaction, disorder, percolation, tunneling states, etc. We propose that the observed metallic behaviour could arise due to a novel possibility of delocalization caused by the interaction between the localized electrons, below a particular concentration at which the interaction energy V_{ee} exceeds the Fermi energy E_F. In the transition region, around a critical $n_s(= n_c)$ the resistivity shows a non-monotonic behaviour as a function of T. Unambiguous metallic and insulating phases are found on either sides of n_s. The new insulating phase below n_c has been argued here to be a Wigner glass where electrons are frozen in random locations by long-ranged interactions among them that are otherwise

trapped in small puddles formed in a 2D electron system due to very low E_F. The experiments also reveal some subtleties in the electrical behaviour which we have tried to put in the right perspectives.

Next we move on to the old problem of the minimum metallic conductivity, σ_{min}, the concept of which was introduced by Mott in connection with Anderson localization. Wherever there is a metal-insulator transition the question of σ_{min} is inevitably associated. Mott was of the view that the MIT across the mobility edge E_c ought to be discontinuous. The conductivity σ would attain a minimum value σ_{min} just before dropping abruptly to zero on the insulating side of the electron spectrum.

We have looked at the general problem of the vanishing of σ_{min} in MIT's in disordered systems. We have considered the basic definition of localization, in terms of the poles and branch-cut of Green's function, and looked into the consequences of the coexistence of poles and branch-cut (in a section of the spectrum of electron states) on σ_{min}. We show that if the intermediate singularly continuous spectrum exists and separates the localized and extended regimes then σ_{min} will be zero and the MIT will be continuous.

The works are organized in the sequence described above. The first chapter, 'introduction', introduces the basic concepts such as types of disorder, scaling theory, conduction mechanisms in Anderson systems, tuuneling phenomena mesoscopic systems etc. that are used in the latter chapters.

Chapter 1

INTRODUCTION

1.1 Disordered systems

In recent decades much interest has been developed in the study of the structure and properties of disordered condensed matter systems. The reasons are two fold: rapid advances in solid state physics and their numerous applications, and the fact that disordered systems - crystals with impurities, liquid metals, amorphous substances and the like - are systems of generic nature, whereas ordered structures such as perfect crystal lattices etc. strictly speaking, are idealized objects.

The theory of ordered condensed matter systems cannot be applied to disordered systems without substantial modifications. The notion of translational symmetry in the crystalline lattice enables one to describe the low lying levels of a macroscopic system in terms of various quasi-particles characterized by quasi-momentum and a dispersion law. However, the energy spectrum of a disordered condensed matter system is more complicated. For instance in the case of disordered materials the spectrum consists of both extended and localized states.

1.1.1 Different types of disorder

The term disorder in the context of disordered condensed matter systems is generally used to refer to a scenario more complicated than that in doped semiconductors. A disordered system has disorder on *every* site, i.e. the potential at each site can be different (see e.g. fig.(1.1)). The site energies ϵ are represented by a probability distribution, $P(\epsilon)$, i.e. the site energy can be anything in a given

range with the corresponding probability. The width of the distribution measures the extent of disorder in the system. Thus disorder is actually a measure of the probabilistic distribution of site energies. The degree or extent of disorder in a typical uniform distribution of site energies measures the difference between the depths of the shallowest and the deepest potential wells, or the spread of site energies in the probability distribution, (see fig.(1.1)).

The probability distribution curve can have any shape, such as Gaussian, rectangular, square or Lorentzian, etc.; a random binary alloy has a bimodal distribution comprising two $\delta-$ functions, the separation between which measures the disorder. Generally, in nature, a random event with no external influence has a Gaussian distribution function (fig.(1.2)).

The above description pertains to what is generally termed as *substituitional* or *compositional* or *cellular* disorder. The underlying lattice structure is normally believed to be intact. Another type of disorder is *topological* or *structural* disorder.

A topologically or structurally disordered system does not have an underlying lattice structure. A topologically disordered system can tentatively be viewed as a system with high density of dislocations. Another way is to treat the system as a collection of microcrystals with random orientations. Of course the order within each microcrystal is the local short range order. A structurally disordered system must contain a sufficient number of defects that destroy the topology of the curvilinear network.

1.2 Anderson model

The idea of localized electron states in disordered systems was first given by Anderson, in his classic paper entitled 'absence of diffusion in certain random lattices' [2]. He considered a tight binding (TB) model of a regular solid, with the disorder introduced by letting the site - energy vary from site to site and is

approximated as rectangular wells of varying depths, ϵ_i (fig.(1.1)). An electron is initially (at time t=0) taken to be firmly localized on a lattice site. Then the interactions between nearest neighbour sites are switched on to allow the electron to diffuse away. The diffusion process is governed by the following TB Hamiltonian.

$$H = \sum_i \epsilon_i a_i^\dagger a_i + \sum_i \sum_j V_{ij} a_i^\dagger a_j \tag{1.1}$$

where ϵ_i are the random site energies and

$$\begin{aligned} V_{ij} &= -V, \quad \text{constant for nearest neighbours and} \\ &= 0 \qquad \text{otherwise} \end{aligned}$$

a_i and $a_i^\dagger$ are the annihilation and the creation operators. The width W of the distribution function for ϵ_i is the measure of disorder. Generally W, normalized by the band width, i.e. $W/(2ZV)$, is taken as the measure of disorder (Z is the co-ordination number of the lattice). Anderson showed that when W/V

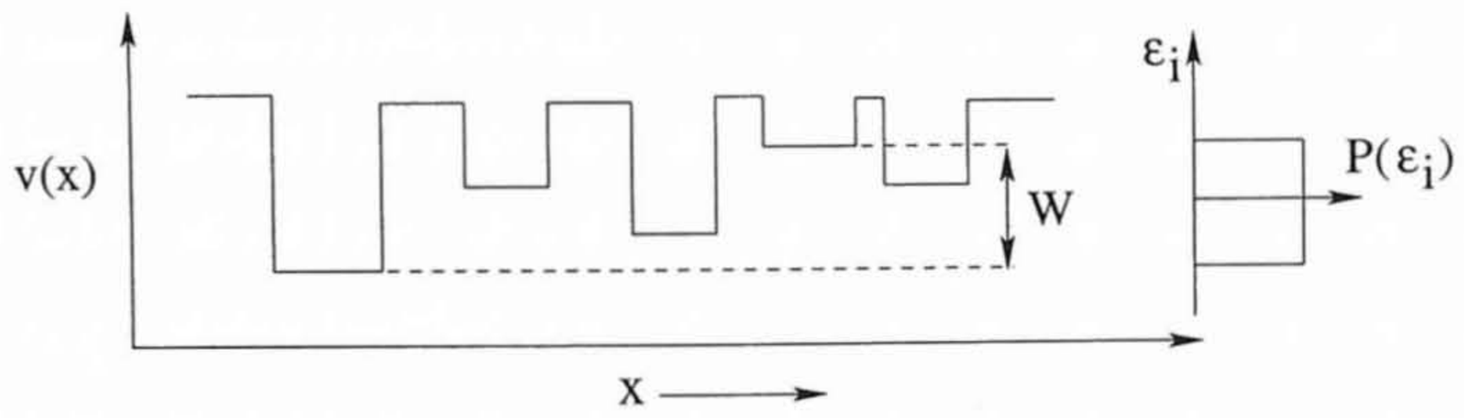
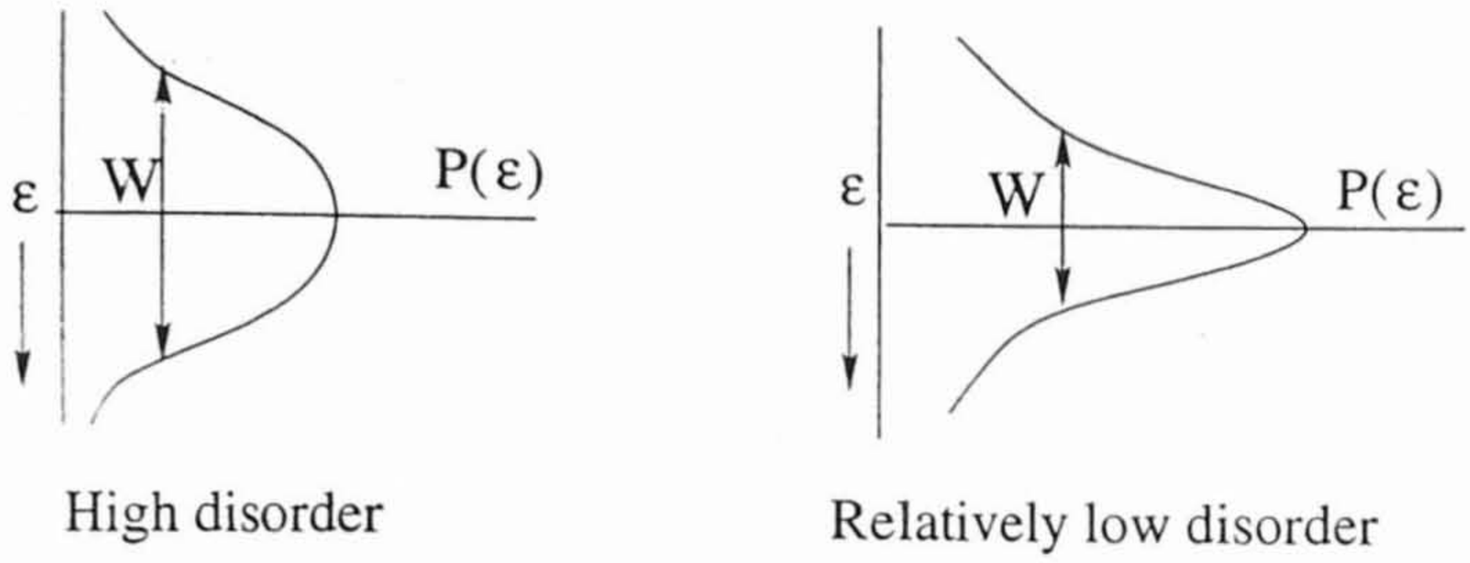


Figure 1.1: Potential energy of an electron in Anderson model

reaches a certain critical value, all states become localized in the band. That is, irrespective of the energy of an electron in the band its probability to be found at the site where it was present at t=0 will be non-zero even at $t = \infty$. In other words, there is a critical value W_c of W such that for $W > W_c$, all the states at the middle of the band and by inference all the states in the band are localized. On the other hand, for $W < W_c$ the states in the middle of the



High disorder Relatively low disorder

Figure 1.2: The extent of disorder

band are extended. Anderson solved the dynamics of an electron in a medium of random ϵ_i's through a renormalized perturbation expansion (RPE) of self-energy of the Green's function, the propagator of the electron. He investigated the convergence/divergence of the RPE at the center of the band, $E \to 0$. Through a laborious calculation Anderson showed that the convergence of the RPE signals the localization of the state under consideration.

A wave function $\psi(r)$ is supposed to be localized if it decays fast enough as $|r| \to \infty$ so that $\int \psi^* \psi \, d^3r$ exists. It generally decays in an exponential way, $\psi(r) \to \exp(-\alpha|r|)$ as $r \to \infty$, where $1/\alpha$ is the localization length.

1.2.1 Mott - CFO model

In 1967 Mott [11, 13] first pointed out that if in Anderson model the ratio W/V lies below the critical value for localization, then only the states in the band tails would be localized. He introduced the concept of an energy E_c, called the mobility edge, which separates the localized states from extended states in the middle of the band. The mobility edge depends on the characteristics of the system and in particular on the degree of randomness. As the randomness increases, the localizability increases leading to an inward movement of the mobility edges. At $W = W_c$ the two E_c's moving away from the two band tails, collapse into each other and all extended states turn into localized states. This transition to an

insulating state is termed as Anderson transition.

Later, Cohen, Fritszhe and Ovshinsky (CFO) [14] arrived independently at the same picture in their amorphous semiconducting alloys. So the model is named as the Mott - CFO model. They also proposed that the tails of the conduction and valence bands could extend through the gap, overlap and pin the Fermi energy (fig.(1.3)). The Mott-CFO model is firmly supported by the experiments.

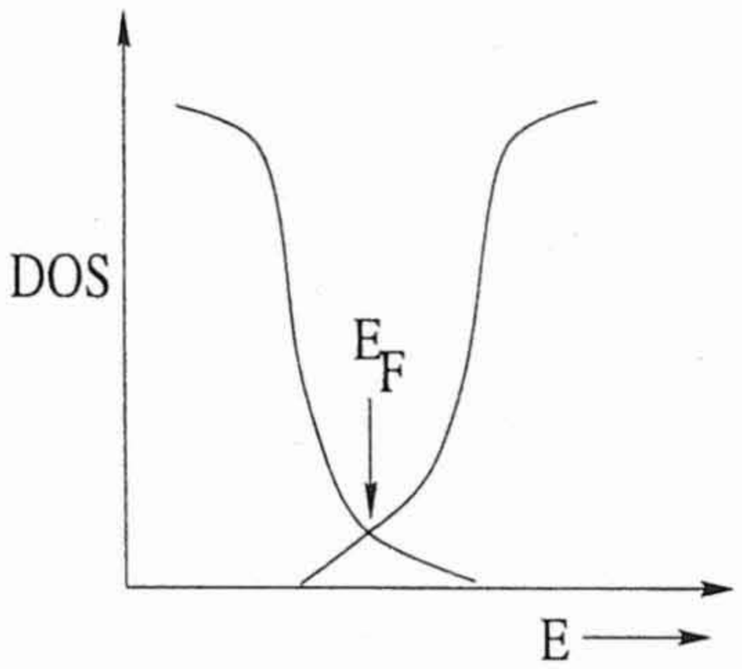


Figure 1.3: The model of CFO

1.2.2 Further developments

Following Anderson, Ziman [16], Lloyd [17] and Brouer [18] tried to simplify Anderson's theory. But they made the mistake of performing configurational averaging to start with. The information about localization was lost in the process. Their negative results conveyed to the future workers on the subject the crucial message that configurational averaging should be done after the quantity of interest has been calculated and that localization occurs due to multiple back scattering from disorder which results in quantum interference.

Thouless [19] clarified the mathematical intricacies in Anderson's paper [2]. Economou and Cohen [27] expressed Anderson's stay put probability in terms of Green's function and the imaginary part of self energy. They also gave a simple criterion to calculate the mobility edges E_c using the self - consistent single - site

approximation, called the coherent potential approximation (CPA) for obtaining the ensemble averaged self energy. Abou - Chacra et al. [32] around this time solved the localization problem exactly for Cayley tree lattice. It provided a lot of insight into the otherwise difficult problem from analytical point of view.

1.2.3 Numerical simulations

Computer simulations on localization are particularly significant due to the difficulties involved in doing analytical calculations and also due to the ambiguities in interpreting the experimental information. The existing theories could not satisfactorily explain simple questions like the location of mobility edges for a given system, the critical disorder W_c to cause Anderson transition, etc. Consequently numerical simulations of Licciardello and Thouless [54] and Weaire and Srivastava [52] and many others [104] proved useful.

The method employed by Thouless and his co-workers is as follows: A lattice of finite size is considered, usually with periodic boundary conditions to avoid surface effects. The results obtained have to be analyzed carefully. For sufficiently large systems the localized and the extended states can be distinguished easily, but the systems of sizes that could be handled on computer in those days were not sufficiently large and hence the distinction between extended and localized states was difficult. Even the extrapolation of the results to an infinite system was not completely reliable. Thouless et al. proposed to use anti-periodic boundary condition and study the sensitivity of the states to change in the boundary conditions from periodic to anti-periodic with increasing system size. We will elaborate on it in a later section on scaling theory.

The above simulations generally predicted mobility edges and therefore metal-insulator transition in 2D systems. However, later works by Licciardello and

Thouless [54] suggested that those states which were earlier interpreted as extended could be localized with large localization length. But there could be a relatively sharp transition between states with short and long localization lengths. These results inspired the scaling theory of localization that formally showed that all states in 2D could be localized at arbitrarily small disorders [57].

Weaire and Srivastava [50] studied the inverse participation ratio

$$\sum_i |a_i|^4 / \left(\sum_i |a_i|^2 \right),$$

where a_i is the probability amplitude on site i. The above quantity represents the inverse of the fraction of sites that lie under a wave function. Weaire and Srivastava [51] also calculated the condition for localization in hypercubic lattices in 4 and 5 dimensions. They found that the critical value of W/ZV increases with dimensionality, but is still a factor of six or seven less than Anderson's estimates.

1.3 Scaling theory

In the scaling theory one tries to understand localization by considering the behaviour of the conductance g as a function of the system size L or of some other variable characteristic of the system size. Although the idea of the scaling theory was already indicated in the works of Wegner [56] and Thouless et al. [19], the first formulation of this idea was given by Abrahams et al. [57].

The main ansatz of the theory states that if one constructs a hypercube of size $2L$ out of hypercubes of size L, then the conductance of the composite cube $\sigma(2L)$ is uniquely determined by that of the initial cube $\sigma(L)$. In other words, the idea is that the change in effective disorder when the system becomes a little bigger is determined by its value at the previous length scale, the only measure of this effective disorder being the conductance.

Consider an electron moving in a disordered medium. The electron wave in the random medium gets scattered repeatedly leading to random changes in the phase

on each episode of scattering. The distance over which the phase fluctuates by 2π defines the mean free path l. Beyond l, the electron motion is not ballistic but diffusive, so that, upon averaging over the impurity configurations, the averaged one electron propagator $< G(r) >$ behaves as $\exp(-|r|/l)$. This means that the scattered components interfere, and for a localized state the interference effects are such that the wave amplitude is large only in a small region of space and falls off exponentially around it.

Thus the microscopic length scale of interest in the localization problem is the mean free path which in turn forms the lower length cut off for diffusive motion. The conductance g_0 at this length scale is the microscopic measure of disorder, being small if disorder is large and vice versa. $g(L)$ has two very different asymptotic forms for $L >> l$ depending on the microscopic disorder.

Abrahams et al. [57] argued that quantum interference effects in a disordered system evolve continuously as a function of scale size. They calculated the functional form of this effect by identifying the leading microscopic contribution to this process and predicted consequences for the observed properties. To the question of what is the measure of quantum interference, following the ideas of Thouless, Abrahams et al. argued that conductance itself is such a measure. It is small if quantum interference is large and vice versa.

Thouless originally considered putting together blocks of random material of size L. A cube of disordered material will have a discrete spectrum and the eigen energies will be distributed randomnly to give rise to a rounded off form of the density of states (DOS). The time taken to cross the cube is $t = L^2/D$ where D is the diffusion constant. So when several such cubes are joined together, it will be very unlikely that the energies of different cubes will match up because of the interfacial perturbation caused by putting the blocks together. The spectra of the cubes will be similar, yet distinct from each other. However, since the

electron spends only a finite time in any cube, the uncertainity in energy can be measured, and it will be given by $\delta E = \hbar/t$.

If δE is small, then the electron will not be able to get into the next cube and hence will be localized. If δE is large, then the time spent in each cube will be less and the electron will easily find a compatible state in the next cube. Therefore the most important quantity is the ratio of δE to the average separation of the eigen energies of a cube, namely dE/dN. The blocks can be characterized by two parameters, the strength $t(L)$ of coupling between the wave functions in two neighbouring blocks and $W(L)$, which is the mismatch between an energy level in one block and the closest level in the neighbouring block.

Finite size scaling

Before studying the scaling by putting the blocks together, we ought to have a criterion for identifying localized and extended states. This can be done by first applying periodic boundary conditions (fig.(1.4)) on a finite block and then studying the effect of changing the boundary conditions to 'anti-periodic' (fig.(1.5)). Consider a system of size L and suppose a localized state lies within the system

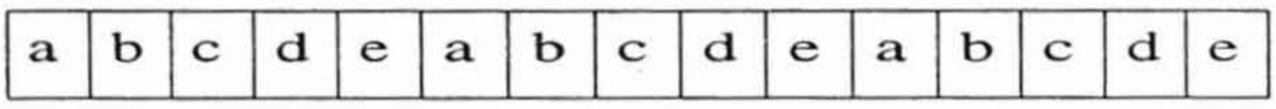


Figure 1.4: Periodic boundary condition

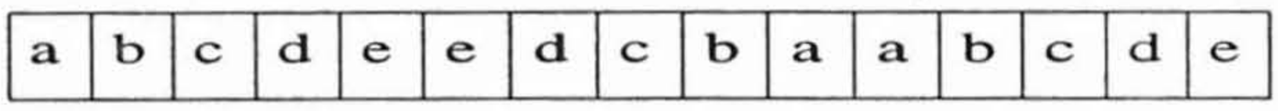


Figure 1.5: Anti-periodic boundary condition

as shown in fig.(1.6a). Such a localized state will be insensitive to the change in boundary conditions. Next consider a system of length L and let the localized state be located at the boundary as shown in fig.(1.6b). Such a localized state will be sensitive to the change of boundary conditions. However, if the system

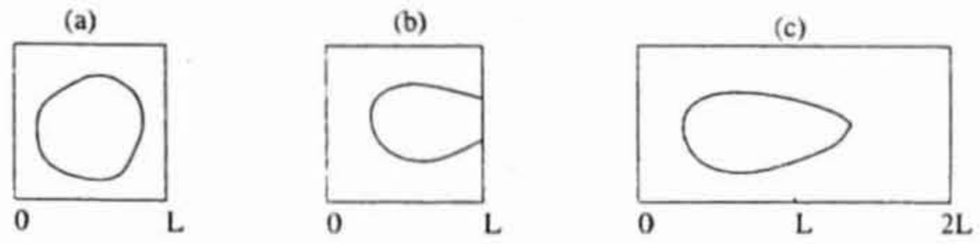


Figure 1.6: Sensitivity to boundary conditions

is scaled to length $2L$, and if the localized state now happens to be well within the boundaries, then it will be insensitive to the change of boundary conditions. Further increase in the size of the system will have no effect on this localized state.

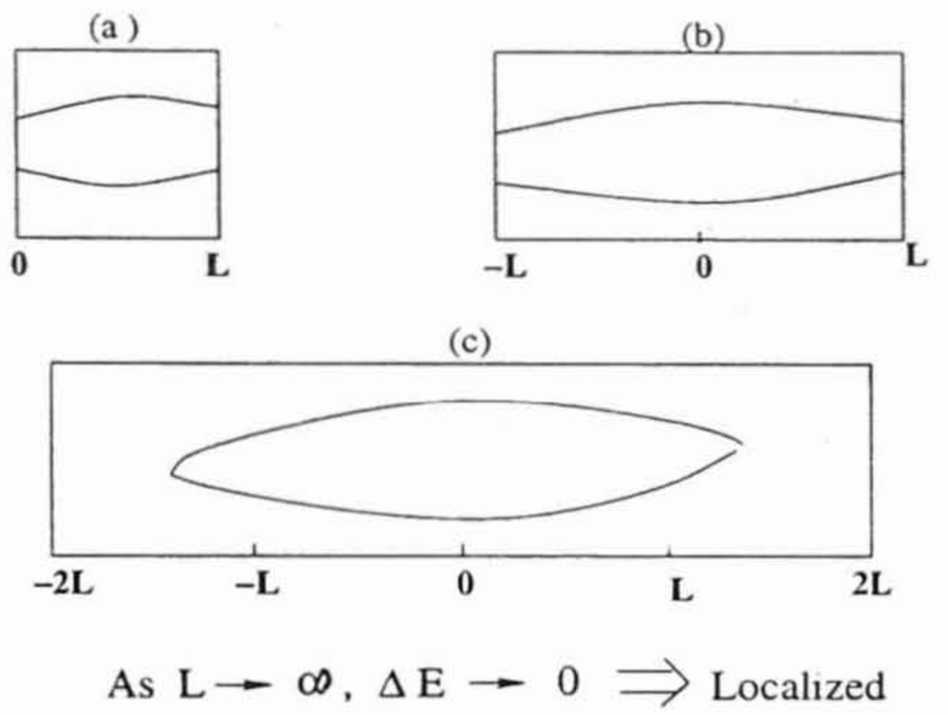


Figure 1.7: Effect of scaling on a localized state

On the contrary, an infinitely extended state will always show sensitivity to the change in boundary conditions no matter how many blocks are put together.

In other words, if the length of the system is less than the localization length, then, even though the state may be localized, it will be sensitive to the boundary conditions. This sensitivity will reduce as the size of the system is scaled up, fig.(1.7). But, for an extended state the sensitivity will keep on increasing with system size, fig.(1.8). The energy shift ΔE_n of the n^{th} energy level is the difference between the n^{th} energy levels calculated with periodic and antiperiodic boundary conditions, $\Delta E_n = |{E_n}^P - {E_n}^A|$. It is found to be of the order of $\hbar/t$, t being the

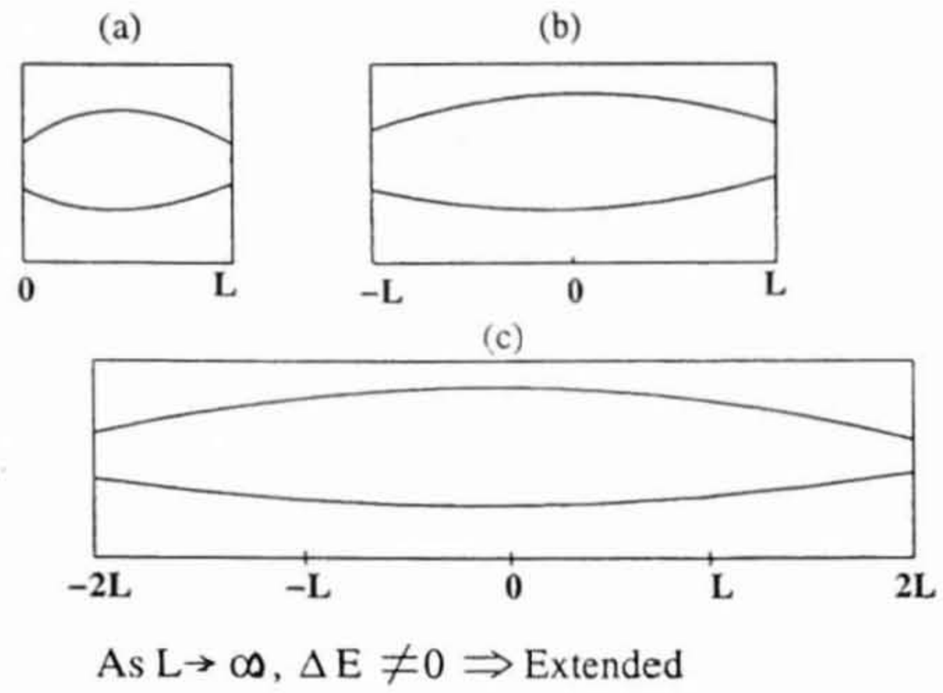


Figure 1.8: Effect of scaling on an extended state

time taken to diffuse to the ends of the wire. The larger the disorder, the greater will be the time taken to reach the ends of the wire.

Let $\Delta E_s = \hbar D/L^2$ be the sensitivity to the change in boundary conditions of a single block. When another such block of length L is attached, the sensitivity of the combined system will be, $\Delta E_c = \frac{\hbar D}{2L^2} = \frac{1}{4}(\Delta E_s)$. Thus we see that when two systems are combined together, the sensitivity of the combined system is reduced by $1/4^{th}$ of the sensitivity for an individual block. Thus as we keep on increasing the length of the system, if ΔE for the combined system reduces rapidly, then the state is detected to be localized or else it is extended. The ΔE which measures the sensitivity of the energy levels to the change in boundary conditions also gives a measure of the strength of coupling of a level in one square to its neighbours.

A finite system will have a discrete set of energy levels. Let dE/dN be the spacing between the levels as in fig.(1.9a). Joining of another system will broaden the energy levels, as in fig.(1.9b). Let ΔE be the range over which the energy levels of the first system vary when a second system is connected. Considering the Einstein's relation for conductance

$$\sigma = \frac{e^2 D}{2}\frac{dn}{dE} \qquad \text{we can write,} \qquad \Delta E = \frac{2\hbar}{e^2}\frac{\sigma}{L^2}\frac{dE}{dn}. \tag{1.2}$$

Consequently, the resistance will be

$$\rho = \frac{2\hbar}{e^2}\frac{dE/dN}{\Delta E}. \tag{1.3}$$

Thus the resistance measures the ratio of the spacing between the energy levels to the sensitivity of the energy levels to the change in the boundary conditions. The latter is also the measure of the coupling between the neighbouring energy levels when the system is scaled. If a state is localized, ΔE will be small and

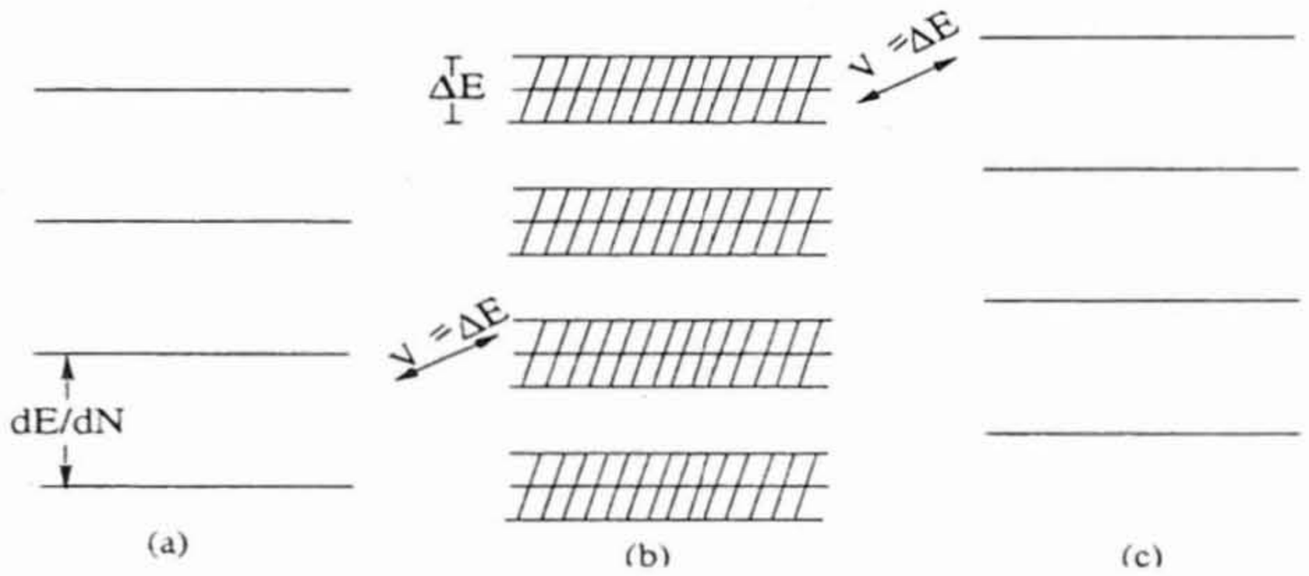


Figure 1.9: Energy level representation of scaling; V is the strength of coupling between two cells.

the resistance of the subsystem will be large. Smaller value for ΔE means that the coupling between the two subsystems is weak, which in turn means that the resistance of the individual subsystem is large, i.e. the state is localized.

Thus, if $\Delta E << dE/dN$, $\rho >> \frac{2\hbar}{e^2}$. So as the system is scaled to larger and larger dimensions, the sensitivity of the energy levels to the change in the boundary conditions becomes smaller and smaller and the resistance of the subsystem becomes greater than $2\hbar/e^2$. This is the argument given by Thouless to show that any system of a given cross-section would behave one dimensionally with localized states only if it becomes sufficiently long. This made Thouless to argue that once the zero temperature resistance of the wire exceeds $2\hbar/e^2$, the resistance will be found to increase exponentially with length instead of linearly.

The above inequalities also indicate that if the uncertainty in energy is large,

then the time the electron spends in each cube is less which would imply that the electron is easily able to find a compatible state in the next cube and thus we have an extended behaviour. When $\rho << 2\hbar/e^2$, Ohmic behaviour is seen and the resistance will add up normally. but for $\rho >> 2\hbar/e^2$ the net resistance is found to increase exponentially. Thus Thouless predicted that all 1D systems with impurity resistance greater than about $2\hbar/e^2$ would exhibit thermally activated hopping conductance at low temperatures and will be insulators at absolute zero. The length of the wire for which the resistance is of the order of $2\hbar/e^2$ is called the localization length, ξ.

Thus $\frac{\Delta E}{dE/dn}$ is the only relevant quantity whose scaling behaviour relates to the scaling behaviour of transport quantities. It can also be called a dimensionless conductance $g_c(L)$,

$$\frac{\Delta E}{dE/dn} = \frac{2\hbar}{e^2}g(L) = \frac{2\hbar}{e^2}\sigma L^{d-2} = g_c(L). \tag{1.4}$$

$g_c(L)$ is often termed as the generalized dimensionless conductance or Thouless number and is related to the conductance $g(L)$ as in eqn.(1.4). In particular, one can write down a single parameter scaling function,

$$\beta(g) = \frac{dlng}{dlnL}. \tag{1.5}$$

For a system of size L, let $g(L)$ be the conductance. Then the conductance for a system of length $(L + dL)$ depends only on the previous conductance, i.e. $g(L + dL) = f[g(L)]$ and

$$\beta[g(L)] = \frac{dlng(L)}{dlnL} = \frac{L}{g(L)}\frac{g(L + dL) - g(L)}{dL} \tag{1.6}$$

The above equation, called the renormalization group equation, has an important feature that the scaling function $\beta(g(L))$ depends on L only through g(L).

Large conductance i.e. $g >> g_c$***:***

In the regime where Ohms law is valid, i.e. $k_F >> 1$, $g(L) = \sigma L^{d-2}$ and

$$g_c(L) = \frac{2\hbar}{e^2}\sigma L^{d-2} \tag{1.7}$$

so that,

$$\beta(g_c(L)) = \lim_{L\to 0} \frac{dlng_c(L)}{dln(L)} = d-2 \tag{1.8}$$

i.e., in the metallic limit, β approaches a value $(d-2)$ asymptotically as $L \to \infty$.

Small conductance i.e. $g << g_c$***:***

For small conductance all the electronic states could be localized so that the scale dependence of $g_c(L)$ and β would be described by

$$g_c(L) = \frac{2\hbar}{e^2}\ g_0(d)\ \exp\left(-\frac{L}{\xi}\right) \tag{1.9}$$

$$\beta = \frac{dlng_c(L)}{dlnL} = \frac{-L}{\xi} \tag{1.10}$$

Also, note that, since β goes to $-\infty$ as the size L approaches infinity from eqn.(1.9) and comparing with eqn.(1.10) one gets

$$\beta = \ln\frac{g_c(L)}{g_0(d)} \tag{1.11}$$

The intermediate perturbative regime:

For weak disorder, i.e. $k_F l \gg 1$, it is possible to calculate corrections to the Boltzmann transport theory result for σ using diagrammatic perturbation theory. It turn out that singular back scattering leads to a significant scale dependent corrections to the conductivity to higher order terms in $1/k_F l$. These terms contribute a correction going as $1/g$ so that for large g

$$\beta(g) = (d-2) - \frac{a}{g} \tag{1.12}$$

For an electron gas $a = g_c = 2\hbar/e^2$. $\beta(g)$ is thus always less than its Ohms law value for a disordered system and hence the conduction is never quite Ohmic. It always increases more slowly with scale size than is suggested by $g = \sigma L^{d-2}$.

The scaling curve can thus be constructed using the eqn.(1.12) for large g and $\beta = \ln g/g_0$ for small g and also the assumption that $\beta(g)$ is continuous and monotonic. The continuous behaviour of $\beta(g)$ is expected because it describes how the conductance of a finite system evolves as a function of scale size. Abrahams et al. calculated $\beta(g_c)$ for $g_c \sim 1$ with some approximation as a function of $\ln g$ for d = 1,2 and 3. The behaviour of $\beta(g)$ is as shown in fig.(1.10). The

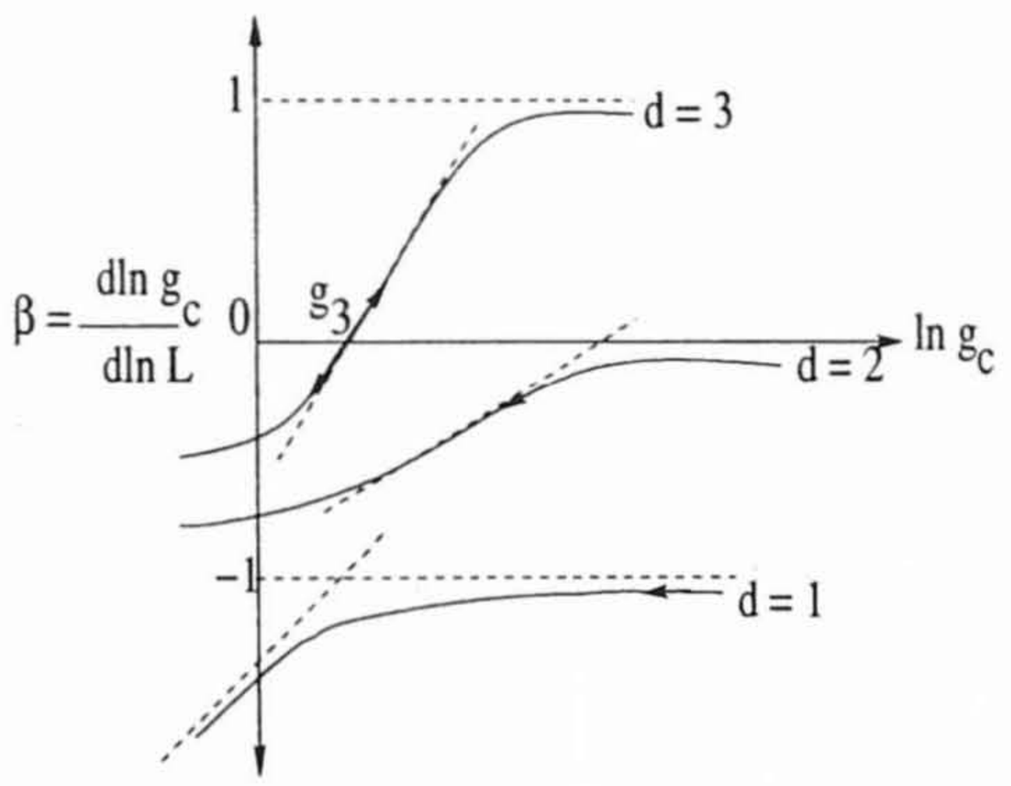


Figure 1.10: Schematic plot of $\beta(g_c)$ vs $\ln g_c$ for d=1,2 and 3.

asymptotics eqn.(1.11) and eqn.(1.12) are shown in dashed lines. From this graph one can draw a number of important conclusions.

For d=1: In this case

$$\beta(g_c) \;=\; d - 2 = -1 \tag{1.13}$$

i.e. the derivative $\frac{dlng_c}{dlnL} < 0$ for all g_c. Therefore the scaling procedure always results in diminishing g_c. This corresponds to $\beta(g_c)$ going downward irrespective

of the starting point. On carrying out the procedure a sufficient number of times, we reach the asymptotics $g = g_0 \exp\left(-\frac{L}{a}\right)$. Thus we find that as $L \to \infty$ both the conductance as well as the conductivity of a 1D disordered system vanish exponentially. This result was known well before the development of the scaling theory of localization.

For d=2: The new result of scaling theory is that $\lim_{L\to\infty} g_c = 0$ in the 2D case as well. In 2D, the conductivity as well as the conductance have the same physical dimension, i.e. the conductance of a square does not depend on its size.

The β function is always negative in this case and does not become zero except at $g_c \to \infty$. This implies that there is no mobility edge and hence no transition to a true metallic conduction. When $g = g_c$ (i.e. the value of conductance g for which $\beta = 0$) is of order unity there will be a cross over at a scale L_s from the slow decrease of eqn.(1.15) to exponential decrease. The localization length is of the order of L_c and is given by

$$L_c = l \exp\left(\frac{g_0 - g_c}{a}\right) \tag{1.14}$$

This is the perturbative estimate of the localization length in 2D. It depends exponentially on the mean free path and consequently localization effects are difficult to observe experimentally for weak disorder. Another striking consequence of the scale dependence of eqn.(1.15) is that a 2D system is non-Ohmic at all length scales. This leads to a characteristic 'non-metallic' resistance increase as temperature decreases. This would imply that even if for small squares the conductance per square is large, it decreases logarithmically as the side L of the square increases so that eventually g becomes small for some large values of L and thereafter the conductance decreases exponentially with L.

If the material parameters or properties are such that the conductance g_0 calculated from Drude's formula is large compared to unity, then for values of L

that are not too large, one can treat the disorder perturbatively. This will give

$$g = g_0 - a \ln(L/l) \tag{1.15}$$

where l is the mean free path, a is a numerical constant and $g_0 = e^2/2\pi\hbar(k_F l)$. This formula is valid so long as the second term is small as compared to the first.

For a film made up of a good material, the 2D localization effects will be tangible only if the film is very large, i.e. $L \approx l \exp(g_0/a)$. Thus, for a film made up of a good metal the 2D localization is indeed 'weak' in certain sense.

At finite temperatures one should replace L by the distance which electrons travel without suffering an inelastic collision. This distance increases with the lowering of temperature. This in turn leads to a logarithmically increasing conductivity which has also been observed experimentally. But the interpretation of this result is unambiguous because a similar behaviour would result from Altshuler et al.'s theory associated with electronic interaction.

For d=3: As is seen in the fig.(1.10), the beta function has a zero on the abscissa at a value g_3 of order unity. This zero is an unstable fixed point which represents the mobility edge. For $g > g_3$, the scaling procedure will monotonically enhance the conductance. For $g < g_3$, $\beta(g)$ is negative. Increasing the length scale from l decreases g so that one moves down on the scaling curve and at large enough length scales, $\beta(g)$ corresponds to the insulator regime.

Thus the conductance g_3 at the scale l corresponds to the critical disorder. The scaling trajectories move away from the critical point $\beta(g) = 0$ which in turn marks a change of regime and is hence identified with the mobility edge.

1.4 Conduction mechanisms in Anderson systems

Just as in crystalline materials, in an amorphous material also it is the position of the Fermi energy E_F relative to the energy bands that determines whether the material will exhibit metallic or insulating (or semiconducting) behaviour. The

difference will be that the band edges will be blurred and each band contains two types of electron states - localized and extended - separated sharply by mobility edges as proposed in Mott-CFO model [11, 14]. In such a situation electrons can participate in conduction at different temperature ranges in the following ways:(fig.(1.11))

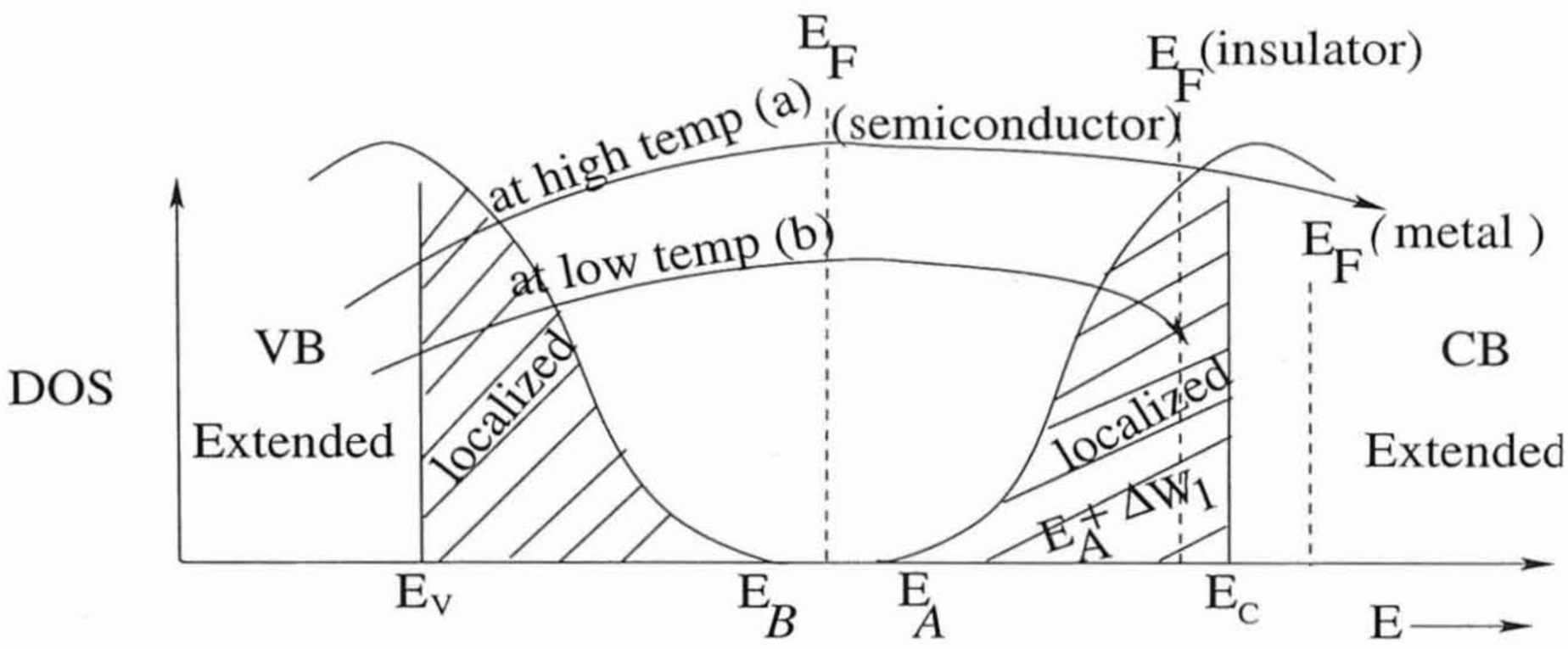


Figure 1.11: Conductivity mechanisms at different temperatures

1. At high temperatures for which thermal energy is sufficient to excite electrons to the extended states beyond E_c in the conduction band (CB), the ordinary conductivity due to electrons drifting in the electric field will occur. This will be of the form

$$\sigma = \sigma_0 \exp\left(-\frac{(E_c - E_F)}{k_B T}\right) \tag{1.16}$$

where σ_0, a function of mobility and the DOS, is the minimum metallic conductivity.

2. At lower temperatures excitations can occur only to the localized states between E_A and E_c. The electrons in these states can contribute to the conductivity only if they are able to acquire sufficient energy, ΔW_1, to hop from one localized site to the other. Thus the minimum activation energy

will be $(E_A + \Delta W_1)$ and the conductivity will be of the form

$$\sigma = \sigma_1 \exp\left(-\frac{(E_A + \Delta W_1 - E_F)}{k_B T}\right) \tag{1.17}$$

where σ_1 is almost 1000 times smaller than σ_0 and it depends on the fluctuations in the electron motion due to phonon interactions i.e. on the rate at which electron tries to jump. This is the thermally assisted hopping. This is illustrated in the figure below. The rate determining process is the

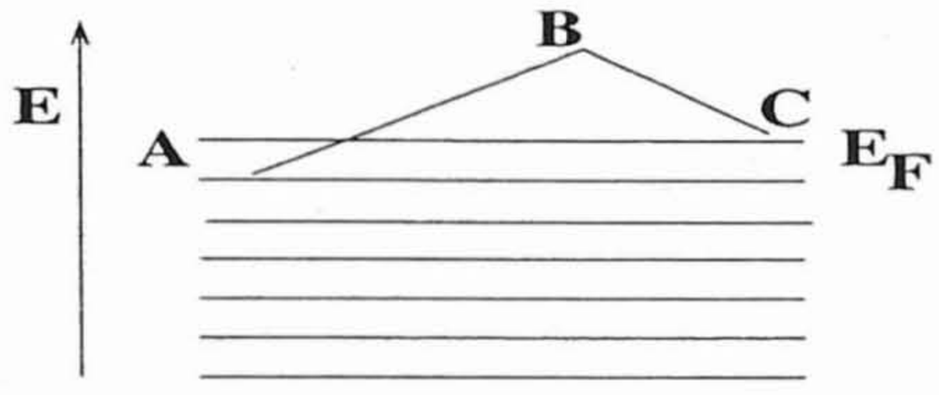


Figure 1.12: Thermally activated hopping

hopping of an electron from a state A below the Fermi energy to one above say B (fig.(1.12)). The probability per unit time that this occurs is the product of the following factors,

(a) Boltzmann factor, $\exp(-W/k_B T)$, where W is the energy difference of initial and final states;

(b) a factor ν_{ph} depending on the phonon spectrum; and

(c) a factor depending on the overlap of the wave functions.

If the localization is very strong, an electron will normally jump to the state nearest in space because the term $\exp(-2\alpha R)$ where α is the inverse localization length, falls off rapidly with distance. This nearest neighbour hopping is called Miller-Abraham hopping [4]. Nearest neighbour hopping is expected only when $\alpha R_0 >> 1$ where R_0 is the average distance to a nearest neighbour. The hopping energy W is of the order of the band width,

$W \sim \frac{1}{R_0^3 G(E_F)}$. Thus nearest neighbour hopping with an exponential factor $\exp\left(-\frac{W}{k_B T}\right)$ is observed only if states are Anderson localized throughout the whole band, so that any mobility edge is in a higher band.

3. At still lower temperatures two other hopping processes are possible. One of them happens if a band of localized states exists around E_F. For the case of amorphous semiconductors it is suggested that there is a high concentration of localized states near the center of the gap that anchors E_F in that region. In such cases just as in (b) thermally activated hopping to the neighbouring

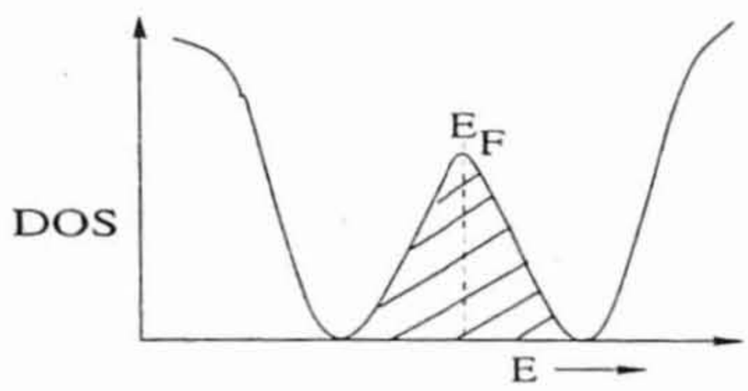


Figure 1.13: Amorphous semiconductors

sites can occur from states that are close to E_F. This will give a conductivity

$$\sigma = \sigma_2 \exp\left(-\frac{\Delta W_2}{k_B T}\right) \tag{1.18}$$

where ΔW_2 is the average energy difference between sites. This will be approximately half the energy spread of the band around E_F. σ_2 will depend on the electron jump frequency.

4. Another possibility arises if αR_0, [1] is comparable with or less than unity, or if the temperature is sufficiently low. Then the phenomenon of variable-range hopping happens. The hopping distance R increases with decreasing temperature. This is elaborated below.

[1] $\alpha = \sqrt{\frac{2mW_0}{\hbar^2}}$ where W_0 is the energy level for an electron in a single well.

At very low temperatures, where $k_BT << \Delta W_2$, the rate of thermally activated hopping to the neighbouring sites will be very small and it is more likely that an electron will be able to find a state of similar energy by tunneling beyond its nearest neighbours to more distant sites. Then there will be a greater selection of possible energies. This is called variable range hopping and it leads to a conductivity of the form exp $\left(-B/T^{1/4}\right)$. This mechanism which was first proposed by Mott can be derived from the following simple argument.

Since the electron states around E_F are localized, their wave function will fall off exponentially with distance R as exp $(-\alpha R)$, where α is a constant. Hence the probability of hopping to R will vary as exp $(-2\alpha R)$. To derive the hopping energy we note that the minimum energy between states around E_F can be derived from the DOS per unit volume, $G(E_F)$ as follows. If in a volume V there is only one state between E and $E + \Delta E$ then

$$dE = \frac{1}{VG(E_F)} \tag{1.19}$$

dE now measures the energy spread between one state and the next and this is only the energy separation between neighbouring sites. Hence the average separation between the neighbouring states, ΔW_3, with the electron being able to sample states within a radius R is

$$\Delta W_3 = \frac{1}{\frac{4}{3}\pi R^3 G(E_F)} \tag{1.20}$$

Thus the farther the electron is able to tunnel, the greater will be the likelihood that it will find a site with small ΔW_3. The probability for such a thermal excitation will be exp $(-\Delta W_3/k_BT)$ and this together with the probability of hopping to R gives the combined probability of the form

$$P = \exp\left(-2\alpha R - \frac{\Delta W_3}{k_BT}\right) \tag{1.21}$$

The maximum probability will occur when the magnitude of the exponent is a minimum i.e. when $\frac{dP}{dR} = 0$ This gives,

$$R \approx \left(\frac{1}{\pi G(E_F) k_B T \alpha} \right)^{1/4} \tag{1.22}$$

and

$$\sigma = \sigma_3 \exp\left(-\frac{\Delta W_3}{k_B T}\right) = \sigma_3 \exp\left(-\frac{B}{T^{1/4}}\right) \tag{1.23}$$

where

$$B = \frac{3\alpha^{3/4}}{4(\pi G(E_F) k_B T)^{1/4}} = 2.75 \left[\frac{\alpha^3}{\pi G(E_F) k_B} \right]^{1/4} \tag{1.24}$$

It is difficult to get good estimates for α and $G(E_F)$ but experiments yield value of B to be around 2. σ_3 is controlled by jump frequency. From eqn.(1.21) we can see that as T is reduced the average hopping length grows as $T^{1/4}$. But when the hopping conduction is governed by the temperature dependence of the form $\sigma = \sigma_3 \exp\ (E_3/k_B T)$ with a constant activation energy E_3, the average hopping length is of the order of the mean separation between the impurities, which does not vary with temperature. To emphasize this characteristic difference, the conduction mechanism leading to Mott's law is referred to as variable range hopping (VRH). In contrast to VRH, E_3 conduction is usually referred to as nearest neighbour hopping.

The index 1/4 is a matter of dispute. A theory due to Efros group [37] shows that when interaction between electrons are introduced into the problem, the index becomes 1/2. This is difficult to be determined experimentally and all the conditions under which 1/2 is to be expected are not entirely clear. The effect of correlation on hopping has been considered by various authors. Pollak [23] and Srinivasan [24] first pointed out that Coulomb repulsion between electrons in occupied centers could lead to ordering, similar to Wigner crystallization, with a reduction in the DOS at E_F or perhaps a gap.

Knotek and Pollak [35] show that the field in which the localized states exist is itself partly determined by the electrons, and a given electron can raise the energies of nearby states above the Fermi level. It thereby creates for itself a sort of electronic polaron, and the electron can only jump to a distant state of very nearly the same energy by taking a 'polaron' with it. This means that simultaneously with its jump, other electrons with energies near the final state must jump into new positions. This reduces the hopping probability.

According to Mott [38, 47] the claims made by Efros et al. [37, 46] that correlation introduces an energy gap, or a $1/T^{1/2}$ behaviour [38], or that deviations at low T as proposed by Kurosawa et al. [40], are not true.

In the 2D case the conductivity is found to have 1/3 power dependence on T,

$$\sigma = \sigma_0 \exp\left(\frac{B}{T^{1/3}}\right) \tag{1.25}$$

The expected value of B in 2D [41] is $B = \frac{3\alpha^2}{N(E_F)k_B}$.

1.5 Tunneling phenomena

Amorphous dielectric solids like glasses exhibit remarkable features at low temperatures which are very much different from their crystalline counterparts. Pohl and co-workers' [26] observation of the anomalous temperature dependence of specific heat and the thermal conductivity below 1K (in comparison with their crystalline counterparts [3]) has led to a lot of theoretical investigations into the acoustic and thermal properties of amorphous insulators. Of the several theories proposed to account for such behaviour [6, 29], the tunneling state model proposed by Anderson, Halperin and Varma (AHV) [29] and independently by Phillips [30] has been the most successful. The first hypothesis of the tunneling model is that in a glass, a certain number of atoms or group of atoms exist, which have two equillibrium positions. These correspond to the minima of an assymmetric double well potential. The tunneling motion of such atoms can be

described as an oscillation around either of the two potential minima and it give rise to two level systems (TLS). At low temperatures the localized oscillators are in their ground states denoted by $|1>$ and $|2>$. These states are not exact eigen states because of the tunneling through the potential barrier. Or in other words, glasses contain localized TLS's characterized by quantum mechanical tunneling. The microscopic origin of such localized states remains unresolved even now. But there is much to be learnt about them from a purely phenomenological point of view. The question, whether there exists a set of tunneling-model parameters and assumptions which are consistent with an increasingly restrictive body of experimental results is also important.

Tunneling states explain and link the observed specific heat and thermal conductivity. Their simplest example is found in alkali halides [21] and also in a partly amorphous material, polyethylene [22]. In a regular lattice of a crystal all atoms or molecules occupy a well defined position, allowing only one possible configuration. In contrast, the random network of an amorphous solid can be realized as a large number of different configurations and certain atoms or group of atoms can occupy at least two different positions or configurations of almost equal potential energy. The amorphous state differs fundamentally from the perfect crystal in that finite displacement of a few atoms does not necessarily increase the internal energy. This would suggest that the TS's corresponding to two neighbouring equillibrium positions could occur naturally in some amorphous solids. Thus on hindsight it can be said that TS should occur in materials with an open structure, and atoms with low co-ordination, possibly only two fold, should be able to move back and forth to give rise to two equivalent configurations. If all atoms are linked to more than two neighbours, then the structure will be very rigid and double well potentials will be unlikely to be formed.

In general, the well will not be symmetric and in particular, a stress applied

to the system will introduce an assymmetry and the potential of one well will be changed relative to the other by $p_0.E$ where p_0 is the dipole moment when the particle is definitely in one well. So an assymmetric well is considered when determining the response of the system to an applied field. In the symmetric case there will be an energy barrier V_0 between the two sites. In the stressed case an energy difference 2Δ is induced between the two sites. Classically, the defect can exist either in site $|1>$ or $|2>$ while quantum mechanically, the defect is considered in both wells simultaneously.

The mathematics needed to treat a quantum defect can be developed by considering a potential as shown in the fig.(1.14). The potential V is considered as the sum of the potentials V_1 and V_2.

The total Hamiltonian is given by

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V_1 + V_2 \tag{1.26}$$

The Hamiltonian for the first and the second well is given by

$$H_1 = -\frac{\hbar^2}{2m}\nabla^2 + V_1 = H - V_2$$
$$H_2 = -\frac{\hbar^2}{2m}\nabla^2 + V_2 = H - V_1$$

$$H = H_1 + V - V_1 = H_2 + V - V_2 \tag{1.27}$$

$$H_{ij} = \begin{pmatrix} <1|H_1|1> + <1|V - V_1|1> & <1|H|2> \\ <2|H|1> & <2|H_2|2> + <2|V - V_2|2> \end{pmatrix}$$

To a good approximation each term $<i|V - V_i|i>$ can be neglected in comparison with $E_i = <i|H_i|i>$. If the zero of energy is chosen as the mean of the two ground state energies E_1 and E_2, then the Hamiltonian matrix becomes

$$H_{ij} = \begin{pmatrix} \Delta & -\Delta_0 \\ -\Delta_0 & -\Delta \end{pmatrix} \tag{1.28}$$

Δ_0 is defined as negative because the matrix element $< 1|H|2 >$ is negative since the negative contribution from $V - V_2$, for e.g. in eqn.(1.27) overwhelms the positive contribution from H_2. Δ_0 can be evaluated for specific potentials. On diagonalizing this Hamiltonian the eigen functions are found to have energies $\pm\epsilon/2$ where $\epsilon^2 = ({\Delta_0}^2 + \Delta^2)$.

Thus in an isolated well the tunneling particle has a series of vibrational states separated by an energy $\hbar\omega$ which is of the order of Debye energy. The separation in energy of the two minima is often referred to as the 'asymmetry' Δ (fig.(1.14)). The two lowest eigen states have relative energies $\pm\epsilon = (\Delta_0^2 + \Delta^2)^{1/2}$ where Δ_0, the coupling energy is approximated by $\Delta_0 = \hbar\omega e^{-\lambda}$. Here ω is the frequency of oscillation in an individual well and $\lambda = d\,(2mV/\hbar^2)^{1/2}$ is the tunneling parameter. In the basis (ψ_L, ψ_R), the wave functions in the left and right wells respectively, the Hamiltonian of a single tunneling system is as in eqn.(1.28). Due to the tunneling, ψ_L and ψ_R are not true eigen states. So in the orthogonal basis with eigen states ψ_+ and ψ_- the Hamiltonian reads as

$$H_{ij} = \begin{pmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{pmatrix}$$

where $\epsilon = (\Delta^2 + \Delta_0^2)^{1/2}$. Thus in the basis (ψ_+, ψ_-) one gets a TLS with energy splitting ϵ. The parameters of the tunneling states (TS) do not have well defined values as a consequence of the random amorphous network. The distribution of coupling strengths is determined by the distribution of barrier heights and asymmetries for the double well potential shown in the fig.(1.14). The eigen states are coupled to the long wavelength phonons through the modulation of Δ_0 and Δ caused by an elastic wave. The resulting variation of E leads to relaxation effects. The modulation of Δ_0 and Δ by the elastic wave leads also to phonon induced transitions between the eigen states of the defect.

The low excitation energies generated by a mechanism which in turn results

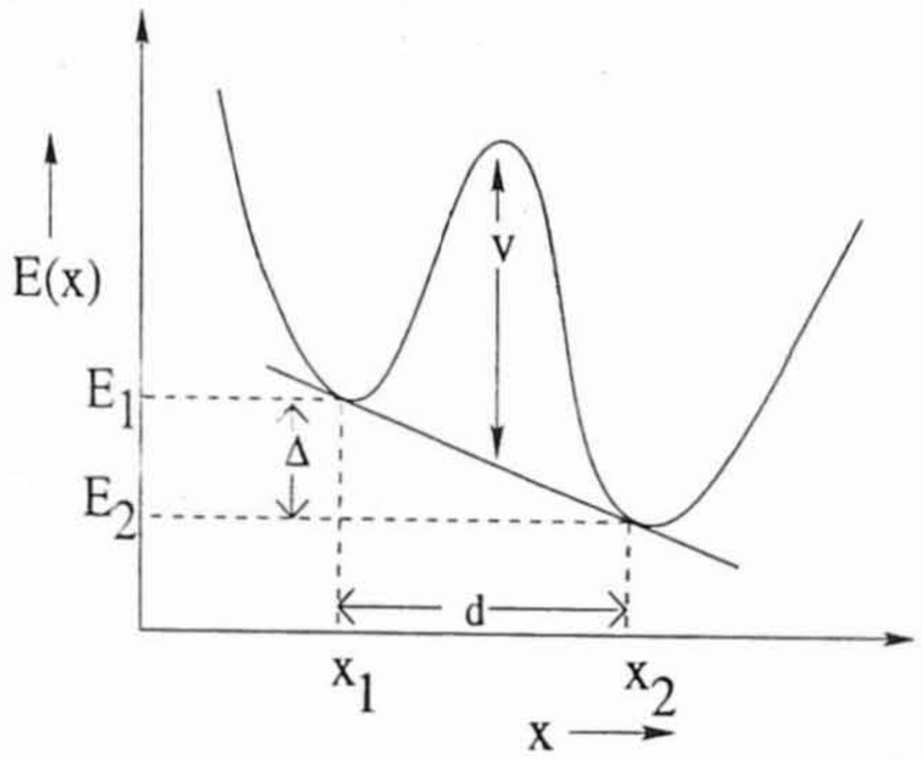


Figure 1.14: Two level system or tunneling states

in atomic tunneling is of the order of $10^{-5}eV < E < 10^{-4}eV$ corresponding to a temperature between 0.1K and 1K.

NH_3 molecule is an example of a system that illustrates the symmetrical double well potential . Two structures are possible for molecules of the type XY_3 namely the planar form and the tetrahedral form. In the tetrahedral form exemplified by NH_3, the three Y atoms form an equilateral triangle but the X atom can have two equivalent positions of equillibrium, one above and one below the plane of the triangle and the potential function for this atom is represented by two wells, centered at the equillibrium positions of the atom with a separating potential hill whose height is conditioned by the magnitude of the molecular binding forces. The two configurations possible for the N atom in the NH_3 molecule represents the two different states of the molecule which form the set of basis states for the analysis of the behaviour of the NH_3 molecule. Finally we note that two level systems can occur due to several reasons:

(a) the separation between energy levels may be so large that the thermal energy may not be sufficient to enable the tunneling entity to go from the ground to excited states. However, if the energy is just enough to cause transition to the first excited state alone, then we get a TLS.

(b) the excited states may be just too far away for an excitation to occur but the ground state may be two fold degenerate as in the case of NH_3 molecule.

(c) as a result of certain interactions like hyperfine interaction, crystal field, nuclear quadrupole interactions etc., the energy level of the atom may get split up into two levels resulting in TLS.

Although the terms TS and TLS are often used interchangeably, there is in fact a distinction between the two. TS is more general and assumes that there is a distribution of values of Δ_0 or equivalently V_0, the coupling energy, as well as E.

1.5.1 Quantum mechanical tunneling of molecular spins

The magnetization measurements by Friedman and his collaborators on crystalline Mn_{12} acetate at temperatures from 1.7K to 3K gave the first direct evidence [123] for the tunneling of a spin through a potential barrier from one orientation to another. The spins of Mn_{12}acetate molecules apparently reverse direction by 'resonant quantum tunneling' from one potential well to another. At low temperatures, the many constituent electronic spins of the molecule freeze into an overall state of fixed angular momentum $10\hbar$. Application of an external magnetic field along the crystal axis destroys the symmetry between the two wells. The quantum tunneling between the two levels on opposite sides of the potential barrier should be greatly enhanced when they have the same energy, or are degenerate. This is the resonant tunneling and it occurs when the applied field strength H is zero and the two wells are completely degenerate. But this resonant tunneling can also happen at a series of other H values also, i.e. whenever the applied magnetic field raises one well above the other just enough so that the energy levels once again coincide - but now for unequal values of $|m|$. For the case of Mn_{12}acetate this happens when H is positive or negative multiple of about 0.45T. When resonant tunneling occurs lots of spins escape quickly into

the positive m well thereby suddenly reducing the sample's negative magnetization. Thus as H is increased, the +m well sinks lower and lower and the levels come repeatedly into resonance, until finally all the spins rest at its bottom and the magnetization of the sample is finally saturated in the other direction. The observations of spin orientation tunneling in lockstep through potential barriers holds promise for future applications. The ultimate size limit for magnetic memories can be reached once it is possible to figure out as to how to store and how to read back information in these paired molecular potential wells. TLS also has some prospect in quantum computing. If, in the absence of an external field, the two wells are degenerate, a spin can in fact tunnel back and forth in a coherent superposition of states and this is exactly what one wants for quantum computing. More works are going on in this system [161].

1.5.2 Dynamical or chaos assisted tunneling

Heller [64] showed long back that discrete symmetries may have 'surprising' quantum effects. For instance, classical trajectories can be trapped in symmetric regular regions of phase space, separated by chaotic regions which behave as impenetrable barriers. Quantum mechanics, however, couples wave functions which describe equivalent motions on both sides of the 'chaotic barrier' [82]. This new type of quantum tunneling is dynamical in nature, and maybe much faster than the ordinary tunneling through a static potential barrier.

The phase-space trajectories on either sides of the chaotic barrier would be deterministic, i.e. given the initial state, the final state after, say a given time, will be predictable. In the normal circumstances when the barrier is non-chaotic, identical states on either side of the barrier can be connected by quantum mechanical tunneling. But for the chaotic barrier unusual thing happens. If the trajectory

on one side of the chaotic barrier touches the barrier it gets connected to an arbitrary state on the other side which cannot be predicted a priori. The reason is that the trajectory evolves non-deterministically in the chaotic case. Thus chaos assisted or dynamical tunneling apparently allows transitions between states of very different energies. We believe that regions of randomness which also have self-similar or fractal character could give rise to dynamical tunneling.

Works of Reichl and Zheng [96] on the 1D quartic double well potential in the presence of a monochromatic external field revealed the appearance of chaotic trajectories with initial energy lower than the barrier height and which are able to increase their energy and cross over the barrier. The phase space chaotic layers increase with the strength of the field and, for external frequencies close to the harmonic frequency within each well, the spreading of chaotic layers is maximum at a given field strength. This barrier crossing due to energy diffusion is a pure classical effect related to chaos and, therefore should not be called tunneling.

Thus the study of quantum tunneling for double well potentials in the presence of a periodic time-dependent driving force became a focus of major theoretical work [96, 114]. Macroscopic quantum tunneling [91], the possibility of tunneling rate enhancement through double quantum wells in semiconductor superlattices [109], intermolecular and intramolecular hydrogen transfer processes [107], tunneling processes of hydrogen isotopes and muon between interstitial sites in metals [103] and Josephson junction in the presence of a microscopic field [112] are some of the applications stimulating these studies [116].

1.5.3 Fluctuation induced tunneling

There is a great deal of evidence [1] that in ultrathin films a few tens of angstroms thick prepared by evaporation onto a substrate kept at not too low a temperature consist of arrays of small islands separated from each other by

a distance of the order of $100A^0$. For electrical conduction to occur electrons have to be transferred from one island to the next across the gap and it is the mechanism of this transfer that determines the resistance of the film.

There are several mechanisms by which the conduction is possible, for e.g. thermionic emission and tunneling. Though thermionic emission, where the current depends exponentially on the height of the potential barrier between islands, is frequently mentioned as a possible conduction mechanism it is found that the tunneling current depends much more sensitively on the separation between the grains than the thermionic current.

In the temperature range where the electrostatic energy required to transfer an electron from one neutral grain to another is appreciably larger than k_BT, the density of thermally excited grains are negligible leading to unusual transport effects in these granular materials. In such cases the conduction is induced by the application of a large electric field. Thus in the limit of low temperature and high electric field, the major contribution to the conductivity is due to field induced tunneling between the neutral metal grains separated by one or more barriers [25]. The low field electrical conductivity of many disordered materials has temperature dependence of the form, $\sigma \sim \exp(-b/T^{\gamma})$ where $\gamma = 1/4$ in many amorphous semiconductors and semiconducting glasses and $\gamma = 1/2$ in disordered materials such as granular metals and some disordered semiconductors. Although $\gamma = 1/4$ behaviour has been justified in terms of Mott's variable range hopping and derived by Ambegaokar [15] there is no definite theory for the $\gamma = 1/2$ behaviour. Ping Sheng et al. [33] proposed a theory which explains the $\gamma = 1/2$ behaviour by a structural effect. They relate the high and low field behaviours through a single structural parameter.

Ping Sheng et al. [55] have also proposed a tunneling conduction mechanism for disordered materials in which there is a modulation of tunneling barriers by

thermal fluctuations with the resulting fluctuating local electric field causing the conduction. Since the granular material which mimic a network of tunnel junctions is situated in a thermal bath there will inevitably be thermal fluctuations that will lead to a range of voltage differences across the junctions.

Later [90] they showed that the whole range of the observed γ values in granular systems can be understood in terms of a general theoretical model that gives $\gamma = 1/4$ for $T \to 0$ and $\gamma > 1/2$ (but < 1) for $T \to \infty$.

1.6 Mesoscopic systems

Mesoscopic systems fall in between microscopic and macroscopic systems in terms of the length scale. A system exhibits mesoscopic behaviour if the system dimension is of the order of either of the three characteristic length scales namely, the de Broglie wavelength, inelastic mean free path or phase relaxation length. Since these length scales are strongly dependent on the material as well as T and magnetic field, mesoscopic transport phenomena have been observed in conductors having a wide range of dimensions from a few nanometers to micrometers. These systems have two important features: firstly, the spectrum of electronic states are discrete and secondly the electronic motion is coherent in the sense that an electron propagates across the whole sample without experiencing inelastic scattering. Its wave function maintains a definite phase or the phase changes deterministically. The electron thus exhibits a variety of novel and interesting interference phenomena. In our work we have mainly dealt with the second case, namely the phenomenon of long range phase-coherence.

Interest to study mesoscopic systems arises since there are many new phenomena that are intrinsic to mesoscopic systems. It is almost like a large molecule, but always coupled, at least weakly, to a much larger essentially infinite system via phonons, many body excitations, etc. Fundamental principles of quantum

mechanics related to the concept of phase of the wave function and statistical physics are amenable to theoretical clarification and experimental examination in these systems. With the advancement of technology, many of the theoretical predictions can now be confronted by experiments. A great majority of mesoscopic conductors are patterned out of a two dimensional electron gas (2DEG) formed at a GaAs-AlGaAS interface.

Many of the rules valid in the macroscopic physics are not valid in the mesoscopic regime. For example, the rules for the addition of resistances, both in series [20, 77] and parallel [95], are different in mesoscopic regime.

Majority of the interesting effects in mesoscopic systems are due to quantum interference effects. These effects are known to be affected by the coupling of the interfering particle to its environment, namely heat bath. The way such a coupling modifies the interference phenomenon has been studied both theoretically [7, 89] and experimentally. The effect of coupling to the environment is characterized by a phase breaking time, τ_ϕ, which is the characteristic time for the interfering particle to stay phase coherent.

We have looked into the problem of the saturation of the phase breaking time or the decoherence time, with the lowering of temperature currently being debated in literature [102, 105, 124]. Theoretically it has been believed so far that $\tau_\phi(T)$ should increase with decrease in inelastic events and should become infinite at $T = 0$ in very large systems. Recent experiments have however found that the phase of the electron wave function does not remain coherent over indefinitely large distances as the temperature is lowered. It saturates at a certain value.

Chapter 2

RESISTANCE OF QUASI-ONE DIMENSIONAL WIRES

2.1 Introduction

In this chapter we study the electronic properties of quasi-one dimensional disordered systems. Borland [8] and Halperin [12] initiated work in this area. Mott and Twose [28] first formulated an approach for the development of localization in 1D systems of large but finite length. A survey of both theoretical and numerical work in this area is given by Ishii [34]. Most of the discussion of this problem considers the solution of the problem with one-point boundary conditions, i.e. they start with a given wave function and derivative (on the amplitude at two neighbouring points in the TB case), and show that the solution grows exponentially with probability unity. It is then argued that an eigen state for a long but finite system occurs at just those energies where an exponentially growing wave function from the left matches an exponentially growing wave function from the right. Wegner [42] had demonstrated the localization without using this approach.

2.1.1 Dimensionality

Dimensionality of a system refers to the number of degrees of freedom in the electron momentum in that system. In other words, the dimensionality of the system is effectively the number of dimensions for which the system size is larger than the inelastic length, which is the distance up to which the electron can travel so that both the initial momentum as well as the energy are destroyed. For example, a wire of cylindrical cross-section (of radius a) is one-dimensional

(1D) if $l_{in} < a$.

Reduction in dimensionality can be achieved by applying a confining potential to a system of electrons. If the confining potential is applied only in one direction, then the electron can move in two other directions, and in this case we will have a quantum well. In a quantum wire there is confining potential in two directions as a result of which electrons can move only along a single direction. If there is a potential confinement in all the three directions then the degrees of freedom for the electron reduce to zero and we have what is called quantum dot. If the number of degrees of freedom (DOF) is labelled as D_f and the number of directions of confinement potential as D_c, then $D_f + D_c = 3$ for all solid state systems. Table 2.1 shows the four possibilities. Traditionally, low dimensional

System	D_c	D_f
Bulk	0	3
Quantum Well	1	2
Quantum Wire	2	1
Quantum Dot	3	0

Table 2.1: System vs dimensionality

systems are labelled by the remaining DOF in the electron motion i.e D_f rather than the number of directions of the confinement potential, D_c.

Since the inelastic length, l_{in} is a function of temperature, one can cross over from 3D to an effectively 1D behaviour in a given wire on cooling. Besides electron-phonon interaction, l_{in} also depends on the scattering of electrons from other electrons and two level systems (TLS or TS). The temperature dependence of the inelastic scattering rate due to e-phonon collisions depends on the phonon dimensionality which is the number of dimensions of the system in which the thermal phonon wavelength λ_{Th} is greater than the diameter of the wire and also on whether $\lambda_{Th} > l_e$ (dirty limit), where l_e is the elastic mean free path [49]. For

example in a wire of diameter a such that $\lambda_{Th} >> a$ and $\lambda_{Th} >> l$, $\tau_i^{ph} \propto T^{-2}$.

Low dimensional electron systems can be fabricated in several different ways. The techniques have been perfected enormously. A detailed discussion of the experimental methods can be found in [143].

Qualitatively, the idea of localization in a random 1D potential can be understood from the arguments of Yuval based on the nature of random walk and uncertainity principle [43]. A wavepacket which diffuses a distance L has an energy spread $\Delta E \propto 1/L^2$ while the energy level spacing varies as $dE/dN \propto 1/L^d$ where d is the dimensionality. For $d = 1$, as L increases, the number of energy levels in the packet decreases. Correspondingly when there is only one eigen state left in the finite packet, localization sets in, i.e.

$$\Delta E \propto \frac{1}{L^2} \qquad \text{while} \quad dE/dN \propto \frac{1}{L}$$

Thus, $\Delta E < dE/dN \Rightarrow$ all states are localized in 1D. Therefore for the 1D case as the packet diffuses a length L, the spread in energy of the wave packet becomes less than the spacing between the energy levels that are contained in the packet. For the 2D case,

$$\Delta E \propto \frac{1}{L^2}, \qquad \frac{dE}{dN} \propto \frac{1}{L^2}$$
$$\text{i.e.} \quad \Delta E = dE/dN$$

i.e. for the 2D case, both the spread ΔE in energy of the wavepacket and the energy level spacing dE/dN decrease as $1/L^2$ and hence no conclusions regarding localization can strictly be drawn. In this sense 2D is truly the marginal case.

2.1.2 Schrödinger's equation in quantum wires

Here we work out the Schrödinger equation under the conditions that give rise to a quasi-1D wire. The equation for a 3D system with potential V is

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(x,y,z) + V(x,y,z) = E\psi(x,y,z) \tag{2.1}$$

Since there is a potential confinement in two directions, say y and z, we can split the potential V and the wave function ψ as,

$$V(x,y,z) = V(x) + V(y,z); \quad \psi(x,y,z) = \psi(x)\psi(y,z).$$

Splitting the total energy E also similarly and further simplifications give

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}\psi(x) = E_x\psi(x) \tag{2.2}$$

$$-\frac{\hbar^2}{2m^*}\Big[\frac{\partial^2}{\partial y^2}\psi(y,z) + \frac{\partial^2}{\partial z^2}\psi(y,z)\Big] + V(y,z)\psi(y,z) = E_{y,z}\psi(y,z) \tag{2.3}$$

The solution of eqn.(2.2) is a plane wave, $\exp(ik_x x)$, which gives the standard dispersion relationship, $E_x = \hbar^2 k_x^2/2m^*$. The eqn.(2.3) is merely the Schrödinger equation for the 2D confinement potential characterizing a quantum wire. For a general cross-section, eqn.(2.3) should really be solved by using a full 2D solution, which is very tedious. So special cases of the solution of eqn.(2.3) for relevant commonly found geometries are taken. Such particular solutions rely upon the ability to further decouple the motion into independent components. For infinitely deep rectangular wires for instance,

$$\psi(y) = \sqrt{\frac{2}{L_y}}\sin\Big(\frac{\pi n_y y}{L_y}\Big); \quad \psi(z) = \sqrt{\frac{2}{L_z}}\sin\Big(\frac{\pi n_z z}{L_z}\Big) \tag{2.4}$$

$$E_y = \frac{\pi^2\hbar^2 {n_y}^2}{2m^* {L_y}^2} \qquad E_z = \frac{\pi^2\hbar^2 {n_z}^2}{2m^* {L_z}^2}$$

$$E_{y,z} = E_y + E_z = \frac{\pi^2\hbar^2}{2m^*}\Big(\frac{{n_y}^2}{{L_y}^2} + \frac{{n_z}^2}{{L_z}^2}\Big)$$

This is similar to 1D infinitely deep quantum well. The confined states of a quantum wire are therefore described by two quantum numbers, (n_y, n_z) in contrast to the sole number required for the 1D confinement potential in quantum wells.

For a circular cross-section, the Schrödinger equation for the motion in the

confined cross-sectional plane of a quantum wire taking into account the cylindrical symmetry has to be solved and is done numerically using for example shooting method [143].

2.1.3 Density of states

The density of states (DOS) changes as we go from 3D crystal to a quantum well (2D) and again to quantum wires (1D) and also to quantum dots (0D). DOS is defined as the number of states per unit volume per unit energy interval in real space and is denoted by

$$\rho(E) = \frac{dN}{dE} \tag{2.5}$$

In the bulk crystal, the three degrees of freedom (3DOF) for the electron momentum map out a sphere in k space, while in quantum well the electron momenta fill successively larger circles. For a quantum wire with just 1DOF, the electron momenta fill states along a line as is shown in the figure below. The total number

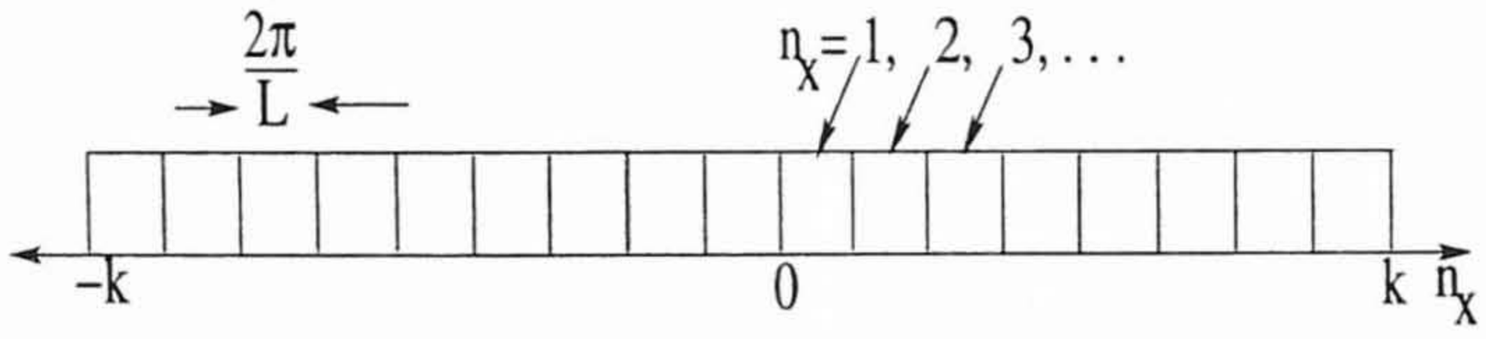


Figure 2.1: Occupation of states in k-space along a 1D quantum wire

of states N is then equal to $2k/\pi$ and the DOS is given by

$$\rho^{1D}(E) = \frac{dN^{1D}}{dE} = \left(\frac{2m^*}{\hbar^2}\right)^{1/2} \frac{1}{\pi E^{1/2}} \tag{2.6}$$

for $E = \hbar^2 k^2/2m^*$. The energy E is measured upwards from a subband minimum. Table 2.2 gives the DOS for bulk, well, wire. We note here that a reduction in DOF for the electron motion leads to a reduction in the functional form of $\rho(E)$ by factors of $E^{1/2}$.

Dimensionality	$\rho(E)$
3D (Bulk)	$\frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}E^{1/2}$
2D (Well)	$\frac{1}{2\pi}\left(\frac{2m^*}{\hbar^2}\right)^{1}E^{0}$
1D (wire)	$\frac{1}{\pi}\left(\frac{2m^*}{\hbar^2}\right)^{1/2}E^{-1/2}$

Table 2.2: Dimensionality vs density of states

If there are many confined states within the quantum wire with subband minima E_i, then the DOS at any particular energy is the sum over all the subbands below that point, which can be written as

$$\rho^{1D}(E) = \sum_{i=1}^{n}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{1}{2}}\frac{1}{\pi(E-E_i)^{\frac{1}{2}}}\theta(E-E_i) \tag{2.7}$$

The quantum wires show maxima in the DOS at around the subband minima,

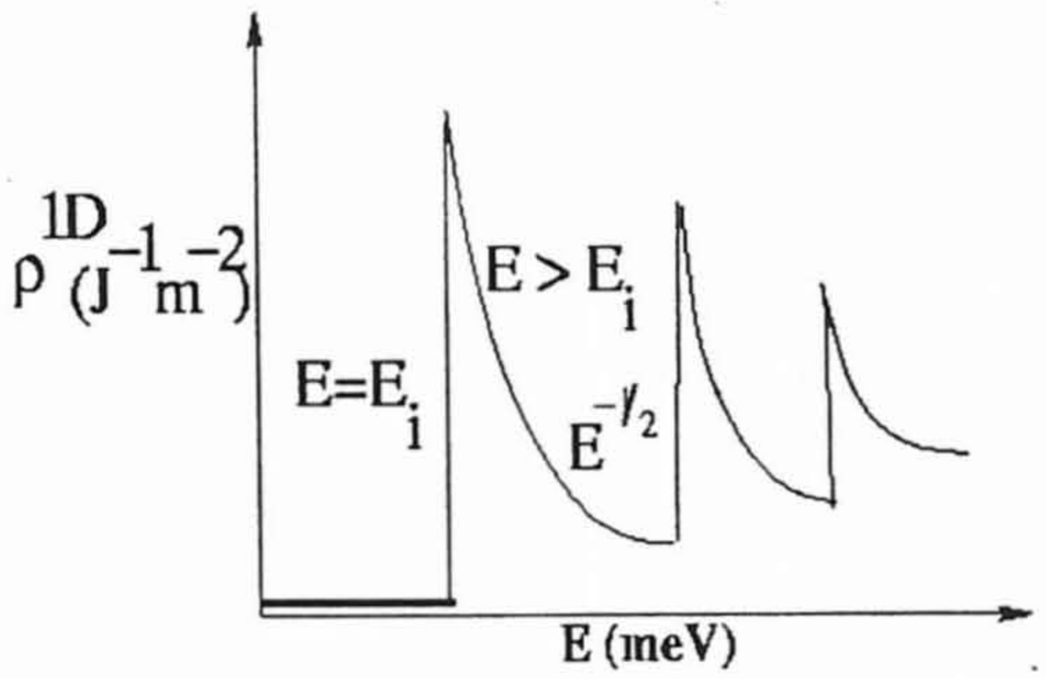


Figure 2.2: Density of states versus energy

i.e. at around the point at which charge would be expected to accumulate. This is in contrast with bulk and 2D cases.

2.2 Thouless' approach

A one dimensional system in the strict sense is a linear chain of atoms where the electrons are bound to move only forward and backward along a particular

direction. In the presence of an obstacle on its path a part of the wave function will be reflected and a part will be transmitted. In a disordered chain this process continues at every obstacle and the transmitted part of the wave function steadily decreases. As a result the conductivity decreases successively and eventually the wave function decays to zero and it is said to be localized. Though it was simple to visualize localization in 1D its experimental verification was not readily possible because of the difficulty in making a 1D wire. At this point Thouless [49, 75] argued that all systems, regardless of their cross-sectional area will behave one dimensionally in so far as localization is concerned, provided that they are sufficiently long or in other words the ratio of length to the cross sectional area should be very large. In practise only quasi-one dimensional (1D) wires could be made, which were actually 3D systems of very small cross-section. Thouless studied the effect of localization in these wires and concluded that they would behave one dimensionally in terms of localization if the diameter is less than the inelastic scattering length and also if the length is greater than the localization length, which is the length of the wire for which resistance is greater than $2\hbar/e^2$. This concept is also known by the term, the maximum metallic resistance. In such a 1D system, the resistance depends exponentially on the length rather than linearly i.e. $(\exp(L/l-1))$ as the temperature is lowered below 10K. For a very disordered wire with $A = 2.5 \times 10^{-11} cm^2$, $(r \sim 250A^o)$. T_L is predicted to be of the order of 1K. By using Fokker - Planck approach Thouless calculated the increase in resistance to the original resistance R_0 and obtained an expression

$$\frac{\Delta R}{R_0} = \frac{\rho_e \sqrt{D\tau_{in}}}{A(\pi\hbar/e^2)} \tag{2.8}$$

where ρ_e is the impurity resistivity, τ_{in}, the inelastic scattering time and $(\pi\hbar/e^2)$ equal to $36k\Omega$, the quantum unit of resistance. He further argued that the effect of localization will only be observed at very low temperature and with very thin wires for the following reason.

Consider the motion of an electron in terms of the motion of wavepackets made up of big localized states. The electron starts as a sharp wavepacket and diffuses, but eventually, the diffusion is limited by the extent of localized states that make up the packet. After a time t, an inelastic scattering process would scatter the electron to a new wavepacket.

At 'high' temperatures an electron will experience frequent inelastic collisions. Each of these collisions will cause the electron to jump from one localized state to another [49, 75]. If the inelastic scattering rate is high, the electron will change states many times before it can diffuse a distance of the order of localization length. As a result the electron will never 'know' that it was in a localized state and the localization will have no effect on the conductance. The effect of localization will only be felt when the mean free path for inelastic scattering, l_{in}, is comparable to the localization length l. This can happen either by reducing the cross-sectional area of the wire and/or increasing the amount of randomness which will decrease l or by reducing the temperature which will increase l_{in}. No matter how large the cross-section is, there will always be a temperature T_L at which l_{in} is equal to l, and this will approximately be the temperature at which localization becomes observable. In addition, the argument that T_L should scale inversely with the diameter of the wire makes this effect not ordinarily observed.

As the temperature is lowered the scattering by phonons become less effective and eventually the electrons will be able to diffuse a distance of the order of localization length between inelastic events. Movement beyond this length is not possible and hence the electron will remain there until another inelastic scattering event will cause a transition to a new packet of states. The size of the localized state is given by

$$l = \left(\frac{2\hbar}{e^2}\right) A\sigma = \frac{2Ak_F^2\lambda_F}{3\pi^2}$$

where λ_F and k_F are the mean free path and the wave number of an electron at

the Fermi surface. The time taken to diffuse this distance is

$$t = \frac{l^2}{D} = \left(\frac{2k_F^4 A^2}{3/\pi^4}\right)\tau$$

where $\tau_{ph} = 2\lambda_F^2/3D$ is the relaxation time and t is the time between two inelastic events represented as τ_{ph}. Therefore the condition for the localization of eigen states to be apparent is approximately

$$\tau_{ph} > \left(\frac{2k_F^4 A^2}{3/\pi^4}\right)\tau \tag{2.9}$$

The ratio of τ to τ_{ph} at room temperature is $(\Gamma - 1)$ where Γ is the resistance ratio which is defined as the ratio of the resistivity at room temperature to the residual resistivity and is an approximate indicator for the sample purity. Originally Thouless had considered e-phonon or e-e scattering for the inelastic process. But then, the dependence of τ_{in} on T was found to be different from that observed experimentally in all samples. Moreover, the lesser experimental value got for $\frac{\Delta R}{R_0}$ implies that τ_{in} is smaller than that considered by Thouless. At this point Lee suggested that τ_{in} must be due to the TLS or TS and later on Black et al. [58] showed that the TS will be dominant under these conditions. Thus it was not certain as to what would be the mechanism responsible for τ_{in}. Thouless' theory based on the localization of electrons is found to give a correct dependence of $\frac{\Delta R}{R_0}$ on T if the inelastic scattering is taken to be due to TS. Thus, even if the temperature is low it does not mean that the effect of localization will be large because τ_{in} would be large. The presence of TLS in the disordered material will also affect τ_{in} and will reduce it and hence the effect of localization can be smaller.

2.2.1 Temperature dependence of e-phonon and e-e interactions

If the localized electron wave packet after diffusing a distance of the order of localization length gets scattered by a phonon, then $\tau_{in} \propto T^{-p}$ where the exponent p depends on whether the material is clean or dirty and whether the

phonons are 1D or 3D [49]

p = 1 for 1D phonons in a clean material

p = 2 for 1D phonons in a dirty material

p = 3 for 3D phonons in a clean material

p = 4 for 3D phonons in a dirty material

If $e - e$ scattering is considered, the relaxation rate is of the form

$$\frac{1}{\tau_{ee}} = \frac{2m\beta(k_B T)^2}{\hbar^3 k_F^2}$$

where β is a numerical constant which is not far from unity.

Schmidt [36], Altshuler et al. [76] as well as Abrahams et al. [80, 80] suggest the e-e scattering rate for the disordered case to be $\tau_{ee} \propto T^{-d/2}$ where d is the dimensionality, rather than T^{-2} which is the case for a pure metal.

$$\begin{aligned} \tau_{ee} &= T^{-2} \text{ for pure metals} \\ &\propto T^{-d/2} \text{ for disordered metals at low temperature.} \end{aligned}$$

For $d = 2$ a logarithmic singularity occurs which leads to $(T \ln T)^{-1}$ behaviour of the life time and a failure of the quasi-particle picture near the Fermi surface.

2.2.2 Experimental status

The first observation of localization effects in 1D wires were made by Dolan & Osheroff [61] in a relatively wide (typically 1μm) very thin ($50A^0$) strips of AuPd alloys made using optical lithography. Later, Garland et al. [62] studied percolative mixtures of Ag particles in KCl. However, measurements at temperatures as low as 0.5 mK showed no evidence for localization and indicated that the effect of localization could be lesser than that predicted by theory. But note that the percolative mixtures are somewhat different from the continuous metallic structures which were considered in the theory. Hence the conditions necessary to observe localization may have not been met in these systems.

Giordano and his co-workers at the same time [63] studied continuous AuPd wires made using a lithographic technique with diameter of the order of 300 A^0. Localization effects were observed in these samples and the increase in R with the lowering of T was found to vary as $1/A$ in good quantitative agreement with theory. The temperature dependent part was found to vary as $T^{1/2}$.

Later in 1980, Chaudhari et al. [69] studied very thin (50 A^0 strips with widths of order 1000 A^0) wires of amorphous WRe made using electron beam lithography. These wires showed localization effects and the resistance rise was found to depend on A & T in good agreement with [63]. Chaudhari et al. made use of the superconductivity of their sample by using the phase slip centers observable below T_c to measure τ_{in}. There was a good agreement with the value obtained in conjunction with the measured value of $\Delta R/R_0$. This was the first direct evidence that the inelastic scattering time are of correct magnitude to explain within the localization picture, the behaviour of R which has been observed.

Overcash et al. [71] worked on freely suspended wires rather than depositing them on substrates or embedding in a matrix. They studied the behaviour of whiskers of Bi and Bi doped with Sb with diameters as small as 1400 A^0, but could not find any evidence of localization in their estimates of τ_i in a manner predicted by Thouless.

So it is concluded that Thouless' estimates are not consistent with the experiments on WRe and AuPd wires. Other experimental results also showed a resistance rise consistent with that found for AuPd and WRe wires.

2.3 Interaction effects

Early studies on the interacting electron gas using perturbation theory in the unscreened Coulomb interaction led to a strong singularity near the Fermi surface. But works of Nozières and Pines [10] removed all the singularities by taking

into account the screening factor. These results when fitted into the general framework of Landau's Fermi liquid theory (FLT) showed that the effects of interaction could be represented by the introduction of a number of Fermi liquid parameters describing the renormalization of physical quantities like specific heat and magnetic susceptibility.

It was generally believed that impurity scattering would not lead to any essential modification of the FLT. But Altshuler et al.'s work [65, 66] showed that interactions in a disordered Fermi liquid do lead to strong singularities near the Fermi level. They treated the disordered Fermi liquid problem by performing a perturbation theory to the lowest order in interaction strength. The disorder is treated by the conventional diagrammatic technique [9], which should be valid in the limit $k_F l >> 1$. For the 1D case the ratio of $\Delta R/R_0$ was found to be

$$\frac{\Delta R}{R_0} = \frac{2-F}{L_L}\left(\frac{4D\hbar}{k_B T}\right)^{1/2} \tag{2.10}$$

where F is the screening parameter and $L_L = R_T A/2\rho_e$ is the size of the localized state. Here the criterion for 1D behaviour is that the diameter of the wire must be less than the coherence length. The dependence of $\Delta R/R_0$ on A, T, and ρ_e is the same as in the localization theory.

2.3.1 Experimental results supporting interaction theory

White et al. [86] have reported the experimental results on ultrathin wires of Cu, Ni and AuPd alloys and also the results of a careful reanalysis of the data in the published literature. In all cases, the quantitative prediction of the interaction model of Altshuler et al. [76] consistently accounts for much of the observed resistance rise and in the case of Cu, it accounts for essentially all of it. So White et al. infer that interaction effects are at least of comparable importance with localization and may dominate over the latter in the metallic samples.

Skocpol et al. [85] fabricated a new MOSFET analogue of narrow metal wires

and demonstrated the simultaneous presence of both localization and interaction effects in good agreement with quasi-1D theory using parameters estimated from 2D results. The main problem concerning localization theory was in τ_{in}, which is a relatively unknown parameter in the case of narrow wires. In contrast, in the case of Si inversion layer in which the conductivity and the diffusion constant of the electron can be easily varied by changing the gate voltage on a single device, much more is known about the relevant length and scales. Thus, in case of narrow Si inversion layers both weak localization and interaction effects are seen.

2.4 Unclear issues

Since the work of Thouless [49, 75] there has been a lot of work on the problem of localization, both in 1D as well as in thin wires using various theoretical approaches. All of these theories basically make the same prediction for the behaviour of R as a function of T. Thouless' result for the ratio of the increase in R to the metallic resistance R_0 is given in eqn.(2.8). From this equation it is seen that the effect of localization is proportional to A^{-1}, ${\tau_{in}}^{1/2}$ and $\rho_e^{1/2}$. It is also evident that all of the temperature dependence comes from that of τ_{in} and hence τ_{in} is the key quantity.

Since there are a number of different scattering mechanisms which could conceivably be important, it is impossible to make an a priori estimate of τ_{in} . The most obvious mechanisms are electron-electron and electron-phonon scattering. But the experimental results are not consistent with either of these scattering mechanisms. This has led to the suggestion that some other scattering mechanism is dominant in these systems [75, 88]. One possibility is that the scattering of electrons from the tunneling levels which is believed to be present in all highly disordered systems [29, 58].

The electron-electron interaction effects also lead to a behaviour similar to

that predicted by theories based on localization. In this case τ_{in} is replaced by $\hbar/k_BT$ [74]. The predictions of the two theories are so similar that it is difficult for experiments to distinguish between them.

The temperature dependent part of resistance is found to vary as $T^{-1/2}$ [68]. This would imply that the inelastic scattering time should vary as T^{-1} and is independent of the cross-sectional area of the wire.

The only scattering mechanism that behaves in this way is the e-tunneling level scattering [49, 58, 75]. Black et al. [58] have used the experimental data for the metallic glass PdSiCu to estimate $\tau_{in} = 2.3 \times 10^{-9}T^{-1}(secK^{-1})$ in this system. Substituting this value of τ_{in} in the above equation, the value of $\Delta R/R_0$ is found to be a factor of seven larger than that observed experimentally. This level of disagreement is reasonable taking into account the fact that this τ_{in} was calculated for a different material than was used for the wires and also the general difficulties encountered in making absolute estimate of the scattering times [73].

So far we have considered the dependence of the resistance rise on the cross-sectional area of the wire as well as on temperature. $\frac{\Delta R}{R_0}$ is found to have a dependence on ρ_e, the impurity resistivity as well. This dependence has been investigated in two ways. First, by depositing the AuPd in two different ways, namely sputtering and thermal evaporation, it was possible to make wires with two different values of ρ_e for the same composition [63, 68]. Secondly, it was possible to anneal the sputtered wires studied previously by gently heating the wire. It is expected that this annealing, which was carried out at temperatures less than 200^0C, well below the melting point of $AuPd$, did not change the cross-sectional areas of the samples. The advantage of annealing was that it allowed ρ_e to vary continuously over a reasonably wide range. It has been observed that as ρ_e is decreased the fractional resistance rise $\frac{\Delta R}{R_0}$ also decreases in qualitative agreement with the equation for $\frac{\Delta R}{R_0}$. The fig.(2.3) shows the results for the

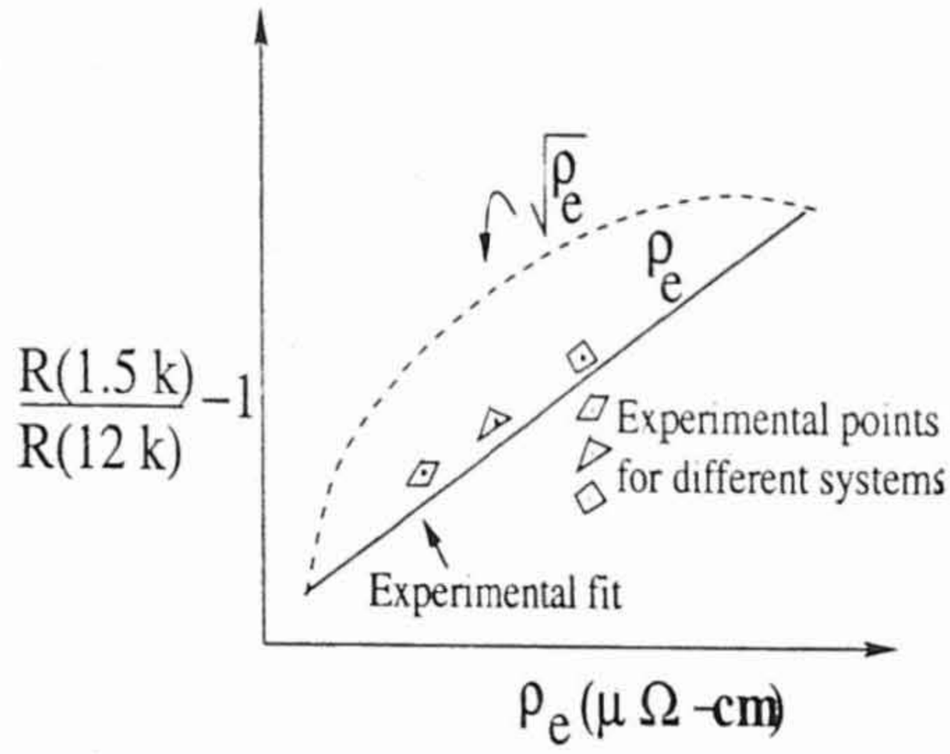


Figure 2.3: Fractional resistance rise vs temperature

resistance rise as a function of ρ_e. $\frac{\Delta R}{R_0}$ is found to vary approximately linearly with ρ_e in contrast with the $\sqrt{\rho_e}$ variation predicted by the theory in dotted line. Thus there is a problem in understanding the variation of $\frac{\Delta R}{R_0}$ with ρ_e. This variation is not consistent with the theories based on e-e interaction effects and those based on localization unless the inelastic scattering time exhibits an unexpected and so far unexplained dependence on ρ_e.

In sum, experimental results showed a lesser effect of localization than was expected by theory. This is deduced from the fact that the inelastic scattering time was shorter and increases less rapidly at low temperatures than that calculated by Thouless [49]. It was also not clear as to what would be the appropriate mechanism for the inelastic scattering.

2.5 Our approach

We have taken up the issue of the ρ_e dependence of $\Delta R/R_0$ within the frame work of the localization theory. We will emphasize on the role of inelastic scattering of electrons from the TLSs in determining the resistance of a thin wire. The element of disorder, which is due to the random distribution of site energies is introduced by treating the inelastic events probabilistically. So, disorder will

not appear in our formulation as an exclusive parameter but will be embedded in the frequency or probability of inelastic scattering from the TSs. It is assumed as discussed earlier that the system has topological disorder that gives rise to TSs which are distributed randomnly in the system.

We consider the movement of an electron as an elastically diffusing wavepacket made up of broad localized states. This narrow wavepacket diffuses along the length of the wire until an inelastic event like a phonon or a TS scatters it into another localized state. It then starts to diffuse again up to localization length and then waits until it encounters another inelastic event. A wavepacket, which comprises group of waves of slightly different wavelengths, strongly localized in a very small region of space is taken to mimic a particle to describe its motion. The energy of an elastically diffusing narrow wavepacket, would not change in the course of diffusion until it meets a phonon or a TLS.

We distinguish the diffusion of wavepackets in terms of the step-lengths travelled on a scale of localization length l and identify two regimes depending upon the temperature and the concentration of the TS present in the system. The range of diffusion of a wavepacket vary from a_0, to l, the localization length.

In the *short-step regime*, the distance travelled between two consecutive inelastic events or the step-length, l_r, is of the order of inter-atomic distance *i.e.* a_0 or a few multiples of it such that l is sufficiently larger than $l_r = ra_0,\ r = 1, 2, 3, ...$; and the *long-step regime* where the step-lengths L_r can be almost of size l, $L_r = rl$ with $r = 0, 1, 2, ...$ Here $r = 0$ corresponds to two inelastic events occurring within a span L_0 such that $l > L_0 > l_r$; and $r \geq 1$ indicate step-lengths protracted beyond l by Mott's variable-range-hopping [13]. If the packet diffuses full localization length l without encountering an inelastic event, it can tunnel into a nearby degenerate or nearly degenerate localized state.

The diffusion process which consists of elastic scattering events contributes

to R. At low temperatures R is large because the distance diffused is large. As T increases, phonon assisted hopping makes the electron jump between diffusion processes. The hopping actually reduces R because the potential fluctuations in the regions which the electron skips while hopping are not felt by it and hence these regions do not contribute to R. The hopping helps the electron to cover larger distances without experiencing much diffusion.

The inelastic life time in the two regimes shall be represented by $\tau_<$ and $\tau_>$ respectively – while $\tau_<$ is dominated by direct inelastic collisions, $\tau_>$ is dominated by incoherence time or the typical time taken in reaching the edge of a localized state. A wire of length L can be imagined to be made up of $s(l_r)$ number of

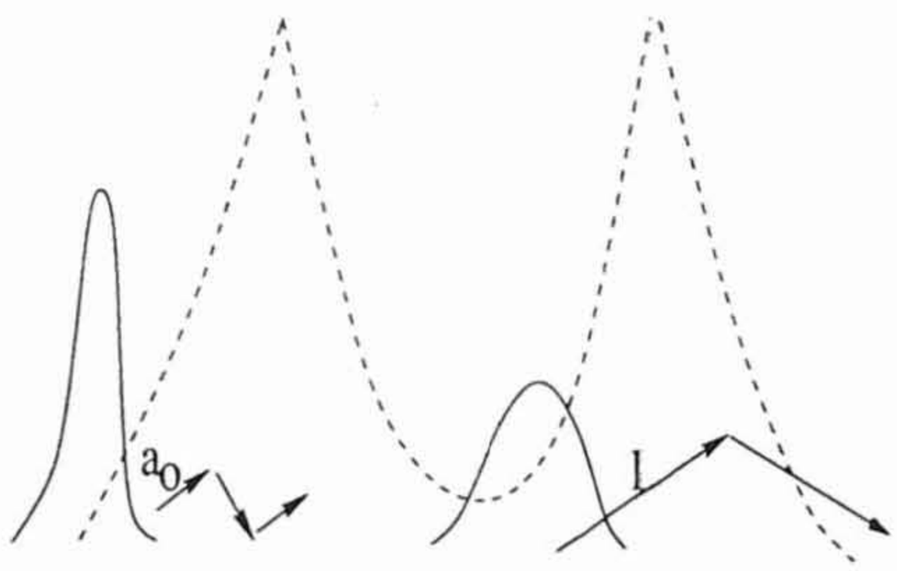


Figure 2.4: Long and short steps of wavepackets; --- represents envelopes of localized wave functions

segments of length l_r and $S(L_r)$ number of segments of length L_r. In general they will peak at different values of segment lengths with the constraint

$$\sum_{r=1}^{N} s(l_r) l_r + \sum_{r=0}^{n} S(L_r) L_r = L \ , \tag{2.11}$$

where $N = L/a_0$ and $n = L/l$.

Treating each diffusion step in terms of a metallic resistor the net dimensionless resistance ρ_e, scaled in $\pi\hbar/e^2$, is just an incoherent sum with segments

contributing as resistances in series:

$$\rho_e = \sum_{r=1}^{N} s(l_r)(e^{l_r/l} - 1) + \sum_{r=0}^{n} S(L_r)(e^{L_r/l} - 1) \ . \tag{2.12}$$

At higher temperatures, inelastic events will be more frequent as a result of which the segment length becomes smaller *i.e.* $l_r/l << 1$ and $L_r/l << 1$. Hence on expanding the exponentials one gets the behaviour at high temperatures which is the metallic one, $\rho_e \sim \rho_0 = L/l$. Thus

$$\rho_0 \ = \ \sum_{r=1}^{N} s(l_r) l_r/l + \sum_{r=0}^{n} S(L_r) L_r/l \ \sim L/l. \tag{2.13}$$

The incremental resistance ratio due to both the packets is given by

$$\begin{aligned} \frac{\Delta R}{R_0} &= \frac{\rho_e - \rho_0}{\rho_0} \\ &= \sum_{r=1}^{N} p_r \left[\left(\frac{e^{l_r/l} - 1}{l_r/l} \right) - 1 \right] + \sum_{r=0}^{n} P_r \left[\left(\frac{e^{L_r/l} - 1}{L_r/l} \right) - 1 \right] , \end{aligned} \tag{2.14}$$

where we have defined fractional contributions to the total length,

$$p_r \equiv s(l_r) l_r/L, \ \ P_r \equiv S(L_r) L_r/L; \ \text{with} \ \sum_{r=1}^{N} p_r + \sum_{r=0}^{n} P_r \equiv (1-\alpha) + \alpha = 1, \tag{2.15}$$

and have assumed metallic behaviour *over the span of each stretch of diffusion* of size l_r or L_r, so that for $l_r, L_r < l$ from eqn.(2.12) we have $R \sim R_0 = L/l$.

In general, the packet will make a relatively fewer excursions over distances larger than l without meeting an inelastic event since the probability for undergoing variable-range hopping is exponentially smaller ($\sim \exp(-T^{-1/2})$) than that for finding an inelastic scatterer ($\sim T^{-1/2}$, see later). So, *on average* we will always take $L_r < l$. Torodov's numerical scaling result [122] that in the localization regime the resistance R of long thin wires will fit a different expression with R proportional to $\sinh L/l$ will also give the same result as eqn.(2.14). Each term in eqn.(2.14) dominates separately in one of the regimes described above.

Short steps: For frequent inelastic scatterings from TSs or phonons p_r is sharply peaked to order $O(N^{-1/2})$ about $\langle l_r \rangle < l$. Then the leading localization correction from the packets able to diffuse over short distances in the range of localization length l, is

$$\frac{\Delta R_<}{R_0} \simeq (1-\alpha)\frac{\langle l_r \rangle}{2l} \simeq (1-\alpha)\frac{\rho_e}{A}\frac{\sqrt{D\tau_<}}{\sqrt{2}(\pi\hbar/e^2)} \ . \tag{2.16}$$

This result is essentially the same as that of Thouless eqn.(2.8) but is derived here more directly from the exponential length dependence of R given by the scaling theory of localization. What we gather here is that Thouless' result belongs to the short-step regime. If $\tau_<$ is small due to frequent scatterings from phonons then this will be the weak localization regime. The term 'weak' is used here in a generic sense and not to refer to the weak localization that arises due to the time reversal symmetry [93]. However, $\tau_<$ can also be small due to scatterings from TSs even at low temperatures if the disorder is sufficiently high. In this situation also, in spite of the disorder being rather high, the effect of localization would be reduced to some extent. Thus at high disorders (and low temperatures) a competition between strong localization and inelastic scattering from TSs – both produced by strong disorder – decides the value of $\tau_<$ or the extent to which the effect of localization is felt.

Long steps: If the inelastic events from TSs and /or phonons are of such frequency that the wavepackets can manage to diffuse over distances of the order of l with some non-zero probability, then on scale l we will have

$$\frac{\Delta R_>}{R_0} = \frac{\alpha \sum_{r=0}^{n} P_r\left[\frac{e^r-1}{r}-1\right]}{\sum_{r=0}^{n} P_r} \approx \alpha\left[\frac{(e^{\langle r\rangle}-1)}{\langle r\rangle}-1\right] \simeq \frac{\alpha}{2}\langle r\rangle \ . \tag{2.17}$$

For peaked distribution P_r, r has been replaced by $\langle r \rangle$, the coarse grained average of L_r/l on the scale l. The last result in eqn.(2.17) is obtained for $\langle r \rangle < 1$, neglecting $\langle r \rangle^3$ and higher powers of $\langle r \rangle$. In this regime although $\langle L_r \rangle < l$, there will be some excursions made by the packets over distances of order l or a few multiples of it.

Thus in a general sense we can include the frequency of inelastic events in our formulation by introducing a probability $P_>$ for a packet to take a step of size l (i.e. move to another localized state after having diffused through one of size l) and a probability $P_<$ of not diffusing (i.e. encountering an inelastic scattering *well* within a distance of l); $P_> + P_< = 1$.

Such a trajectory can be represented as a sequence of randomly arranged vertical partitions and horizontal bars. The partitions represent steps of 'zero' size on a scale l and the bars represent steps of an average size of order l. Thus the partitions, $n_<$ in number, represent inelastic events, and the bars, $n_>$ in number, represent diffusion steps with, $n_> + n_< = n$. This will enable us to estimate the coarse grained average $\langle r \rangle$ which will be the average occupation fraction in a box bounded by vertical partitions, i.e.

$$\langle r \rangle \simeq \overline{n_>}/(\overline{n_<} - 1) \approx \overline{n_>}/\overline{n_<} \ . \tag{2.18}$$

The most probable values $\overline{n_<}$ and $\overline{n_>}$ are found by maximizing the binomial distribution $W(n_>) = n! P_>^{n_>} P_<^{n_<} / n_>! n_<!$. Using Stirlings approximation and maximizing, we get

$$\langle r \rangle \simeq P_>/P_< \ . \tag{2.19}$$

The probabilities $P_>$ and $P_<$ defined in the strictly 1D model must be related to the physical decay or diffusion rates in the quasi-1D wire. In a thin wire, such that $d \ll l_{in}$ [94] the minimum energy states will be uniform across the wire, with roughly A/a_0^2 chains of states exponentially decaying along the wire. For time intervals greater than A/D, the diffusing packets can be taken as uniform in the transverse direction while diffusing 'one-dimensionally'at a rate D/l^2 along the wire. The 1D diffusion probability $P_>$ then depends directly on D/l^2. [1]

[1] If a step of size l is taken in time t in a medium of diffusion constant D then $l \sim \sqrt{Dt}$, and the jump frequency $P_> = 1/t \sim D/l^2$.

The incoherence time $\tau_>$ is related to the decay time τ_l of any one of the localized states that make up the packet. Since there are A/a_0^2 chains of states across the wire, the packet decay rate, $1/\tau_>$, must be related to the 1D decay probability summed across the wire, $\sum P_< = (A/a_0^2)P_<$. That is. the decay in any one of the chains should bring about incoherence and decay in the overall combination. Since the incoherence time of the packet comes from the decay of any of the localized states, the rate per chain $(1/\tau_>)/(A/a_0^2)$ is to be related to the 1D probability $P_<$.

Equating the ratio of probabilities to the ratio of relevant rates, i.e.

$$P_>/P_< = (2D/l^2)/(a_0^2/A\tau_>) \ , \tag{2.20}$$

we finally get

$$\Delta R_>/R_0 = \alpha {\rho_e}^2 D\tau_>/\left\{A{a_0}^2\left(\pi\hbar/e^2\right)^2\right\} \ . \tag{2.21}$$

Our next task is to determine $\tau_>$, the packet incoherence time. Each localized state used in the construction of a packet has an energy width $\hbar/\tau_l$ and the incoherence time $\tau_>$ for the diffusing electron should be associated with it. Many localized states of width $\hbar/\tau_l$ will form a packet which in turn diffuses until it gets scattered. Thus the width of the localized state will affect the intrinsic energy width of the packet and hence the packet incoherence time $\tau_>$. Since we do not know the details of how a particular packet is constructed, we must consider a typical diffusion path-length and work backwards.

A free wavepacket made up of plane waves of momentum $\hbar\langle k\rangle$ broadens as it moves, with the co-ordinate space width $\Delta x \equiv \langle(x - \langle x(t)\rangle)^2\rangle^{\frac{1}{2}}$ proportional to the distance $\langle x(t)\rangle$ travelled. Since $\Delta x \geq \hbar/\Delta p$, the width in co-ordinate space is inversely proportional to the energy width and so

$$\Delta x \ \geq \ \frac{\hbar^2 < K >}{m\Delta E}. \tag{2.22}$$

Thus in the energy space its width narrows such that $\Delta E \geq \hbar K/\langle x(t)\rangle$ (with the constant $K \sim \hbar k/m$). We *assume* that for an elastically diffusing wave packet the same type of relation holds,

$$\Delta E \geq \hbar K/\sqrt{2Dt}\ . \tag{2.23}$$

Since the localized states decay in τ_l, the intrinsic energy width of a packet should be,

$$\frac{\hbar}{\tau_>} \geq \frac{\hbar K}{\sqrt{2D\tau_l}}\ . \tag{2.24}$$

The K is estimated by considering a narrow packet of size $\sim a_0$ and initial intrinsic width $\hbar/\tau_0$ that does not narrow in its short life time τ_0. That is

$$\hbar/\tau_0 \ \geq\ \hbar K/\sqrt{2D\tau_0}, \ \text{ or } \ \sqrt{2D/\tau_0} \geq K. \tag{2.25}$$

Using the equality sign for a rough estimate we obtain from eqn.(2.24)

$$\tau_> \approx \sqrt{\tau_0\tau_l}\ . \tag{2.26}$$

Substituting in the expression for $\Delta R_>/R_0$ we get,

$$\frac{\Delta R_>}{R_0} = \alpha\left(\frac{\rho_e^2}{a_0^2 A}\right) D\sqrt{\tau_l\tau_0}\Big/\left(\pi\hbar/e^2\right)^2\ . \tag{2.27}$$

Thus we obtain

$$\frac{\Delta R_>}{R_0} \sim \rho_e A^{-1} T^{-1/2} \tag{2.28}$$

in agreement with the experimental behaviour. Using the parameters of [70] one can find $\Delta R_>/R_0$ as follows,

Numerical values

$$\begin{aligned} D &= \frac{1}{\rho_e}\frac{\hbar}{e^2}\frac{4\pi\hbar}{mk_F} \\ \frac{\Delta R_>}{R_0} &= \alpha\frac{1}{D^2}\left(\frac{\hbar}{e^2}\right)^2\left(\frac{4\pi\hbar}{mk_F}\right)^2\frac{D\sqrt{\tau_0\tau_{in}}}{a_0^2 A\pi\hbar/e^{2^2}} \\ &= \alpha\frac{1}{D}\frac{16\hbar^2}{m^2k_F^2}\frac{\sqrt{\tau_0\tau_{in}}}{a_0^2 A} \end{aligned}$$

From Chaudhari and Habermeir's work [70]

$$\frac{\hbar}{mDk_F A^{1/2}} \approx 10^{-2} \text{ and we set } \alpha = 1$$

$$\tau_{in} = \frac{1}{4.3 \times 10^8 T}\text{sec}$$

By transmission electron diffraction it is found that at 4.2 K

$$D = 1.7cm^2sec^{-1};\ k_F = 2.73 \times 10^8 cm^{-1}$$

$$\therefore \tau_{in} = \frac{1}{4.3 \times 10^8 \times 4.2} = 0.0553 \times 10^{-8}\text{sec}$$

We have found that

$$\tau_0 = \sqrt{\frac{2Dm^2}{\hbar^2 k^2}} = 34 \times 10^{-18} sec$$

$$\text{Hence } \tau_> = \sqrt{\tau_0 \tau_{in}} = 13.74 \times 10^{-14} sec$$

$$\therefore \frac{\Delta R_>}{R_0} = \frac{16}{a_0^2}\left(\frac{\hbar}{mDk_F A^{1/2}}\right)^2 D\tau_> = 3.73 \times 10^{-2}$$

Experimental results: From the graph given in [70], $\ln T(4.2K) = 1.44$

$$\frac{R(T) - R(13K)}{R(13K)} \approx 2 \times 10^{-2}$$

Thouless' case:

$$\frac{\Delta R_<}{R_0} = \frac{(1-\alpha)\rho_e \sqrt{D\tau_<}}{A\sqrt{2}\left(\frac{2\hbar}{e^2}\right)}$$

$$\text{Here } \alpha = 0$$

$$D\tau_< = \frac{1}{2} l_{in} l_{el} = 2 \times 10^{-12}$$

The area:

$$\frac{\hbar}{mDk_F A^{1/2}} \approx 10^{-2} \quad \therefore A = 6.2 \times 10^{-18} m^2$$

$$\therefore \frac{\Delta R_>}{R_0} = \frac{4\pi\hbar}{mDk_F} \frac{\hbar}{e^2} \frac{D\tau_<}{A\sqrt{2}} \frac{e^2}{\pi\hbar} = 0.0161 \times 10^3 \tag{2.29}$$

Thus Thouless' result is found to be anomalously large [70, 81]. Large τ_i and the erroneous assumption of a ρ_e independent $\sqrt{D\tau_i}$ were apparently responsible for Thouless' high value.

Thus we've got

$$\frac{\Delta R_>}{R_0} = \rho_e A(\pi\hbar/e^2)\left[(1-\alpha)\sqrt{\frac{D\tau_<}{2}} + \frac{\alpha\rho_e D\sqrt{\tau_l\tau_0}}{\pi\hbar/e^2}\right].$$

This expression covers the physical conditions ranging from the extreme ones where an electron can barely diffuse a few atomic spacings, to the moderate ones where it can make some excursions of the order of localization length. The conditions allowing many and longer excursions can be taken into account by including higher powers of $\langle r\rangle$ in eqn.(2.17).

2.6 Discussion and comments

Here we have derived an expression for the increase in resistance to the metallic resistance, $\Delta R/R_0$ in the framework of localization theory. We have considered the inelastic events probabilistically, the main cause to be from TLS. We find that the electrical resistance of quasi-1D systems is sensitive to the frequency of inelastic scattering events. The identification of the physical conditions under which Thouless' results [75] should be valid and those that would have been present in the experiments [72] done to verify his results, calls for new experiments under controlled conditions of disorder and temperature to study in detail the roles of inelastic scatterings from TSs and phonons separately in the electrical transport in quasi-1D systems. This should give more insight into the microscopic details of electron diffusion in the backdrop of localization. Experiments at very low temperatures should possibly reveal something new arising from the interaction between TSs which can change the nature of tunneling from coherent to incoherent [124, 125].

It should also be interesting to investigate the conditions under which the τ_{ee} takes over from τ_{TS}, and also the nature of this transition. This transition is expected to be different from the weak [93] to strong localization cross-over.

The scaling theory of localization asserts, besides arguing the absence of extended states in 1D and 2D, that in 2D there can be a transition from strongly localized (SL) to weakly localized (WL) regime depending upon the sheet resistance value $R_{\square}$. A great deal of effort has been devoted to extending the study of localization as well as strong localization(SL) to weak localization (WL) transition [118] in the quasi-1D limit, still it has not been demonstrated in quasi-1D with the same clarity as in 2D.

Chapter 3

INTRINSIC PHASE-DECOHERENCE IN MESOSCOPIC SYSTEMS

3.1 Introduction

One of the fundamental properties of an electron under quantum mechanical conditions is that the phase of its wave function remains coherent over a length of time and space. The electron loses the phase coherence if it interacts with its environment. The coherence-decoherence transition defines the transition from quantum mechanical behaviour of a 'closed' system to the classical behaviour of the same system when it is treated as 'open'. What should comprise 'a system of interest' and its 'environment' with which it may be coupled, depends on how we want to define the problem; the experiments are designed accordingly. For example in our problem of the movement of an electron in a random potential, the electron and the impurities or the disordered potential comprise the system of interest while other electrons, phonons and TLSs etc. form parts of the environment.

For this problem it is now established that the elastic scatterings of the electron under study from the impurities do not dephase it, or randomize its phase [20]. On each such scattering episode the momentum of the electron changes and also the phase of the single-electron wave function, however the changes are in a deterministic manner in that these changes are correlated and in principle computable. Normally, the phase relaxation length, or the length over which the phase has reversed, can be much larger than the elastic mean free path. The inelastic scattering events due to electron-phonon (e-ph), electron-electron (e-e) or

e-TLS interactions, on the other hand randomize the phase of the electron wave function. It was believed until recently that in the limit of temperature $T \to 0$ the inelastic events could be minimized and consequently the phase-decoherence time τ_ϕ and the phase-coherence length L_ϕ could be arbitrarily large.

Under normal conditions achievable in experiments a disordered system can be viewed as a jigsaw of phase-coherent units, where each unit is of mesoscopic length scale and contains many elastic scatterers. To study the long-range phase-coherence one ought to do experiments on a sample of mesoscopic size and weak localization is an appropriate phenomenon to investigate for analyzing different scattering processes for it is sensitive to phase and momentum relaxation. All electrons incident in the same state acquire the same phase shift after going through a given set of elastic scatterers so much so that a time reversed course of the same collisions can restore the original phase of the wave function. An inelastic collision in the course of these events destroys the phase memory of the electron irrevocably.

3.2 Saturation of phase-decoherence time

Some recent experiments [102, 124] along these lines have shown that τ_ϕ, and in turn L_ϕ, approaches a *finite* temperature independent value below a temperature that may lie between a few mK and 10K depending on the system under study. It has been observed in a wide variety of disordered conductors that τ_ϕ saturates to a value between 10^{-9} sec and 10^{-12} sec below 4K depending on the system. It is further claimed that this phase decoherence is intrinsic in character, that is, it should not depend on the coupling with extrinsic environmental factors. This led to the suggestion that the decoherence could be caused by the zero point oscillations of the electrons [124]. This point of view was, however, refuted on the simple ground that the energy of the zero point oscillations cannot

be transferred in the course of inelastic collisions of the electron in question with the electrons around it.

Not withstanding the mechanism of dephasing, which is a matter of intense debate [167], the result is undoubtedly of fundamental importance and of far reaching consequences. A number of phenomena, including electron localization, that depend on quantum interference would require rethinking. As for localization, the experimental result [124] poses a serious puzzle by indicating that the zero temperature dephasing length $L_\phi(T = 0)$ is much smaller than the typical localization length ξ. This would have the serious implication that large localized states (or weak localization, WL) would not exist. There ought to be a competition between quenched or static disorder and the factors that limit the intrinsic decoherence time τ_ϕ in deciding the extent of localization even for $T \to 0$. Consequently, there could be a lower critical value of disorder below which localization may not happen. (If $L_\phi \sim \frac{\xi}{(k_F l)}$, localization will occur only if $\xi < L_\phi$, i.e. $k_F l < 1$, which implies the WL regime for which $k_F l \sim 1$ should actually be non-existent].

3.3 Sources of dephasing

Phonons are the most obvious source of dephasing, but they have to be ruled out in the temperature range in which τ_ϕ has been observed to saturate. The inelastic processes that may persist at such low temperatures are e-e and e-TLS interactions.

While the e-e interaction is generally considered to be a good candidate as a phase randomizing agent at low temperatures it should be noted that the samples in the experiments in question have fairly low concentration of electrons, $\sim 10^{12} cm^{-2}$ [128]. The e-e interaction energy should be considerably small in these samples as compared to that in the earlier experiments, when the electron

density used to be much higher. It is therefore not clear as to what extent will these interactions be instrumental in the dephasing phenomena. These could at most be quasi-elastic which would imply that there would have to be many collisions of this kind before the electron's phase would change by 2π. Instead of thinking in terms of many colliding electrons it helps to consider one electron subjected to a random time and space dependent electric field created by all the other electrons. This is the electric noise inside the system. It is however certain that if τ_ϕ saturates, then as a consequence, the e-e interaction correction to conductivity will also saturate. It will be of interest to examine the factors that can saturate τ_{ee}.

We will investigate in some detail the interaction of electrons with TLSs as a plausible mechanism of the phase decoherence. In this scenario one studies the movement of an electron under the combined influence of static or quenched disorder and a dynamical environment due to an atom or a group of atoms moving back and forth between two locations in space which correspond to minimum energy states separated by a potential barrier in the configuration space. While the movement of an electron under the influence of a static disorder is diffusive, the dynamical disturbances in space caused by TLSs can make the electron move into another state inelastically even at $T = 0$. We expect that the inelastic scattering from TLSs should dominate at very low temperatures when other sources of inelastic scattering have diminished or become ineffective. Inelastic scattering from TLSs as the source of decoherence of an electron has been discussed in the literature [97]; here we have a very different mechanism to propose for the dephasing phenomenon.

Ovadyahu [97] first found in some of his indium oxide samples with low resistivity ($k_F l > 2$) that inelastic scattering time was much shorter than the e-e interaction time. The results fitted well when e-TLS scattering was invoked as

the phase-breaking mechanism. Zawadowski et al. [97] considered non-magnetic TLSs having degenerate Kondo ground states. In a certain temperature range the TLSs exhibit non-Fermi liquid (NFL) behaviour which apparently is the signature of dephasing. They propose that the scattering of an electron from a TLS of this type, changes the state of the TLS and thus the environment of the electron changes. This causes the dephasing. Imry et al. [141] propose a perturbative theory in electron-environment interaction where τ_ϕ is much longer than the quasi-elastic scattering time τ. The scattered electron undergoes a phase-shift due to the motion of the scatterer. The phase-shift changes the conductance and also causes dephasing. If the defect motion is slower than the time scale of electronic motion only the conductance changes, but if the defect moves faster than the electronic motion then dephasing also happens.

3.4 Our proposal

Our arguments are somewhat similar to those of Imry et al. [141] but only at the beginning. We propose a novel mechanism for the saturation of τ_ϕ which accounts for the T-independence of τ_ϕ. First of all we propose that the phase-shift of an inelastically scattered electron should depend not only on the fact that the scattering it is undergoing is inelastic in nature, but also on the character of the scatterer. The latter should be particularly significant in the case of dynamical scatterers like TLSs, whose character depends on the nature of the tunneling - whether it is coherent or incoherent.

We can formally write,

$$\tau_\phi = f(\tau_{in}, c), \tag{3.1}$$

where c is a parameter signifying the character of the inelastic scatterer. In the case of e-TLS scattering, $\tau_{in}(= \tau_{e-TLS})$ would predominantly depend on temperature and concentration of TLSs. While its dependence on concentration of TLSs

is obvious, we understand the dependence of τ_{e-TLS} on T like this: first of all, the tunneling will have to be assisted by phonons if λ is larger than a certain λ_{min} [29, 98] where $e^{-\lambda}(\simeq \Delta_0)$ represents overlap between wave functions for the two potential wells in the TLS. Since λ depends inversely on T, the tunneling will be increasingly more difficult as $T \to 0$ and at some point it will be impossible for those parameters of the TLS that determine λ_{min}. Below this value of T the system will freeze into one of the configurations represented by the two wells. Thus as T decreases, the tunneling rate of this type of TLSs decreases and consequently the scattering rate τ_{e-TLS}^{-1} decreases. In simple terms the rate of tunneling becomes slower than the time scale of the electron movement. However, if the TLS is such that $\lambda < \lambda_{min}$, then tunneling continues to happen even if $T \to 0$. Such TLSs are particularly significant for the saturation of τ_φ.

We will now discuss the parameter c in the eqn.(3.1). The character of a TLS can depend considerably on its interaction with other TLSs. Note that the motion of the tunneling entity (an atom or bunch of them) produces a strain field. If the TLSs are far away from each other or the temperature is not low enough to preclude phonons, then the strain field may not affect the other TLSs because it may get weakened or dissipated by phonons. But if the concentration of TLS is high, or there are intermediary impurities, then the strain field produced by one TLS can affect the nature of oscillation of the other TLSs if the temperature is so low that the dissipation of the strain field by phonons can be ruled out. While an isolated TLS generally oscillates between two wells coherently, the interaction between TLSs can make the oscillations incoherent. This crossover as a function of decreasing temperature will have its influence on the phase-shift of the electron scattering off the TLS; it should add to the change in the phase of the electron.

If the mean interaction between the TLS is represented by an energy J then

one can combine the local parameter Δ_0 with it and describe the TLS-TLS interaction by a dimensionless parameter [120]

$$\mu = J/\Delta_0. \tag{3.2}$$

If J dominates over the local coupling energy Δ_0 (i.e., interaction between TLSs is as large as, or larger than, the coupling between wave functions in the two wells of a TLS) then μ will exceed 1 and the local tunneling motion will become incoherent. In glassy systems Δ_0 will have a wide distribution which can vary as k_BT [125]. Consequently μ can be taken as proportional to T^{-1}. Note that τ_{e-TLS} is also $\propto T^{-1}$. In the background of the above discussions, the implications of both μ and τ_{e-TLS} being proportional to T^{-1} are important in so far as the phase change of the electron is concerned.

Let us consider the two situations, $\lambda > \lambda_{min}$ and $\lambda < \lambda_{min}$, separately. In fact both the situations are important at the same time because TLSs satisfying either conditions would be present in the system.

In the TLSs for which $\lambda > \lambda_{min}$ the tunneling, which must be assisted by phonons, will increasingly slow down with decreasing temperature. As a result τ_{e-TLS} will increase at a rate $\propto T^{-1}$. But, while the tunneling rate slows down, the *nature* of tunneling changes from coherent to incoherent at the same rate, namely T^{-1} due to increasing TLS-TLS interaction. If according to Stern et al. [113] e-TLS scattering is turning from inelastic to quasi-elastic and then to elastic with decreasing T and is therefore able to change only the conductance, the phase-shift in the scattered electron is certainly brought about by the latter factor discussed above, namely the coherent-to-incoherent crossover in the nature of TLSs.

The TLSs with $\lambda < \lambda_{min}$, in which the tunneling occurs in spite of the absence of phonons, can, in principle change the phase of the electron scattering off them even as $T \to 0$. This is true independent of whether the energy exchanged in

the scattering process is sufficient for it to be fully inelastic. The phase of the scattered electron in any case changes because the tunneling in these TLSs also becomes incoherent with decreasing T due to long-range interactions among the TLSs.

The incoherence of the tunneling in both types of TLSs increases with decreasing T and accordingly the amount of the phase change of the scattered electron increases. At sufficiently low T when the phase change is about 2π, the decoherence time τ_ϕ will saturate and become temperature independent.

3.5 Discussion and comments

The above mechanism for saturation of decoherence time τ_ϕ is plausible although it is based on heuristic arguments. A good amount of further experimentation is required to ascertain a number of finer points.

First of all it must be checked whether the systems that exhibit τ_ϕ-saturation always have TLSs present in them. This is necessary in order to establish that the suggested mechanism is really a universal one.

Experiments are required to identify the types of TLSs, at least the two types discussed above. Having done this it is necessary to study in greater detail the coherent-incoherent tunneling crossover as a function of T and whether both the above types of TLSs are affected equally as T decreases.

Experiments are also needed to ascertain if the e-e interactions in *dilute* electron systems indeed involve sufficient energy to be classified as inelastic at low temperatures.

Finally, it could well be as suggested by Imry et al. [141] that there may be just a temperature range over which τ_ϕ remains saturated, but at $T << \hbar/\tau_0$ (τ_0 being the saturation value) the τ_ϕ may diverge. Only very careful experimentation can resolve these issues.

We may mention in passing that it is the rapid development of quantum information processing [129] that has led to renewed interest in the study of dephasing effects. The studies proposed above would be very vital in this modern context for one of the major obstacles in the way of implementation of quantum computers is the relatively short dephasing time in the solid state devices.

Chapter 4

METAL-INSULATOR TRANSITIONS IN TWO DIMENSIONAL SYSTEMS

4.1 Introduction

No solid has a perfectly regular structure of an ideal solid and hence disorder is an essential ingredient of the quantum theory of solids. If the disorder is not much, the electrons will be accelerated by the electric field and the electrical resistance will be found to be less. The thermal motion of atoms causes some dynamical disorder which decreases as the temperature is lowered and the resistance of a metal decreases. At very low temperatures there will be only residual resistance which is entirely due to the presence of impurities and disorder in the metal.

For 2D case it was argued in [44] that if the film sheet resistance $R_\Box > R_{2D} \approx 8\hbar/e^2$ all electronic states would be localized. This concept of maximum metallic resistance led to the scaling theory of localization which argued that true metallic states do not exist in 2D. The scaling parameter in this case, which is the sheet resistance of the film determines whether the conductor falls into the strongly localized (SL) or weakly localized (WL) regime. For strong disorder the electron transport occurs by thermally- activated or variable-range hopping between localized states. Consequently the resistance increases exponentially with decreasing temperature. As the film sheet resistance decreases and the disorder becomes weaker, it crosses over to the WL regime where the resistance increases only logarithmically with decreasing temperature.

Microscopically it is the competition between the localization length ξ and the inelastic scattering length (l_{in}) on which this crossover depends. In systems

where $\xi < l_{in}$, the electrons are SL and in systems where $\xi > l_{in}$ the electrons are WL. Therefore, although there is no true metal-insulator transition (MIT) in 2D, a crossover from weak to strong localization with increasing disorder (i.e sheet resistance) does exist and this crossover appears to be continuous.

Even if a 2DES were conducting at high temperatures, as the temperature is lowered, an electron begins to settle down with a sequence of phase coherent scatterings from impurities. These elastic events give rise to a logarithmically increasing resistance. Altshuler et al. [74] showed that weak e-e interactions between the conducting particles would also give rise to a similar logarithmic correction to resistivity. This result was extensively supported by the experimental evidence [61, 78] and it was generally accepted that the presence of any amount of disorder in a 2D system would give rise to these logarithmic corrections for any energy in the band. But the experimental results of Kravchenko et al. [121] and other subsequent works [133]on high quality 2D samples challenged this understanding.

The clear distinction between a metal and an insulator is properly made only at the absolute zero of temperature. If the resistance is finite at $T = 0$ then the system is metallic, or else is insulating. It is impossible experimentally to reach the absolute zero of temperature and hence to characterize the sample at $T = 0$. But then using a single scaling parameter it was possible to collapse all the resistivity versus T data for different carrier densities onto two separate curves, one in the insulating regime and the other in the metallic regime. The collapse of all the data onto two separate branches can be taken as an evidence that this is a true quantum phase transition between 2D insulating and metallic states. Also, the ability to scale the data over several orders of magnitude of temperature in the metallic branch showed that as $T \to 0$ the resistivity remains finite, consistent with the definition of a metallic state but in dramatic contrast

with the earlier results.

4.2 Ways to make a 2DES

There are two ways of producing a two dimensional electron system (2DES) and they are briefly explained below.

4.2.1 Trapped electrons on liquid He

In this method the electrons are confined to the neighbourhood of a surface is by trapping them above the surface of liquid He. The small polarization that they induce in the liquid makes them attracted to the surface of liquid He. Since the liquid is a good insulator they cannot penetrate into it. The application of an additional electric field normal to the surface will bind the electrons more tightly to the surface. The trapped electrons move parallel to the surface. Typical density of trapped electrons is of the order of $10^8 cm^{-2}$.

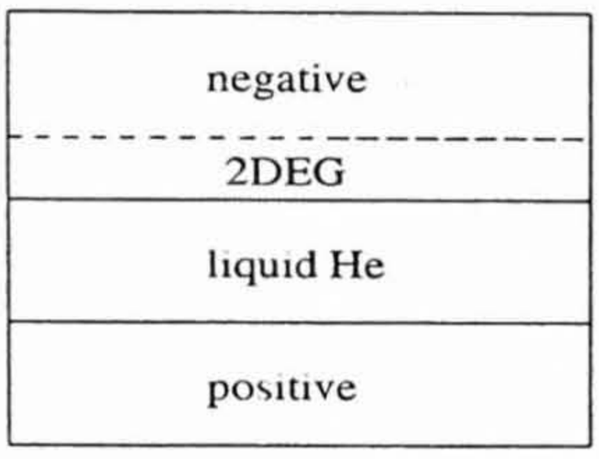


Figure 4.1: Trapped electrons in liquid He

4.2.2 Semiconductors and heterojunctions

Electrons can also be trapped at a semiconductor surface. In metal oxide semiconductor (MOS) devices, a p-type semiconductor, usually Si, has an insulating layer, such as SiO_2, grown on top of it. A metal electrode known as gate, is grown on top of the oxide layer. A positive voltage is applied to the gate so that the electric field lowers the energy of the conduction band close to the

surface. If the field is strong enough, electrons are trapped in a narrow layer on the semiconductor side of the interface between the semiconductor and the oxide. These trapped electrons are free to move parallel to the surface, and a current can be made to flow along the surface between two electrodes known as source and drain. When a voltage is applied to the gate, the positive carriers near the oxide surface can be driven into the bulk. This induces negative charges at the interface between Si and SiO_2. Further increase in voltage will produce conduction electrons which appear in a narrow layer near the interface, with thickness of the order of $100A^o$ or less. The sign of these charges are opposite to that of the bulk carriers in Si is hence is called as inversion layer. If an n-type Si is used instead of a p-type, there will be an accumulation layer, because carriers of the same sign as in bulk will be induced. Thus electrons can move freely in the

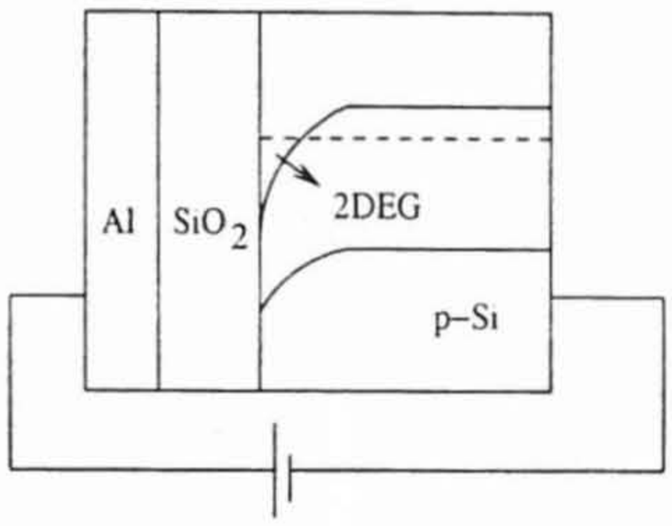


Figure 4.2: 2DEG in Si MOSFET

layer while their motion perpendicular to the condenser plates is restricted due to the quantization of the energy levels. Therefore the electrons constitute a 2DS for low energies. The great advantage of this type of device is that the number of electrons trapped on the surface can be controlled by adjusting the voltage applied to the gate which makes it useful for the study of 2D physics.

Heterojunction is another type of device which has a junction between two different semiconductors such as GaAs/AlGaAs. In this case though the number of electrons cannot be directly controlled it can be arranged in such a way that

the electrons are trapped in regions of very high purity and so are much less scattered than they would be in MOS device. In these semiconductor devices, MOS or heterojunctions, a much higher density of electrons of the order of 10^{11} or $10^{12} cm^{-2}$ can be obtained than is possible above a liquid He surface. The dielectric constant is also much higher than in the He vapour, so the electrons interact less strongly with one another.

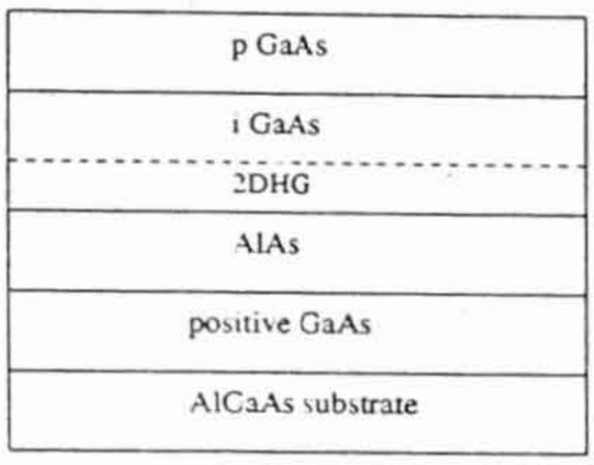


Figure 4.3: 2DHG in GaAs/AlGaAs

4.3 Recent experimental works

Experimental works of Kravchenko et al. [121] revealed for the first time a genuine metallic phase and a MIT in Si MOSFETs with very low disorder. Later experiments on the 2DEG formed in GaAs/AlGaAs heterostructures also gave the same result [135, 136]. Very low concentration of electrons in these samples apparently plays the central role in this context. If the concentration of a 2DEG is reduced, the e-e interaction energy, V_{ee}, reduces, but at the same time the Fermi energy E_F also reduces considerably. Interesting thing is that while at high electron concentrations $V_{ee} < E_F$, with decreasing concentration at one point the decreasing V_{ee} exceeds E_F, i.e. $V_{ee} > E_F$. The strength of this interaction is measured relative to E_F in terms of a dimensionless quantity [31]

$$r_s = V_{ee}/E_F. \tag{4.1}$$

where $V_{ee} = e^2/\epsilon r$; ϵ is dielectric constant and r is the average distance between carriers. Note that

$$[V_{ee}]_{2D} = \frac{e^2\sqrt{n_s\pi}}{\epsilon\sqrt{m}}, \quad E_F = \frac{\hbar^2 n_s \pi}{m} \tag{4.2}$$

$$\text{So} \qquad r_s = \frac{V_{ce}}{E_F} = \frac{e^2}{\hbar^2\epsilon}\sqrt{\frac{m}{n_s\pi}} \tag{4.3}$$

Smaller mass m will increase E_F for a given concentration n, and therefore low carrier mass systems are usually characterized by small r_s values. Thus the effective mass also plays a role in affecting the different properties [169]. Experimental evidence shows that a high value of r_s, usually > 5, is a prerequisite for the observation of MIT.

r_s also gives a measure of the average inter-particle separation $\overline{r}$ in units of Bohr radius a_B, $r_s = \overline{r}/a_B$, with $a_B = \hbar^2\epsilon/me^2$ and $\overline{r}$ the radius of a circle containing one electron on average, $\overline{r} = 1/\sqrt{n_s\pi}$ where n_s is the number density.

$$r_s = V_{ee}/E_F = \overline{r}/a_B = \frac{1}{\sqrt{n_s\pi}a_B} \tag{4.4}$$

Large value for r_s implies that the system is dilute – i.e. $r_s >> 1$ or $E_F << V_{ee}$, and low r_s would imply a dense system, i.e. $r_s << 1$, or $E_F >> V_{ee}$. At low r_s, the electrons form a weakly coupled liquid while at large r_s they undergo a phase transition and crystallize.

Kravchenko et al. performed experiments on Si MOSFETs in a temperature range 0 to 8K and concentration varying from $7.12 \times 10^{10} cm^{-2}$ to $13.7 \times 10^{10} cm^{-2}$. Their samples had a peak mobility of $40,000 cm^2 V^{-1} s^{-1}$ at 4.2K. The experimental results revealed that, starting from a low concentration say about $(7.12 \times 10^{10} cm^{-2})$, as the concentration is increased the system crosses over from an insulating phase to an intermediate phase at a critical concentration $n_c \sim 8.4 \times 10^{10} cm^{-2}$ and then to a fully metallic phase at a concentration of $11 \times 10^{10} cm^{-2}$ fig.(4.4). The phase of the system in the concentration range above

$8.6 \times 10^{10} cm^{-2}$ is in contradiction to the widely accepted result of complete localization in 2D. In the range of concentration from $8.6 \times 10^{10} cm^{-2}$ to $11 \times 10^{10} cm^{-2}$, the system goes over from an insulating phase to a metallic phase in a somewhat gradual manner with decreasing temperature. In this range of concentration, the crossover happens at a critical temperature of 2K. Later on, the experimental

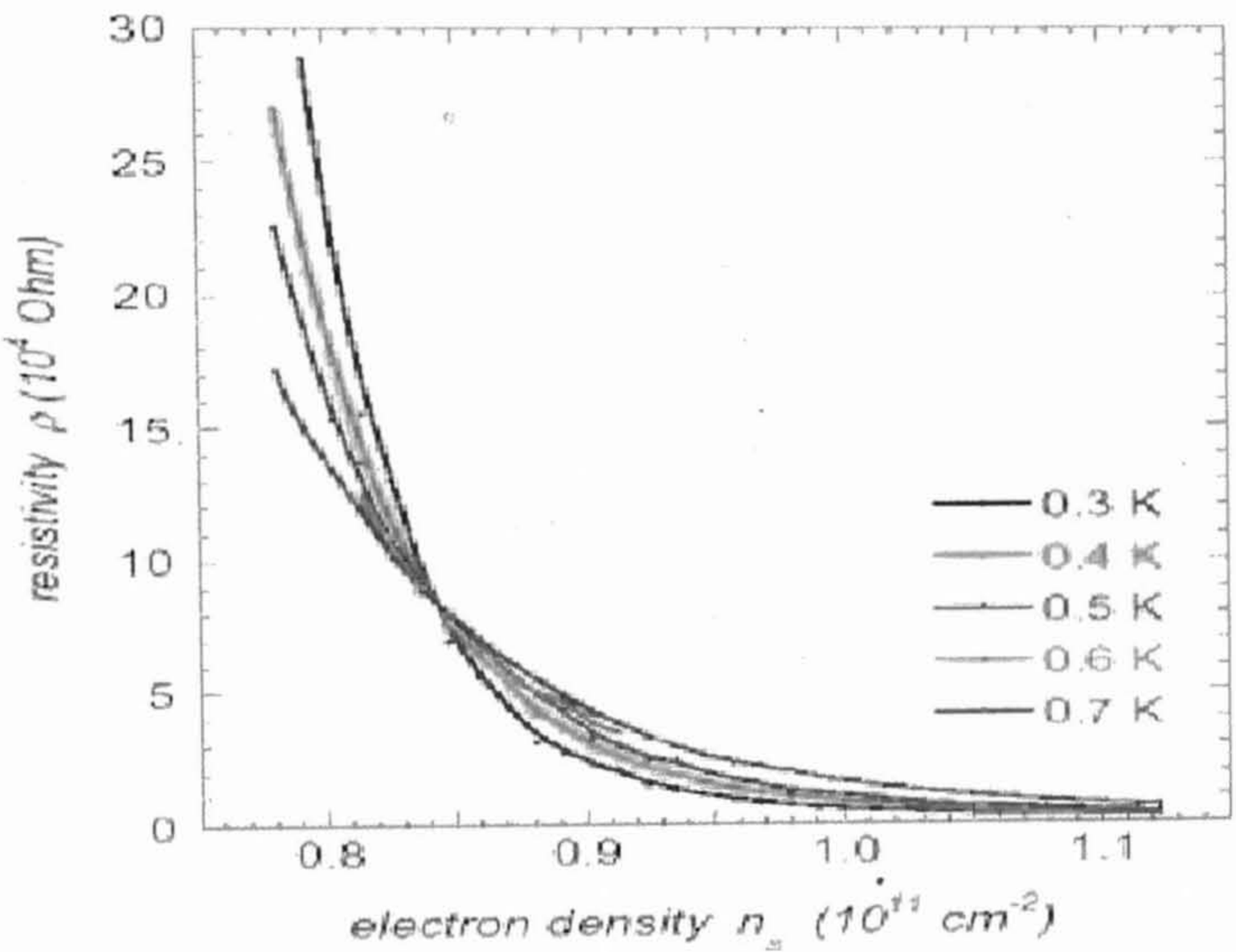


Figure 4.4: Resistivity vs concentration at different temperatures

works of Simonian [126] and Hannien [135] showed the existence of a metallic phase even in 2 dimensional hole gas (2DHG). Hannien performed experiments on the 2DHG in GaAs/AlGaAs heterostructures for concentration varying from $1.09 \times 10^{10} cm^{-2}$ to $6.4 \times 10^{10} cm^{-2}$, in a temperature range 0 to1.2K. As in the case of Si MOSFET, for a concentration range $1.19 \times 10^{10} cm^{-2}$ to $2.5 \times 10^{10} cm^{-2}$, the system exhibits an intermediate phase and above it a fully metallic behaviour is seen. In the intermediate range the system undergoes an insulator to metallic behaviour with the decrease in temperature at a critical temperature of 0.2K. As the carrier density is reduced, r_s increases, until at $r_s > 5$ the interactions

between electrons become weak, but sufficiently stronger relative to E_F and a metallic state is found to be formed. Early studies of weakly interacting 2D disordered systems ($r_s \sim 4$) [83] demonstrated both weak localization and weak e-e interactions causing a logarithmic reduction of the conductivity as $T \to 0$.

4.3.1 Comparison of new and old samples

The MIT was observed in samples of high quality with a mobility about ten times higher, and electron concentrations about 8 to 9 orders of magnitude smaller than the samples used in the earlier experiments. The main factor which distinguishes the new samples from the earlier ones is the high mobility of the order of $30,000 - 70,000 cm^{-2}V^{-1}s^{-1}$ [121, 150] whereas in the earlier samples it was around $2000 - 6500 cm^{-2}V^{-1}s^{-1}$. Earlier samples which favoured the scaling theory result had a concentration of $n_s \sim 10^{19} cm^{-2}$ [92]. The low mobility in old samples indicates that the sample had high disorder but then the high density of electrons would lead to large screening of impurities. Thus the effective disorder felt by an electron in the earlier samples was still considerably low. The recent samples also correspond to low disorder regime – high mobility indicates low disorder with marginal screening at low density of electrons

Kravchenko et al. measured the resistivity of the electron gas as a function of T for several electron densities n_s, and also as a function of n_s for several temperatures. Samples with ultrahigh mobility (upto $\sim 70,000\, cm^{-2}V^{-1}s^{-1}$ of Si MOSFET) at zero magnetic field and low electron densities, a little higher than a critical value, $n_c \sim 10^{11} cm^{-2}$, revealed that the conventional weak localization observed at $T \geq 1 - 2K$ is overpowered by a sharp drop of ρ by an order of magnitude as the temperature is decreased. No signs of electron localization are seen down to the lowest possible temperature of $20mK$. For concentrations below the critical concentration, the resistivity increases monotonically as $T \to 0$

indicating an insulating state studied earlier [119].

4.3.2 Mobility as a function of temperature

In a semiconductor, the electron gas may be described as degenerate or non-degenerate depending on whether or not the mobile electrons are sufficiently numerous to make quantum restrictions on the motion important. A conduction electron gas is degenerate when the electrons are numerous and T is rather small. It requires $(E_F - E_c) >> k_B T$ and the properties are dominated by the changing occupancy of states at E_F, with E_c the mobility edge. An electron gas is non-degenerate or classical when the electron density is very small and/or T is high.

High temperature case:

In the high temperature range where the dominant effect of scattering is from phonons, the carrier mobility is inversely proportional to $T^{3/2}$ for a non-degenerate case and is inversely proportional to T for a degenerate case.

Low temperature case:

In the low T range, the dominant scattering effect comes from ionized impurities. The mechanism of scattering process is such that the impurity ions deflect electrons passing close to them and thereby reduce their velocities in the original direction. The mean free path of these electrons is inversely proportional to their concentration and is *independent* of temperature for the degenerate semiconductors. For the non-degenerate case, the carrier mobility due to scattering from ionized impurities is proportional to $T^{3/2}$. Table 4.1 summarizes the T dependence of μ.

4.3.3 Mobility as a function of concentration

Experimentally one observes a non-monotonic dependence in the low temperature mobility as a function of electron density. Starting from the high density

side, the mobility is found to increase with decreasing concentration, reaches a maximum value called the peak mobility μ_{max} at a concentration n_{max} and then decreases with further decrease in concentration. The peak mobility is actually a rough measure of the amount of disorder determined primarily by oxide charge scattering and the scattering due to surface charge roughness of the $Si - SiO_2$ interface for the case of MOSFET systems. The mobility of MOSFETs can be defined only on the metallic side of the transition $n_s > n_c$ and is limited by scattering from surface roughness and ionized impurities. In high mobility samples such as the ones that showed MITs, high resistivity Si material was used and therefore scattering by ionized donors can be ignored.

The carrier density is varied by applying a voltage to the gate electrode which is separated from Si by insulating SiO_2 (see fig.(4.2)). At the interface a triangular potential well, 'the inversion layer' is formed of which only the lowest subbands is occupied at low temperature. The increasing and the decreasing parts of the mobility with concentration reflect scattering by different scattering processes. Starting at high electron densities and high applied gate voltages, the carriers are pulled towards $Si - SiO_2$ interface and they experience strongly the surface roughness. Upon lowering the gate voltage, the 2D gas moves away from the interface and hence the mobility increases. On the other hand the random ionized impurities invariably present at the interface as a result of fabrication process becomes more and more effective at lower electron densities due to the reduction in electronic screening.

Temperature	$Degenerate$	$Non-degenerate$
High	$\mu \propto T^{-1}$	$\mu \propto T^{-3/2}$
Low	$\mu = const$	$\mu \propto T^{3/2}$

Table 4.1: Temperature dependence of mobility.

A high peak mobility and the associated low values of n_{max} at which the mobility peak occurs is taken as a signature of good quality MOSFETs [108, 149] because it signals both low surface roughness and low density of ionized impurities, which is controlled by working under very clean conditions in particular for the oxidation process.

Klapwick et al. [149] claim that an $n_c > n_{max}$ has never been reported in Si MOSFETs, samples with the highest peak mobility, $\mu_{max} \sim 7 \times 10^4 cm^2 V^{-1} s^{-1}$ have $n_c \leq n_{max}/2$ whereas samples with a more modest peak mobility of $2 \times 10^4 cm^2 V^{-1} s^{-1}$ typically have $n_c \leq n_{max}/5$. Thus the critical density n_c differs for different materials. It is of the order of $10^{11} cm^{-2}$ in n-Si and p-SiGe, an order of magnitude lower for p-GaAs and even lower for n-GaAs. It is reported that [151] the precise value of n_c depends on the sample quality, with larger mobility samples having lower concentration, n_c.

Sarachik [158] plotted the critical density n_c vs the scattering rate $1/\tau$; $\tau = \mu m^* c/e$ using the data reported by different groups for five different electron and hole systems in 2D and observes that the critical density n_c, that marks the onset of strong localization is shown to be a single power law function of the scattering rate $1/\tau$ deduced from the maximum mobility, i.e.

$$n_c = A\left(\frac{1}{\tau}\right)^{\beta} \tag{4.5}$$

where $A \approx 2240\, cm^{-2} s^{\beta}$ and $\beta = 0.67$. This implies that in the limit of zero scattering rate the critical density $n_c \to 0$. The plot is shown in fig.(4.5). Below the curve there is a strongly localized phase and above it there is a metallic temperature dependence. This empirical relation implies that a transition to strong localization is triggered by the degree of disorder in the system. As the transition is approached with decreasing concentration the screening becomes less and less effective and as a result interactions become stronger. But both disorder and interactions are inextricably linked.

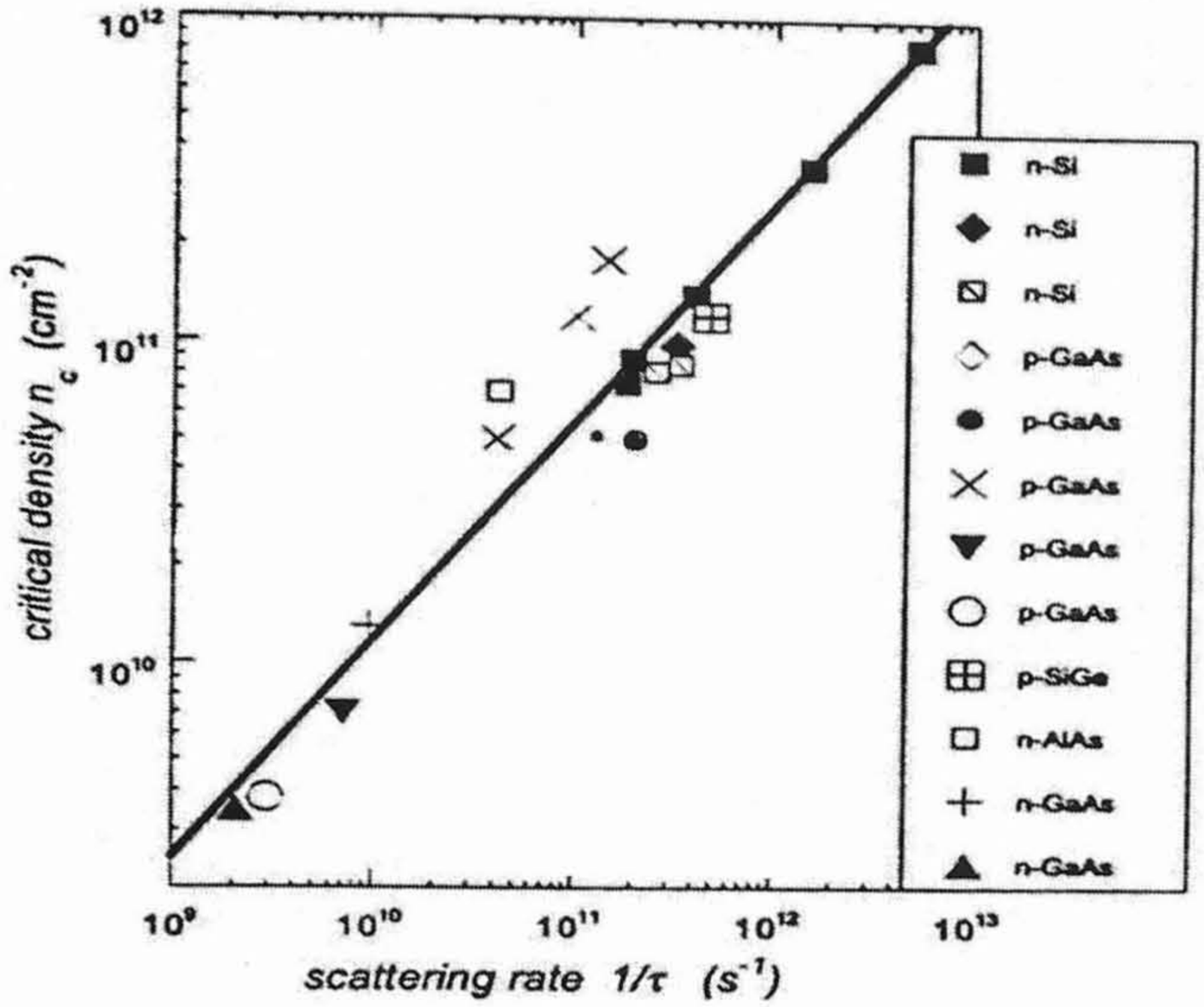


Figure 4.5: Critical electron density vs scattering rate

4.4 Proposed models

Out of the several models proposed [144] some of them are briefly given here. Disorder and correlations can lead to at least two types of localization. In the presence of disorder, Anderson [2], Abrahams et al. [57] and many others showed that a system of *non-interacting* electrons in 2D cannot sustain static conductivity no matter how small the disorder is; this is called Anderson localization. But strong correlation among charge carriers (relative to E_F) at low concentration of electrons can cause a very strong localization in *disorder-free* systems which can lead to Wigner crystallization. The electrons arrange themselves as far apart from one another as possible to minimize their repulsive potential energy and form a crystal. In 2D they form a triangular lattice.

Real systems include both e-e interactions as well as e-impurity interactions, the former apparently dominate in low-electron density regime while the latter

in the high-density regime. Between these two extremes of electron concentration, disorder and correlations compete with one another to decide the nature of localization [163].

While according to the one parameter scaling theory of localization a 2DES is always an insulator, the scaling theory put forth by Finkelstein [99] which includes the combined effects of both interaction and disorder predicts the possibility of a metallic state even in the limit of zero temperature. One reason why Finkelstein's theory did not gain much acceptance is that the scaling equations have the peculiar feature that the scaling variables diverge at some finite value of length scale. Castellani et al. [130] reconsidered the problem of 2D metallic behaviour and argued that for weak disorder the theory remains under control over a large temperature range, provided the renormalization of the energy scale relative to the length scale is taken into account. In fact, this renormalization allows the possibility of a metallic state with finite resistance in 2D.

Azbel [117] found that a system of non interacting 2D electrons in a model disorder potential with a set of special scatterers at B=0 and T=0 is localized only when $E_F < E_c$. At all energies above E_c extended states exist. According to Azbel the disagreement between his results and those of Abrahams et al. might indicate that the resistance strongly depends on the range of scattering centers. Azbel's result might be applicable for the 2DES in Si MOSFETs because the prominent scatterers in these samples, particularly at low electron densities have been shown to be short-ranged [87], similar to the model potential.

A theory developed by Si and Varma [131] takes into account the renormalization of compressibility which becomes important at low electron densities (i.e. large r_s) in which case the screening length s is greater than the mean free path l; $s > l$. At high electron densities, the screening length, s is less than the mean free path, and the fact that the compressibility (which is proportional to the inverse

screening length) is unrenormalized, as was taken in earlier RG approaches, is valid. They argued that for large r_s, the interactions become unscreened at low temperatures and the conductivity approaches zero as might be expected near the MIT. This leads to a MIT controlled by whether s is larger or smaller than l. In sum at high densities the screening is good, r_s is small, compressibility is high and $s < l$, which should imply a metallic phase. At low densities r_s is large, interactions become unscreened at low temperatures and compressibility approaches zero for $s > l$, and an insulating phase is expected.

Experimental works of Dultz and Jiang [155] as well as Ilani et al. [156] in p-GaAs/AlGaAs also found the compressibility tending to zero near MIT. This is what one expects if the insulating phase is one in which the long range Coulomb interactions become unscreened [131], as would also be the case in a disordered Wigner crystal [132].

Dobrosavljević et al. [127] proposed a scaling analysis and showed that a disordered 2D system of interacting electrons should scale either to a perfect conductor or to an insulator in the limit of zero temperature. These authors point out that the metallic state is very unlikely to be a Fermi liquid since if the interactions were turned off metallic behaviour would disappear and the system would become an insulator.

Chakravarty et al. [132] considered the effect of disorder on a model of a 2D non-Fermi liquid. They showed that for sufficiently strong interactions, a non-Fermi liquid state of interacting electrons is stable in the presence of disorder and is a perfect conductor. They [145] subsequently showed that the insulating state is due to the formation of a Wigner solid and the transition from insulator to metal is due to the melting of this glass into a non-Fermi liquid state characterized by short-range magnetic singlet correlations. Experimental evidence for Wigner crystallization was reported by Pudalov et al. [119] and also by Simmons

[134]. Yoon et al. [146], based on transport studies in clean p-GaAs/AlGaAs heterostructures suggested that, the insulating phase is a Wigner crystal and is not due to single particle localization.

Mills et al. [147] did not observe insulating behaviour at much lower densities where interactions are strong. The MIT in interacting 2DEG was proposed to be similar to superconductor-insulator transition in thin films [138, 157]. Also the conducting phase was reported to be suppressed by a magnetic field.

There have been several suggestions that some of the unusual behaviour observed in dilute 2DES at low temperatures can be explained by mechanisms that are classical in nature. Altshuler and Maslov [148] had proposed a mechanism based on charging/discharging of traps in the oxide close to the 2D layer in Si MOSFETs.

Klapwick and Das Sarma [149] proposed a scenario based on the scattering of electrons on charged ion at the oxide-semiconductor interface under conditions when the number of electrons and ions are comparable. They showed that this could lead to a very large magnetoresistance observed on the insulating side of the transition. Das Sarma and Hwang [159] calculated $\rho(T)$ on the metallic side of the transition based on the assumption that n_c carriers are frozen to interface impurities and the MIT occurs when there are no free electrons left.

Klapwick et al. [149] highlight that the observed MIT occurs at electron densities where the ionized impurity scattering dominates. In particular, the 2D MIT is seen clearly in samples with high μ_{max} and usually with $n_c << n_{max}$. In this situation the electron densities are sufficiently low as a result of which the screening low and hence are in a regime where carrier scattering and transport are dominated by ionized impurities. This has the implication that the electrons are facing random localized impurity ions which are poorly screened. Thus screening is an important ingredient in understanding the observed 2D MIT.

Meir [153] proposed that MIT results from percolation in an electron liquid. In this scenario puddles of charges are formed in a percolation landscape. Due to the low density, the screening of disorder is weak and hence these potential fluctuations give rise to density puddles. Between the puddles transport is via quantum point contacts (QPC) or saddle points and between such tunneling events dephasing takes place. That is, the time a particle spends in a puddle is greater than the dephasing time. Each QPC is characterized by a critical energy E_c such that the transmission through it is given by $T(\epsilon) = \theta(E - E_c)$. Then the conductance through the QPC is given by the Landauer formula

$$\begin{aligned} G(\nu, T) &= \frac{2e^2}{h} \int d\epsilon \left(-\frac{\partial}{\partial \epsilon} f_{FD}(\epsilon) \right) T(\epsilon) \\ &= \frac{2e^2}{h} \frac{1}{1 + \exp\left(\frac{(\epsilon_c - \nu)}{k_B T} \right)} \end{aligned} \tag{4.6}$$

where ν is the chemical potential and f_{FD} is the Fermi Dirac distribution function. The system here is viewed as being composed of classical resistors, with the resistance of each one of them given by the above expression.

At low temperatures the resistors are divided into two groups, the conducting ones, $\nu > \epsilon_c$ with conductance of about $2e^2/h$ and the insulating ones, $\nu < \epsilon_c$ with conductance nearly zero. Thus in brief the system is made up of puddles connected to one another via metallic (m) or insulating (i) QPC's. In this background Meir explains the MIT in the following way.

Suppose the concentration of electrons is very low. Then the chemical potential ν will be less than ϵ_c and i-QPCs will dominate. Consequently no conducting channels will exist across the system, and hence is in an insulating phase with resistance increasing with decreasing T. Ultimately, $R \to \infty$ as $T \to 0$. On increasing the concentration, when the critical percolation threshold is reached, there will be one conducting channel across the system. For a range of concentration just above n_c the system will contain more of i-QPCs and m-QPCs scattered

across. Suppose we're in this range of concentration and then start to increase the temperature: at $T = 0$ only m-QPCs contribute as the R of i-QPCs is infinitely high. As T is increased R will initially increase because of the m-QPCs which are actually contributing to R. When the temperature exceeds a certain value, hopping conduction begins to set in and the i-QPCs also start to contribute to the overall conductance. Since the critical percolation cluster is very ramified there will be many such i-QPCs in parallel to the main conducting network as a result of which the net conductance will decrease. Thus R decreases with increasing temperature beyond a particular temperature.

If the concentration is increased, the percolation cluster widens with an increase in ratio of the m-QPC over i-QPCs. As a result, above a particular concentration, there are only m-QPCs and then as T increases R will also increase continuously. The fact that only deep inside the metallic regime the overall resistance R increases with increasing T suggests that the density at which R is approximately temperature independent is not the true critical point. The true critical point is deep into the metallic regime. So one should be cautious in associating the temperature independent critical point with the experimentally observed temperature independent point as is done routinely in the experimental interpretations.

This theory does not explain what makes a contact metallic or insulating.

4.5 Synthesis of available information and our proposals

The new result on MIT in 2D disordered systems, which arises by changing the electron-concentration [121], is generally dealt with without reference to the old results [57], where samples with high electron density and considerably low mobility showed localization of all states without any MIT. We take the view that the subject of MIT in 2D systems should be examined in its entirety. The

main question to be settled ought to be whether the old belief, largely generated by the scaling theory of localization [57], that there is no MIT in 2D disordered systems at T=0 is after all correct, or not? Could it be that the validity of the old results was conditional? If so, one should know the conditions clearly besides understanding how a new set of conditions, as in the new experiments [121], gives rise to a metallic state.

We have attempted to piece together a good cross-section of available experimental information and some of the existing theoretical ideas to understand how the insulating state at the high end of electron density changes into a metallic state as the density reduces and how the system enters into an insulating state again at the low end of the density. There seems to be unambiguous evidence that in contrast to the old belief [57], a metallic state does appear in 2D dirty systems. So MIT certainly takes place in these systems. In fact, it happens twice as a function of electron density, once at the high density end and again at a very low density. The insulating phase at high density is due to Anderson localization, whereas the one at the low density end apparently has a different origin. The nature of the intermediate metallic state is interesting too. Our analysis reveals some loose ends which require some more experimentation to be tied up.

4.5.1 Mobility, disorder and screening

Electron density, n_s, and mobility, μ, are the two gross parameters that distinguish the samples in the new experiments from those in the earlier ones. So, starting from the old scenario one should understand how the electron-transport-properties change as n_s decreases and μ increases, say simultaneously. Note that μ is controlled at the stage of preparation of the sample to start with. That is, one can make samples with *intrinsically* high or low mobilities, and the intrinsic factors that control this decide the amount of disorder in the sample. But the

electron mobility μ, in a sample with a given amount of intrinsic disorder, also depends on n_s– it increases with decreasing n_s, reaches a maximum and then decreases again. We will refer to the n_s dependence of μ only in special circumstances. In general the understanding will be that we have to interpolate between the old results in *high* n_s and *high disorder* limit and the new results in *low* n_s and *low disorder* limit.

In spite of the above clarification it should be noted that both the old and the new experiments were *effectively* in the low-disorder regime. In the old samples the high disorder was screened by the high n_s of electrons, so the disorder actually felt by a conducting electron was sufficiently low. In the new samples the screening effect is marginal, but then, the intrinsic disorder is low. Thus, the effective disorder can be assumed to be low more or less uniformly over the whole range of n_s of interest. We should, therefore, understand the *two* MITs in 2D systems mainly as a function of n_s only.

4.5.2 Interaction energy versus Fermi energy

As a function of decreasing n_s the e-e interaction energy, V_{ee}, decreases because the average separation between the electrons increases. But at the same time the Fermi-energy E_F also reduces, i.e. the average kinetic energy E_{kin} reduces. If we look at the decreasing trends of V_{ee} and E_{kin}, we find that while E_F is always larger than V_{ee} at larger values of n_s, around $n_s \simeq 10^{15} cm^{-2}$ it is overtaken by V_{ee} (see fig.(4.6)). This marks an interesting scenario: For $n_s < 10^{15} cm^{-2}$, V_{ee} remains greater than E_{kin} while both keep on decreasing as n_s decreases. From eqn.(4.2) note that in 2D $V_{ee} \sim \sqrt{n_s}$ while E_F has a stronger dependence on n_s, which goes as $\sim n_s$. Consequently, as n_s decreases, V_{ee} becomes stronger *relative* to the faster-decreasing E_F *or* E_{kin}. In fact, as n_s decreases two things happen to V_{ee}: not only does an electron feel its interaction with neighbouring electrons

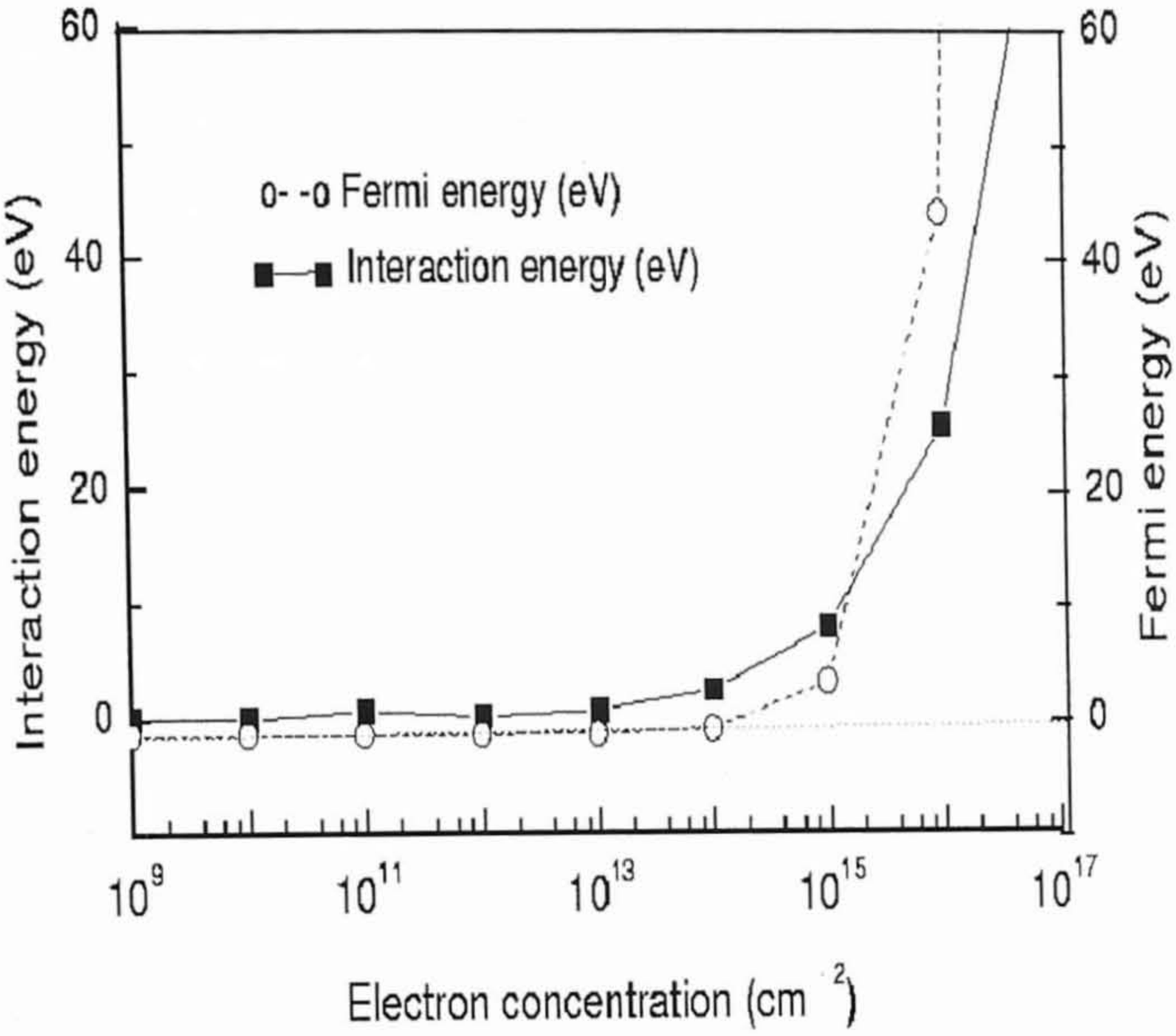


Figure 4.6: Dependence of V_{ee} and E_F on n_s

more strongly, but the interaction also becomes more and more long-ranged. The latter happens simply because of the reduction of the electron population in the medium; as n_s decreases the screening of each electron by the intermediary electrons will reduce. Now if the temperature is also low so that $E_F > k_B T$ we will have an interacting electron system in a practically phonon free environment. All this we find forms an ideal setting for delocalization of electrons mediated by e-e interactions.

4.6 Interaction induced collective hopping leading to new metallic phase

The above quantum correlations among the electrons which are otherwise localized in the Anderson-sense in a medium of random potential suggest that

the Hamiltonian should be,

$$H = H_1 + H_2, \tag{4.7}$$

$$\text{where} \qquad H_1 = \sum_{\alpha} h_1(\alpha), \tag{4.8}$$

represents the one-electron part, and

$$H_2 = \sum_{\alpha\beta} e^2/\kappa_0|\vec{r}_\alpha - \vec{r}_\beta|, \tag{4.9}$$

represents the interaction Hamiltonian. The summation in H_1 is over all electrons, and in H_2 over all electron pairs, κ_0 is the dielectric constant of the medium. In the absence of e-e interactions, $H_2 = 0$ and we have just the Anderson Hamiltonian for a single non-interacting particle in a disordered potential. For H it is necessary to use many-electron wave function, ψ, which can always be represented as a superposition of Slater determinants S,

$$\psi_I = \sum_J A_{IJ} S_J. \tag{4.10}$$

Here I, J denote snapshots of electrons in different positions at different points of time and the co-efficient A_{IJ} gives the overlap between these two configurations. Ideally a complete orthonormal set of one-electron wave functions should constitute the set S. However, for a disordered system with localized states one can use either atomic type wave functions, such as Wannier functions or the solutions ϕ for the non-interacting system. Abrahams and Miller [4] have found the latter to be,

$$\phi_i = \chi_i \pm \sum_{j\neq i} (J_{ij}/\Delta_{ij})\chi_j \equiv \chi_i + \sum_{j\neq i} a_{ij}\chi_j, \tag{4.11}$$

where $\Delta_{ij} = \epsilon_i - \epsilon_j$, the difference between the energies on sites i and j; J_{ij} is the transfer integral and χ_i is a site function localized on site i. The above form of ϕ_i is valid in the Anderson localization regime,

$$J_{ij}/\Delta_{ij} << 1. \tag{4.12}$$

For the typical separation between two localized states $r_{ij} >> a_B$, the Bohr radius, J_{ij} has the form

$$J_{ij} = \epsilon_0 \exp(-r_{ij}/a_B), \tag{4.13}$$

where $\epsilon_0 \sim e^2/\kappa_0 a$ and $r_{ij} = |\vec{r}_i - \vec{r}_j|$.

Note that in the presence of e-e interactions, localization not only requires eqn.(4.12), but also that there exists a dominant A_{II} such that

$$\psi_I = S_I + \sum_J A_{IJ} S_J \text{ with } A_{IJ} << 1. \tag{4.14}$$

When the number of $A's$ are comparably large, we have a delocalized ψ and a continuous current can result, flowing from one macroscopic configuration of electrons to the next.

By a variational method it is found that [4] the amplitudes a_{ij} and a_{ik} of χ_j and χ_k in ϕ_i of eqn.(4.11) are comparable in magnitude if $\Delta_{jk} < J_{ij}$. Pollak and Ortuño [101] proposed in analogy with this condition for delocalization that, for two dominant configurations K and L, $|A_{IK}| \sim |A_{IL}|$ if

$$\Delta_{kl} \equiv |H_{KK} - H_{LL}| < J_{KL} \tag{4.15}$$

where J_{KL} is the many-electron transfer integral.

To understand the onset of correlated electron motion, following Pollak and Ortuño [101], we note the following aspects: (a) The hopping probability of an electron may depend on preceding hops of other electrons in the neighbourhood; (b) several electrons may participate in a single hopping excitation; and (c) as indicated above, correlation in the motion of electrons can be inherent in the many-electron wave functions. To study the transition from one-electron to many-electron hopping transport, first recall the one-electron hopping rate,

$$\nu_{ph} \exp(-2r_m/\xi) \exp(-\epsilon/kT), \tag{4.16}$$

where ϵ is the activation energy for hopping through singly occupied localized states of size ξ; r_m is the percolation distance or the length associated with the critical percolation resistance or the largest resistance R_m in the current carrying percolating network; and ν_{ph} is a typical phonon frequency. Delocalization in a system consisting predominantly of localized states can happen if the latter are connected by hopping events and form a percolative network whose nodes are the localized states. For a given distribution of localized states there will be a largest gap in space that must be covered for the percolation to happen. r_m is this distance in units of Bohr radius a_B.

The above should be compared with the many-electron hopping rate

$$\nu_{ph}\gamma \exp(-2r_m/\xi)\exp(-2\overline{r}/\xi)\exp(-\epsilon-\overline{\epsilon})/kT). \tag{4.17}$$

The first exponential factor reflects the fact that one electron must still jump over the critical percolation distance. As a result of this hop there will be local short-ranged rearrangements of other electrons near the initial and the final sites of the long hop. The second exponential accounts for these short hops with $\overline{r}$ representing the variance of r_{ij}, the separation between localized states. The local rearrangements affect the occupancy of (near by) localized states in a region, and also cause shifts in the locations of electrons in these localized states so as to minimize the energy of a configuration of electrons. This causes relief in Coulomb energy and effects a lowering of the activation energy as represented by the third exponential. γ measures the relative importance or effectiveness of Coulomb interactions over phonons. The transition from one configuration of electrons to the one after the collective hopping of this type is generally referred to as "polaron transition" [46, 47]. Often a number of electrons hop comparable distances. These are called "cascade transitions" [79] and presumably happen far away from the threshold of many-electron hopping [38, 46, 67, 79].

At low temperatures ν_{ph} in eqns.(4.16 & 4.17) becomes irrelevant and can be

dropped without affecting the plausibility of the physical phenomenon described above. Experimentally it has been shown explicitly by Marnieros et al. [160] that at sufficiently low temperatures e-e interactions alone can cause variable-range hopping transport which can be independent of phonon distribution. By comparing eqns (4.16) and (4.17) the following conditions are obtained for one-electron and many-electron hopping [101]:

$$\gamma \exp\left(-2\overline{r}/\xi\right) \exp\left(\overline{\epsilon}/kT\right) < 1 \Longrightarrow one-electron\, hopping; \quad (4.18)$$

$$> 1 \Longrightarrow many-electron\, hopping. \quad (4.19)$$

That is, the transition from one process to the other happens when

$$-2\overline{r}/\xi + \overline{\epsilon}/kT + \ln\gamma = 0 \quad (4.20)$$

Taking $\overline{\epsilon}$ to be a fraction of the typical Coulomb energy and $\overline{r}$ as fraction of the typical separation between the electrons, one can find that the transition from one-electron to many-electron hopping should happen if,

$$\xi e^2 n_s > kT\kappa_0. \quad (4.21)$$

That is, if the density n_s is decreasing, then T should also reduce for e-e interactions to dominate and cause many electrons to hop collectively. One can also compute the electron concentration for the onset of many-electron quantum correlation effects [101]. In 2D it turns out to be of the order of $(\pi\overline{r}^2)^{-1}$ i.e. less than $10^{15} cm^{-2}$, in agreement with the threshold value below which V_{ee} exceeds E_F or E_{kin} as is seen in fig.(4.6).

4.6.1 Coulomb gap

Another consequence of the fact that long-range interactions among electron are important in the present context is the formation of the so called 'Coulomb gap' – a deep depletion of one particle DOS near the chemical potential [39]. Due

to Coulomb effects, one-electron hops near chemical potential inevitably involve a non-zero excitation energy which measures the Coulomb gap. It naturally has implications on the electrical conduction [162]. For instance, Efros and Shklovski [37] argue that the T dependence of variable-range hopping resistivity should get modified as $\exp(T^{-1/2})$ as opposed to Mott's law of $\exp(T^{-1/4})$.

It is of interest for us to understand the dependence of Coulomb gap on n_s and quenched disorder in the system. The gap is proportional to V_{ee} and is inversely proportional to the dielectric constant. The decreasing n_s reduces V_{ee} and consequently the gap reduces. Similarly, decreasing disorder increases the dielectric constant and decreases the gap. Thus in the systems of our interest the Coulomb gap should be very small due to low concentration of electrons and high mobility in samples. This should ease the conditions for electrical conduction.

Thus it is our understanding that starting from the old situation of Anderson type insulating phase, if n_s is reduced, then below $n_s \simeq 10^{15} cm^{-2}$, the system enters the phase where V_{ee} begins to dominate over phonons as well as impurity scattering (due to the low T and disorder), and a metallic phase is produced due to delocalization by the V_{ee} instigated collective hopping of electrons. One should not deduce from the last paragraph above that the conditions would improve indefinitely for conductance if n_s kept on reducing. The disorder and its continuously reducing screening, and the ever increasing dominance of V_{ee} over E_F again change the scenario to suit a very strong insulating phase as we argue in the following.

4.6.2 Mobility revisited

Besides being exhibited in terms of n_s and T dependence of resistance [121], the new insulating phase and the MIT have also been seen in terms of sudden drop in electron mobility [106] and a change of sign of the electronic compressibility

[156]. The latter two studies give insight into the microscopic nature of the new insulating phase.

Interestingly, a clear signature of a strong insulating phase at very low n_s was found by Jiang et al. [106] way back in 1988, well before the Kravchenko et al.'s [121] discovery. They found that mobility dropped much faster than that

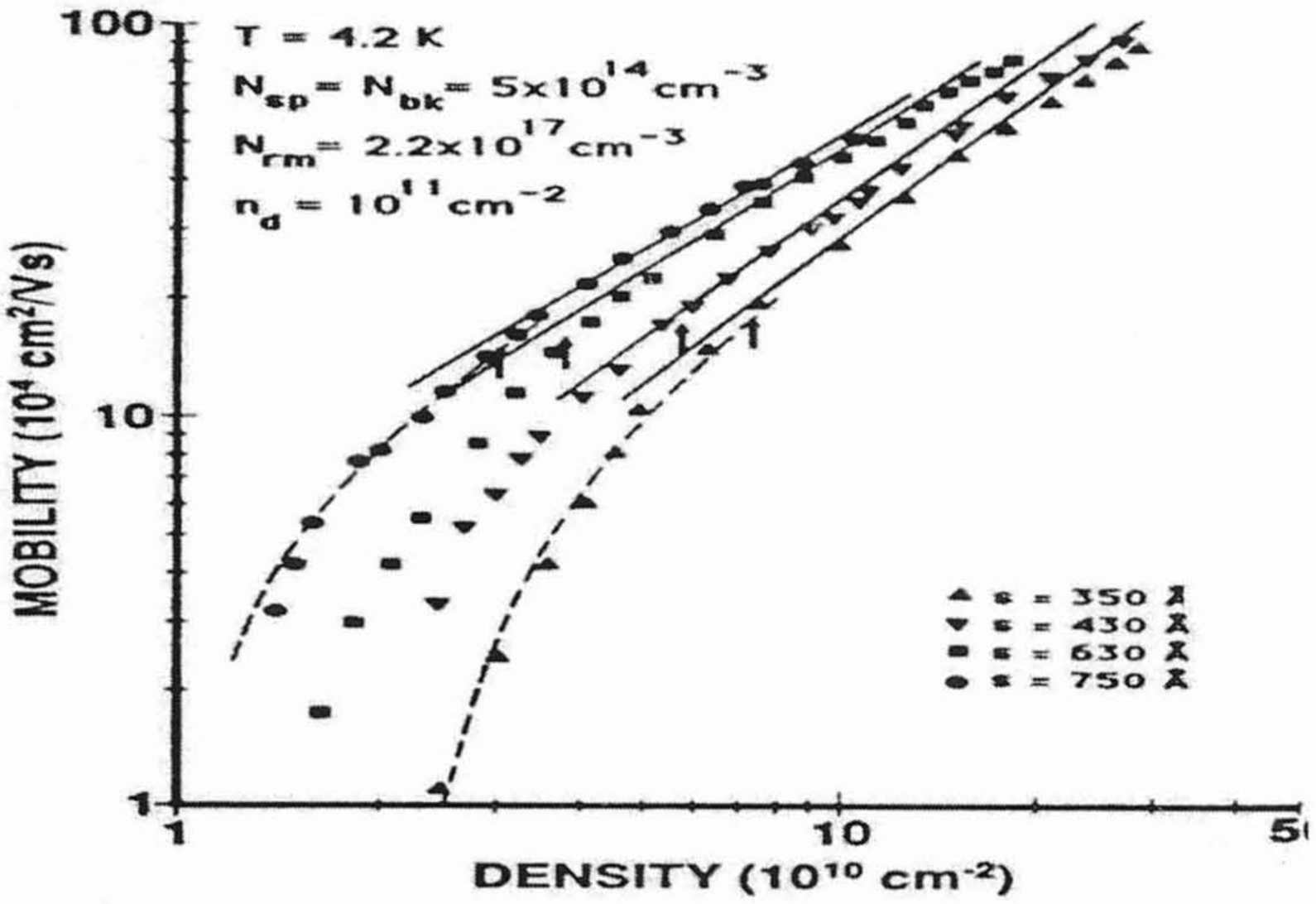


Figure 4.7: Mobility versus electron density. The arrows indicate the densities at which mobility drops faster than linearly for different concentrations

expected from impurity scattering for n_s below a characteristic density n_c, typically around $7 \times 10^{10} cm^{-2}$. For $n_s > n_c$, the mobility increases linearly, which is indicative of metallic behaviour. Thus n_c marked a transition from a metallic state to an apparently insulating state of rapidly decreasing mobility. The n_c was found to decrease with the increasing spacer thickness in GaAs/AlGaAs heterostructures at temperatures $\sim$ 4K. The rapid decrease in mobility is attributed to the fluctuations in the density n_s, the effect of which is apparently felt stronger with thinner spacers. That is the fluctuations need to be stronger to be felt in thicker layers, hence *perhaps* lower n_c. It is however not entirely clear as to why

n_c ought to be smaller for thicker spacer layer. Jiang et al. [106] found metallic behaviour (i.e. linear increase of mobility with n_s) for n_s as low as $1.4 \times 10^{10} cm^{-2}$.

4.6.3 Thermodynamic property– Compressiblity

The rapid density-fluctuations were investigated in great detail by Ilani et al. [156] in very sensitive experiments using single-electron transistors above 2D hole gas in GaAs/AlGaAs heterostructures. Measuring chemical potential c as a function of n_s they investigated electronic compressiblity, dc/dn_s with n_s changing around n_c. Compressiblity is related with the ability of an electronic system to screen a charge brought from outside to a close proximity of the 2DHG. Mobile electrons accumulate in its vicinity to screen it. If the electrons happen to be localized, they will not be able to move and thereby screen the charge. So, a system, which cannot redistribute its charge, is considered to be incompressible. These measurements indeed showed that the electron system was strongly fragmented (i.e. highly non-uniform distribution of electrons) when it was in the incompressible state. The ν is found to increase as n_s decreases on the metallic side. This *negative* compressibility reaches a maximum and then begins to decrease. This marks the transition to an insulating phase. Dultz and Jiang [155] found that the insulating phase remains incompressible over entire range of magnetic field B. In fact n_c increases as B increases, as one would expect.

4.6.4 Breakdown of screening

The breakdown of screening at low values of n_s was also studied by Wilamowski et al. [164] around the MIT in modulation doped Si/SiGe quantum wells using conduction electron spin resonance (CESR) in a temperature regime, $kT << E_F$. In this limit the 2DEG exhibits Pauli paramagnetism, so that the magnetic susceptibility χ_m is proportional to the DOS at E_F, $D(E_F)$, which in turn is proportional to the Thomas-Fermi screening wave-vector q_{TF}. Thus

CESR measures q_{TF} and it is found to be constant upto $n_s \sim 3 \times 10^{11} cm^{-2}$ (with decreasing n_s) as one expects in 2D systems. For smaller values of n_s, q_{TF} drops somewhat gradually to become zero at $\sim 7 \times 10^{10} cm^{-2}$. This divergence of screening length (q_{TF}^{-1}) marks an insulating phase (fig.(4.8)). In these experiments screening does not pertain to that of an external charge but refers to the partial shielding of the random potential by the electrons inside the system from being felt by the conducting electrons. That the screening wave-vector should

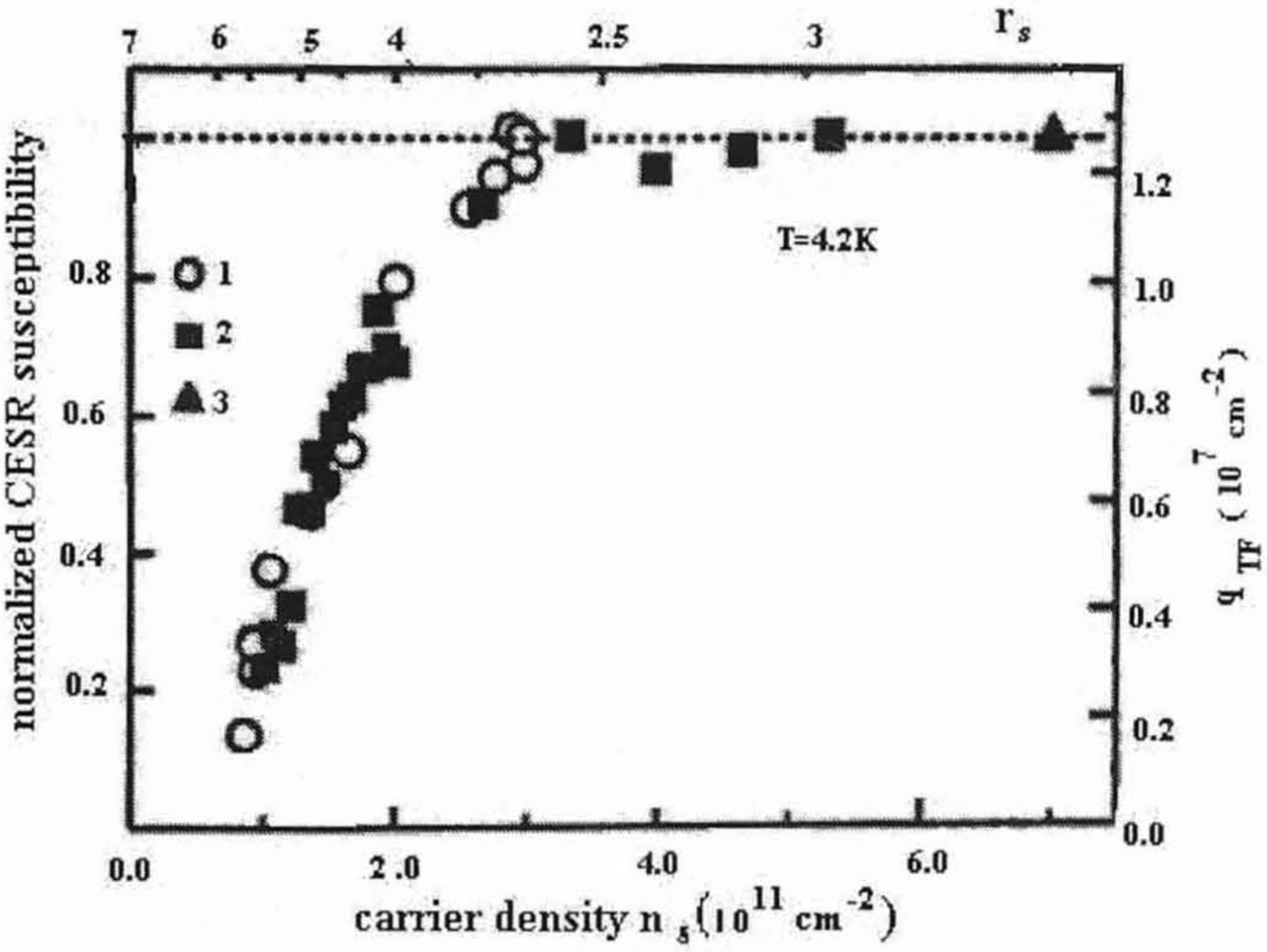


Figure 4.8: Screening length vs concentration

be a constant in 2D systems as a function of n_s is a result of the Thomas-Fermi theory which employs free electron approximation according to which the density of electron states should be a constant as a function of energy. Wilamowski et al.'s [164] data indicate that the Thomas Fermi approximation remains valid up to n_s value as low as $3 \times 10^{11} cm^{-2}$. This might appear somewhat surprising because as we have argued earlier, e-e interactions play important role at such low

densities. But recall, in the absolute sense e-e interaction actually gets weaker as n_s decreases; at very low n_s it gets stronger only relative to E_F, which decreases more rapidly than V_{ee} with n_s. The weakly interacting electrons can be treated as free (or nearly free) if the disorder is also very weak, which incidently is the case in the samples of our interest here because the mobility is very high in them.

For $n_s < 3 \times 10^{11} cm^{-2}$ the q_{TF} falls monotonically [164], i.e. the screening length increases. The diminishing q_{TF} indicates reduction of compressibility of the electron system. That is the electrons are becoming more and more rigid in their movement which happens if they are getting localized. There are two possible scenarios: (a) with reduction of screening the disorder is felt more, which can lead to greater localization in Anderson's sense; or (b) the n_s goes below the percolation threshold and electrons get localized in isolated packets, or clusters.

4.6.5 Sub-percolation threshold region

Wilamowski et al. [164] believe in (a) and argue that around $n_s \simeq 7 \times 10^{10} cm^{-2}$, when q_{TF} vanishes and screening length diverges, the amplitude of potential fluctuation δV, felt by the electrons, diverges. We don't find it convincing because a diverging δV would imply an infinite quenched disorder in the system, which is in sharp contrast to the fact that the samples under study have very high mobility and therefore very weak intrinsic disorder. We are therefore of the view that below $n_s \simeq 3 \times 10^{11} cm^{-2}$ the scenario (b) comes into play. Just below this value of n_s the system will get divided into large fragments of 2DEG. The fragmentation will increase as n_s decreases. Visualizing the fragments as lakes in a rugged terrain of fluctuating potential with the E_F defining the surface of the lakes, we see that with decreasing n_s as E_F goes down the lakes become smaller and less deep. Tunneling events that may occasionally connect them will also reduce with the increasing separation between the lakes. This will result in the

electron system becoming more and more rigid or less compressible.

We can consolidate on this scenario by recalling the parameter $r_s = V_{ee}/E_F \propto 1/(a_B\sqrt{\pi n_s})$ [110] and introducing an $r_d = e\delta V/E_F$ (following [164]) which measures disorder, relative to E_F or E_{kin}. We have seen that with decreasing n_s, E_F decreases faster than V_{ee}, and therefore r_s increases. This has vital implications in making e-e interactions more and more relevant in spite of getting weaker. With decreasing n_s, r_d also increases because (i) E_F decreases; and (ii) more and more of *actual* δV is felt by electrons as the screening weakens. Since the bare (or unscreened) δV is small, at a particular small value of n_s the r_d will exceed r_s, because in

$$\frac{r_d}{r_s} = \frac{e\delta V}{V_{ee}}, \tag{4.22}$$

the δV cannot increase beyond its bare value but V_{ee} keeps on reducing with decreasing n_s. At this value of $n_s = n_s^c$ (say) the disorder effects, howsoever weak they may be, will dominate over e-e interaction effects. In this limit the delocalizing effects of e-e interaction will become ineffective and the electrons will be strongly localized in very narrow regions of space. Note that the electrons will be localized by the finite and small extents of the lakes or more appropriately 'puddles' (since at n_s as low as n_s^c the regions that confine electrons will be very small in extent as well as depth) rather than by quantum interference effects that cause Anderson localization. The crossover point, $r_d < r_s$, we suggest, will be at $n_s = n_c$ and will mark the MIT; this should coincide with the breakdown of screening (i.e. $q_{TF} = 0$, or $q_{TF}^{-1} = \infty$) and compressibility.

We suggest that this insulating phase should be a Wigner glass. When $r_d = r_s$, the disorder and interaction effects together pin the electrons down to the randomly distributed puddles. Further reduction of n_s below n_c shrinks the puddles more and makes the pinning stronger. If one could control δV and reduce it, the MI transition point would shift to a lower value of n_c because $r_d/r_s = 1$

would require a smaller V_{ee}, i.e. r_s would be larger. Thus Wigner crystal would correspond to a much larger r_s than that required by Wigner glass.

4.6.6 Summary

In sum, we propose that there are two MITs in 2D disordered systems. Starting from the *high* n_s and low mobility end, which corresponds to the old experiments, we interpolate between this end and the other one with *low* n_s and high mobility. The insulating phase at the *high* end, characterized by $r_s << 1$, is the same old Anderson insulator. If we continuously reduce n_s and increase the *intrinsic* mobility, at one point r_s will exceed 1 (around $n_s \sim 10^{15} cm^{-2}$) and e-e interactions will dominate over E_{kin} and a metallic phase should result due to delocalization from Anderson localized states by collective electron hopping. Such a metallic state should persist as r_s grows with decreasing n_s. The $r_s = r_d$ should trigger the second insulating phase, which we argue should be a Wigner glass state. In fact, the *low* end MIT should be a continuous one; it ought to build up gradually from $n_s \simeq 3 \times 10^{11} cm^{-2}$ downwards.

While there are many experiments in the region of *low* end MIT, experiments are required near the *high* end, say around $n_s \sim 10^{15} cm^{-2}$ to check how the metallic state evolves from the Anderson insulator as n_s is reduced.

4.6.7 MIT at non-zero magnetic field

Curious observations have been made about the similarities in the nature of MIT at low n_s in the absence of magnetic field ($B = 0$) and that of the MIT in the quantum Hall effect (QHE) setting when there is a strong magnetic field (B) perpendicular to the 2DHG systems [139]. The similarities might indicate some commonalities in the underlying physics of the MITs in $B = 0$ and $B \neq 0$ situations. For one thing, it is indicated that the two MITs are quantum phase transitions in that they happen when the system is in a degenerate state

[152, 165].

The most intriguing feature in Hannien et al.'s [139] experiment is the initial decrease of n_c with increasing B. This means that some of the states that are localized (for $n_s < n_c$) at $B = 0$ gets delocalized when B is switched on and hence n_c^B is pushed below $n_c^{B=0}$. We have two plausible explanations for this surprising result. First, at $B = 0$ and $n_s < n_c$, besides the confinement within the boundaries of the randomly scattered small puddles, there could be a novel weak-localization due to quantum interference over a cluster of puddles – an electron may tunnel through a set of suitably placed puddles and make a closed trajectory; the time-reversed paths through these puddles may interfere constructively and give rise to a weak-localization. This will be destroyed due to breaking of time-reversal symmetry as soon as B is introduced and we will have some delocalization due to variable-range hopping. So, now when B is non-zero, the MIT will happen at a smaller n_c. Note that as n_c reduces, due to non-zero B, the average puddle-size would also reduce and the average spatial gap between them will increase. This will make the tunneling between them more difficult and therefore less probable. It remains to be understood how the decreasing trend of $n_c(B)$ with increasing B comes about; how it saturates at a minimum value of n_c; and finally why at higher values of B the MIT happens at larger n_c's. Clearly, both B-induced delocalization as well as B-induced localization are involved in the QHE regime [137] in giving rise to the observed $n_c(B)$ behaviour [139]. The B- induced localization can be better understood in the following picture.

Note that in the presence of magnetic field the electron wave function assumes a tubular shape. Such a tube-like wave function, whose width is twice the cyclotron radius, spreads along the equipotential lines that mark the boundaries of the puddles. At low n_s and non-zero B only the lowest Landau levels (LLL's) are filled and since B is small, the LLs overlap considerably and the cyclotron orbits

are large, so that the cross-section of tubular wave functions is large. As a consequence of the latter there will be large scale overlap of wave functions spreading around the peripheries of the puddles. This will result into a lot of quantum interference which will cause both localization and delocalization. The possibility of delocalization will reduce n_c but the possibility of localization will not allow it to become too small. As B increases and tubular wave functions shrink and their mixing will reduce and will be restricted more to the nearby energies. While the mixing of wave functions on neighbouring puddles helps delocalization the reduction in widespread mixing reduces the chances of localization by quantum interference. Thus we can imagine delocalization in a more channelized manner with reducing possibilities of localization by interference. This will reduce n_c with increasing B. A minimum will be reached with decreasing overlap of wave functions on neighbouring puddles. As the wave function shrinks closer to the boundaries of the puddles and delocalization effects due to overlap of wave functions reduce, the MIT can happen at relatively larger puddles, i.e. higher n_c. Thus, in this picture (in which the earlier picture of 'weak-localization' is, in a way, also included) we can account for the $n_c(B)$ behaviour qualitatively.

We can conclude that the zero-field density-driven MIT and the MIT in the QHE setting share the common feature that both involve transition to insulating states that arise due to breakdown of percolative type delocalization. Both the MIT's are quantum phase transitions too.

4.6.8 Two allied results

Finally we will address two more fine observations in the experimental results. They both pertain to the metallic phase, i.e. $n_s > n_c$. The resistivity (ρ) measurements of Hanein et al. [135] show that at the lowest temperatures in their experiments the ρ showed a tendency to saturate or flatten out to a constant

value or a very weakly temperature - dependent value rather than decrease indefinitely; see fig.(4.9). That is the metallic phase does not approach an ideal metallic state or a superconducting state as in [138]. This result is important for one can argue that it is possible that after an initial levelling off, the ρ might begin to rise at much lower temperatures and it may turn out that the newly discovered metallic phase is in fact an insulating phase which requires extremely low temperatures to show up. It will require very careful experimentation at very

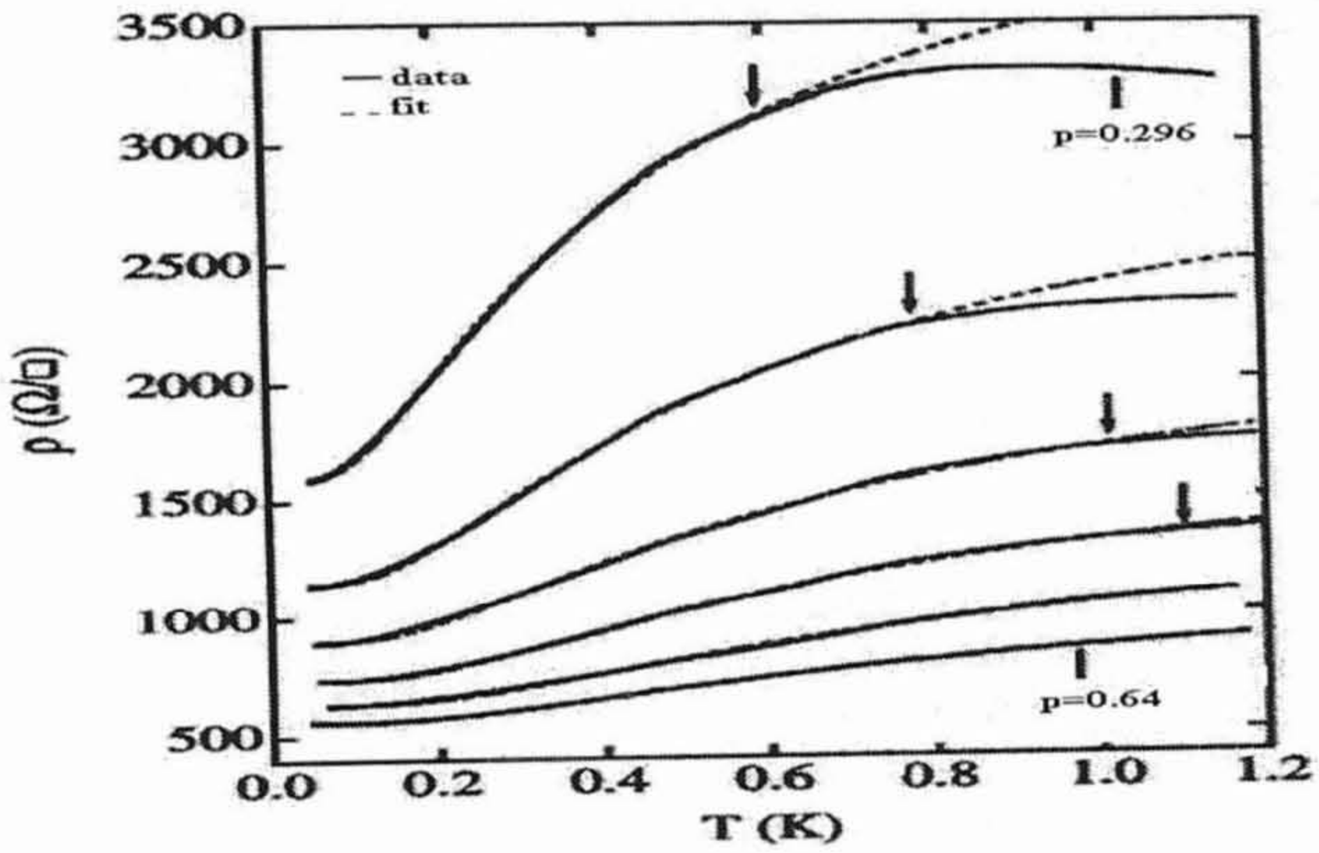


Figure 4.9: Support for the saturation of resistivity

low temperatures to resolve this issue, but on the basis of the available information if we believe that the metallic phase is indeed metallic and that ρ saturates at very low temperatures, then we suggest that the saturation of ρ could be due to the presence of two-level systems (TLSs) [170]– TLSs provide the dominant source of inelastic scattering at very low T, moreover the tunneling in them becomes incoherent because of TLS-TLS interactions which become more and more prominent as $T \to 0$; both these factors can make the phase of the electron wave function saturate to a T–independent value. This will restrict the ρ from going to zero in the $T = 0$ limit.

The above argument of phase decoherence should be understood carefully because if the saturation of phase coherence time is a real phenomenon [170] then it might also indicate the absence of weak localization, which will strengthen the states of the metallic phase in 2D disordered electron systems, besides supporting the saturation of ρ.

Another important experimental observation due to Hanein et al. [135] is shown in fig.(4.10). The interesting thing about this result is that on the metallic side, in the vicinity of the MIT the ρ increases as T decreases, reaches a maximum and then begins to drop at lower T. The last one is particularly intriguing since it indicates that an otherwise insulating behaviour turns metallic by the lowering of T. Again it seems likely that the saturation of phase-coherence time (and length) for $T \to 0$ is important in this connection. According to the percolation picture [115] just above n_c on the metallic side there will be an infinitely connected channel, i.e. a lake open at at least two ends. This will have a highly ramified and tortuous structure; in fact it will be a fractal [115]. This structure makes the electrical conduction very slow and diffusive and gives rise to a high

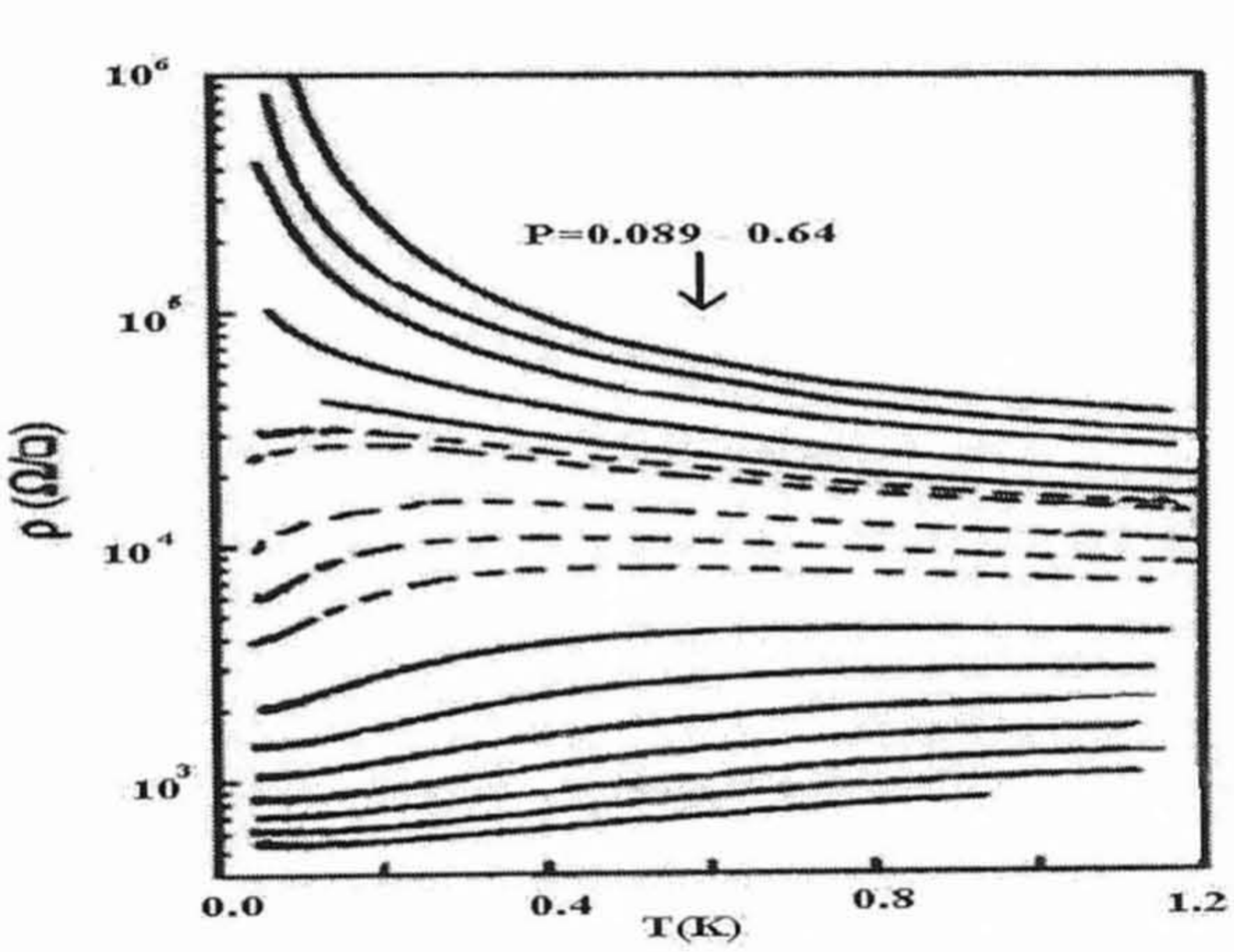


Figure 4.10: Resistivity vs temperature for various concentration

resistance. Consequently, as T decreases ρ should increase. However, as $T \to 0$ phase-decoherence also sets in, i.e. the phase-coherence time τ_ϕ as well as the length L_ϕ tend to saturate to constant values. Since this limits the quantum interference, it give rise to delocalization. Thus as $T \to 0$, two competing phenomena happen – on one hand resistance in the conduction channel increases due to its tortuous structure, but on the other hand conditions also become favourable for delocalization to some extent due to the saturation of phase-coherence. This competition should give rise to a peak in the $\rho - T$ behaviour. The observed peak fig.(4.9), we suggest, has its origin in this competition.

Chapter 5

THE MINIMUM METALLIC CONDUCTIVITY

5.1 Introduction

Most part of our work deals with metal-insulator transitions (MIT). The question that naturally arises in this context is whether the transition is of first order or second order. A first order transition is one where a discontinuous change in the order parameter occurs at the (transition or) critical point. The order parameter in the case of metal to insulator transition is the conductivity σ.

It has been a long standing problem as to whether the M-I transition driven by disorder is first or second order. Or put in another way whether or not there exists a minimum value of conductivity, namely σ_{min}, on the metallic side just before the transition happens to the insulating phase.

The concept of σ_{min} was introduced by Mott [11] in connection with Anderson localization. Mott was of the view that the MIT across the critical energy termed as the mobility edge E_c, the concept of which emerged from the Mott-CFO model [13, 14], ought to be a discontinuous one, i.e. a first order phase transition. Though there were some experiments in favour of this proposal [45] later experiments [84] proved it to be wrong except in certain special circumstances, e.g. in the presence of magnetic field. In this chapter we focus on the general problem of vanishing of σ_{min} in MITs in disordered systems including the MIT driven by the variation of carrier concentration.

By examining the basic definition of localization in terms of poles and branch-cuts of Green's function we look at the consequences of the co-existence of poles and branch-cuts in a section of the spectrum of electron states [111]. Accordingly

we propose three sections in the spectrum: point spectrum corresponding to the poles of the Green's function, continuous spectrum represented by the branch-cut of the Green's function and a singularly continuous spectrum where poles appear inside the branch-cut. We have defined each part of the spectrum in terms of the stay-put probability and its time integral and propose that if the intermediate, singularly continuous, spectrum exists and separates the localized and extended regimes then σ_{min} will be zero and MIT will be continuous.

5.2 Mott-CFO model

Anderson treated the diffusion of electrons in random lattices, i.e. the problem of localization and delocalization of an electron in a medium of random potential in terms of the convergence and divergence of a renormalized perturbation expansion of self energy. It has also been cast in terms of Green's function having simple poles or branch cuts along the real energy axis with the poles corresponding to a discrete set of localized states and the branch cuts to the continuum of extended states [2, 27]. Anderson worked out a critical value of disorder above which the states at the middle of the band, and by inference all the states in the band, are localized.

Mott later on considered this problem for disorders less than the above critical value. He proposed that for disorders less than the critical value, both localized and extended states would be present in the system and that there would be a particular energy, called mobility edge E_c, which would separate the localized states from the extended states. This energy E_c would depend on the degree of randomness. Cohen, Fritzsche and Ovshinsky also arrived at the same picture in their model for amorphous semiconducting alloys. Thus the model, in which extended states exist in the middle of the band and localized states at either ends of the band, is termed as Mott-CFO (MCFO) model.

According to the MCFO model, the regime of exponentially localized states tailing deep into the band gap and the extended states at the center of the band are separated sharply from one another by a pair of energies called the mobility edges E_c and E_c'. This indicates that the simple poles of the Green's function lie on either sides of the cut and that the poles and the branch-cut do not overlap as is shown in fig.(5.1). Mott suggested that the transition from delocalized

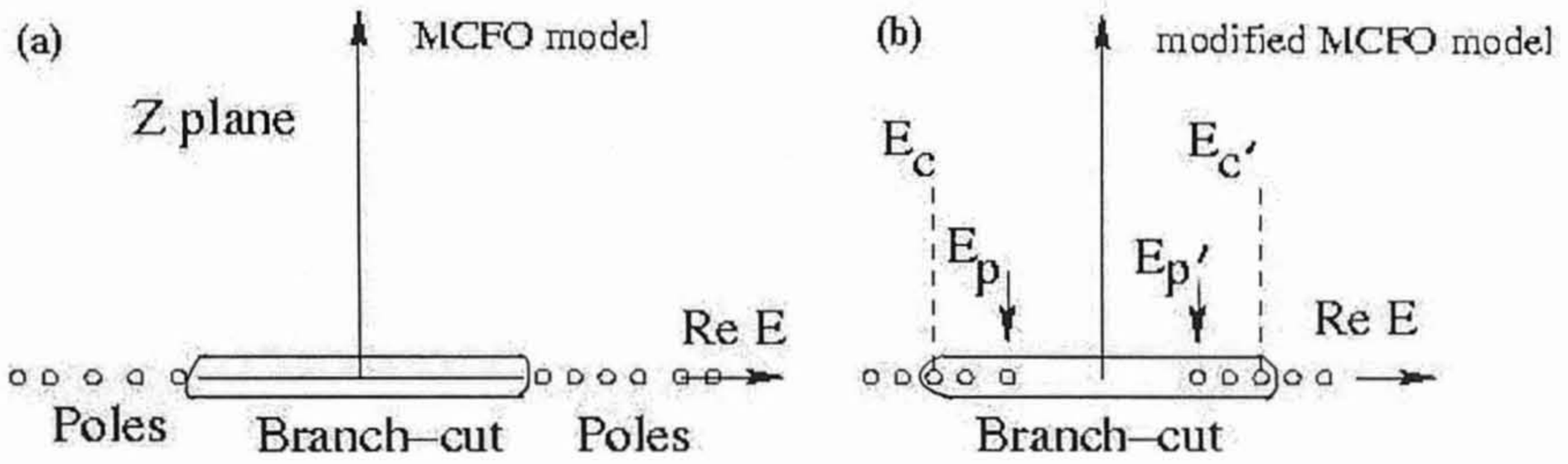


Figure 5.1: Branch-cuts and poles of the disordered Green's function

states to localized states should be sharp in that the conductivity should attain a minimum value, called the minimum metallic conductivity, σ_{min} at E_c before becoming zero on the localized side. This minimum value of conductivity appears as a pre-factor in the expression for the hopping conductivity in the vicinity of E_c,

$$\sigma = \sigma_{min} \exp\left(-(E_c - E_F)/kT\right) \tag{5.1}$$

where E_F is the Fermi energy, E_c the mobility edge and k the Boltzmann constant. As $(E_c - E_F) \rightarrow 0$, $\sigma \rightarrow \sigma_{min}$. Mott's calculation of σ_{min} is as follows:

5.3 Mott's calculation of σ_{min}

From Kubo-Greenwood formula for the conductivity

$$\sigma \propto |D|^2_{av}\{N(E_F)\}^2\,, \tag{5.2}$$

$$\text{where,} \qquad D = \int \psi_1^* \frac{\partial}{\partial x}\psi_2\, d^3x\,, \tag{5.3}$$

gives the transition between states ψ_1 and ψ_2 or the overlap between them.

$$|D|^2 = \frac{\Omega}{v}|\delta|^2\,; \quad v = \frac{4}{3}\pi l^3. \tag{5.4}$$

where l is the length over which the phase memory lasts, so v represents the volume over which ψ retains the phase memory and Ω is the volume per electron; and δ represents the overlap of the phase coherent regions. Note that

$$\begin{aligned}\delta &= \int_v \psi^*_{k'} \frac{\partial}{\partial x}\psi_k\, d^3x \\ &= \frac{1}{\Omega}\int_v \exp\{i(k-k').r\}\, d^3x \\ &= kv/\Omega\,, \text{ if } kl\theta < 1 \\ &= 0 \qquad \text{otherwise}\end{aligned} \tag{5.5}$$

Here θ is the scattering angle. Averaging over all angles θ between 0 & $1/kl$

$$|D|^2_{av} = \pi a/3\Omega$$

Taking Ioffe-Regel limit, $l \sim a$ and substituting in eqn.(5.2) we get

$$\sigma_{min} = \frac{0.03e^2}{\hbar a} \approx \frac{610}{a}\, ohm^{-1}cm^{-1} \tag{5.6}$$

where a is the average inter-atomic distance.

The questionable assumptions that have gone into this result are

- the phase of the wave function fluctuates from site to site and
- the wave function is treated as a plane wave even near the E_c

Experiments in the 1970's [45] showed good agreement with the value in eqn.(5.6). Computer simulations by Licciardello and Thouless [44] for 2D systems showed a constant value of $\sigma_{min} = 0.16e^2/\hbar$ for all 2D systems.

However experiments in 1980's [84] done under better experimental conditions (i.e. lower temperatures) gave a contradictory result in that there existed no σ_{min}. These experiments show that the conductivity σ approaches zero, as $E \rightarrow E_c$ from the extended side almost linearly indicating a second order phase transition.

5.4 Modified MCFO model

The experimental results in the 1980's tentatively indicate that there could be a transition point E_p below which $\sigma(E)$ becomes almost linear in range (E_p, E_c) which is different from the behaviour typically exhibited by extended states that exist in the range E_p and E_p'. Before going into the details of the nature of the states in the vicinity of the mobility edges on the extended side which has already been studied in [111] we first analyze some of the issues that are involved in this problem.

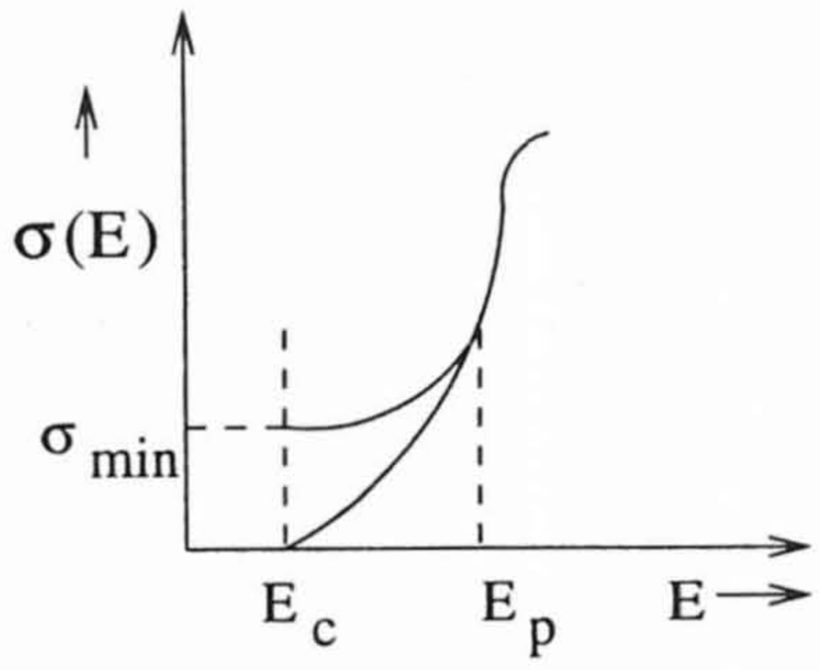


Figure 5.2: Conductivity vs energy plot showing σ_{min}

5.5 Issues involved

1. The conventional transport theory holds when $k_F l \gg 1$ i.e. $l \gg a$ where l is the length over which the phase memory in the wave function lasts and a is the inter-atomic distance. Perturbation theory can be used for calculating the disorder induced corrections to the conductivity. But this breaks down when $k_F l \lesssim 1$ i.e. $l \leqslant a$ (Ioffe-Regel criterion)[5]. As emphasized by Mott [59] localization effects start to set in when $l \sim a$.

   Thus it is more appropriate to start with localized states even though the full effect of localization would not have set in when $l \sim a$. More specifically, a plane wave like approximation for the wave function in Mott's calculation of δ in eqn.(5.7) will not be good in this region of the spectrum.

2. In the case of second order phase transition, the transition from one phase to another is characterized by the divergence of a characteristic length as the transition point is reached from either side. Hence if MIT is a second order phase transition this criterion should hold. It is well known that as E_c is approached from the localized state, the size of the localized state, $l \to \infty$. But the characteristic length which would diverge when E_c is approached from the side of the extended states above E_c remains unknown.

3. One possible reason for the observation of σ_{min} in the earlier experiments [45] could be the fact that those experiments were done at higher temperatures compared to the extremely low temperatures of the newer ones [84]. At relatively higher temperatures the inelastic scattering may have increased the conductivity. In the energy range where the states are localized or pseudo-localized the phonon-assisted hopping can help in the conduction process thereby showing residual conductivity. This residual conductivity might have been mistaken for σ_{min} in the earlier ones. If so, we also learn

that in the energy range (E_p, E_c), in the vicinity of E_c where the newer experiments show lower σ compared to the older results (fig.(5.3)), the states may be 'pseudo-localized'.

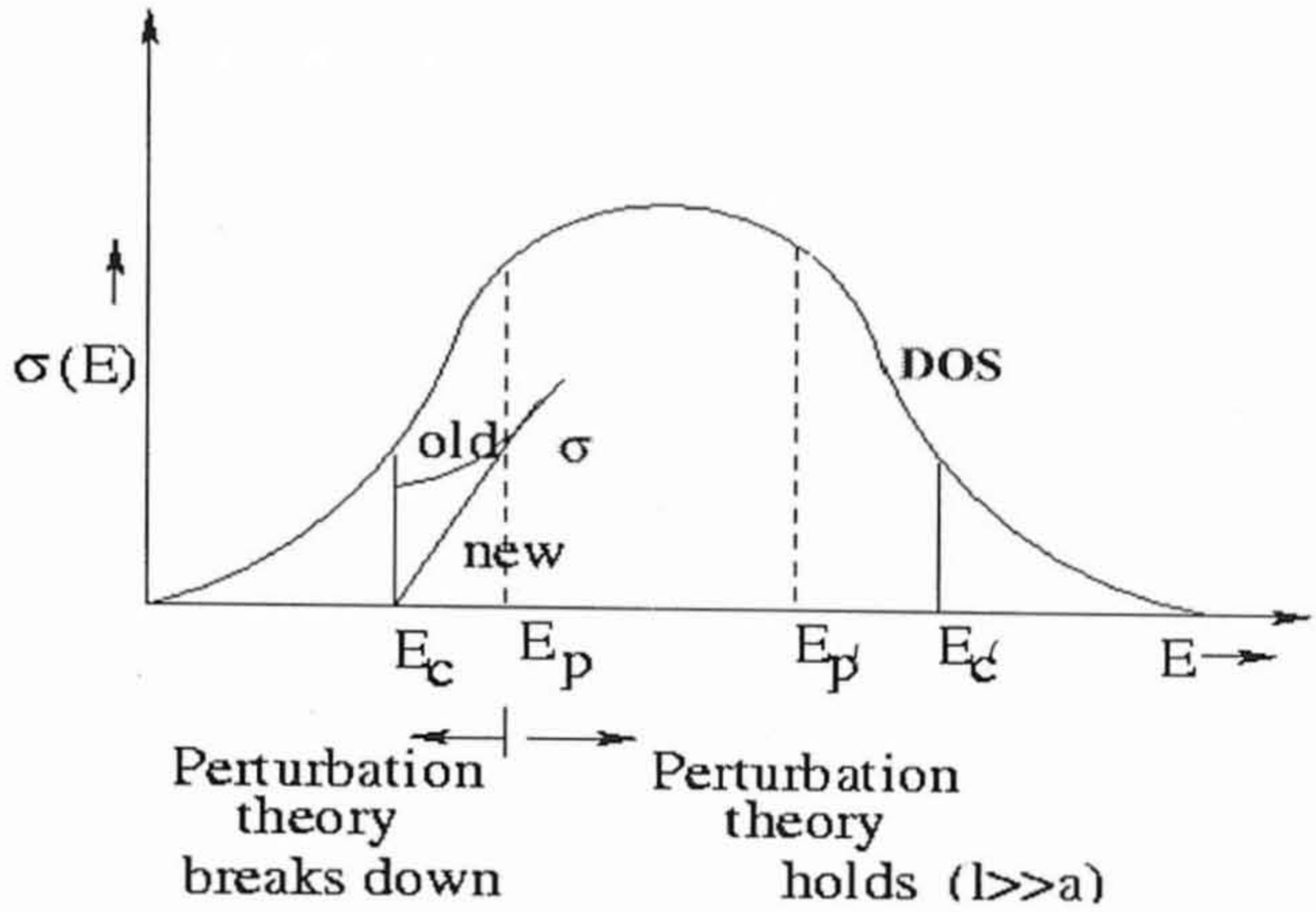


Figure 5.3: Conductivity vs energy

4. The wave function in the region (E_p, E_c) may be a 'fractal' so far as the variation of its phase is concerned. That is, instead of the phase fluctuating from site to site as is commonly assumed, the phase may fluctuate over larger length scales and the magnitude of the fluctuation may be different at different length scales.

In the next section we discuss a new proposal for the nature of the extended states that exist near E_c and study how the above mentioned issues are accommodated into it.

5.6 Precise definition of localization

One way to decide about the localizability of the eigen state is to consider what happens to a particle which is initially localized in a certain region of space

as its environment changes. The presence of localized eigen states in the neighbourhood of the region considered leads to a finite probability for the existence of the particle considered in any one of the localized states. Since the particle can in principle return to the original state there will be a finite probability of rediscovering the particle at the initial region as $t \to \infty$. But if there are a few extended states in the neighbourhood of the region considered, the particle will diffuse away and the probability of its being felt in the initial region will approach zero as $t \to \infty$. Thus following Anderson, the criterion for the nature of the eigen state is the behaviour of the probability of rediscovering the particle in an initially $(t = 0)$ localized state as $t \to \infty$. This stay-put probability, denoted by $P_a(t)$, which is the probability of rediscovering a particle at an arbitrary site 'a' at time t if initially (at $t = 0$) it was there with probability unity can be written in terms of Green's function $G_{aa}(E \pm is)$ as

$$\lim_{t\to\infty} P_a(t) = \lim_{s\to 0}\left[\frac{s}{\pi}\int_{-\infty}^{\infty} G_{aa}(E+is)G_{aa}(E-is)dE\right] \tag{5.7}$$

where

$$G_{aa}(E+is) = \left\langle a\left|\frac{1}{E+is-\hat{H}}\right|a\right\rangle$$

in the complex energy space. Eqn.(5.7) can also be written as

$$P_a(t) = \int_{-\infty}^{\infty} f_0(E)dE \tag{5.8}$$

where

$$f_0(E) = \lim_{s\to 0^+}\frac{s}{\pi}G_0(E+is)G_0(E-is) \tag{5.9}$$

is a non-negative quantity. The Green's function can be expressed in terms of self energy as

$$G_{00}(E \pm is) = \left[\frac{1}{E \pm is - e_0 - \Sigma_0(E \pm is)}\right] \tag{5.10}$$

where Σ_0 is the self energy and e_0 is the potential offered by the region '0' (the region under consideration is represented as '0'). Using eqn.(5.10) and the relation

$$n_0(E) = \frac{1}{\pi} \lim_{s \to 0^+} ImG_{00}(E - is) \tag{5.11}$$

for the DOS, $f_0(E)$ can be written as

$$f_0(E) = n_0(E) \lim_{s \to 0^+} \frac{1}{1 - \left[\frac{\Sigma_0(E+is) - \Sigma_0(E-is)}{2is}\right]} \tag{5.12}$$

From eqn.(5.12) we see that for $f_0(E) \neq 0$ one should have either

$$n_0(E) \neq 0, \tag{5.13}$$

or

$$Z_0(E) = \lim_{s \to 0^+} \frac{1}{1 - \left[\frac{\Sigma_0(E+is) - \Sigma_0(E-is)}{2is}\right]} \neq 0 \tag{5.14}$$

We know that the extended states do not contribute to $P_a(t)$ and consequently for extended states $f_0(E) = 0$ which implies that $Z_0(E) = 0$. Thus if $Z_0(E) \neq 0$, the states are localized. From eqn.(5.14) it follows that a branch-cut in $G_{aa}(E \pm is)$ along the real axis corresponds to extended states and the localized states correspond to $Z_0(E) \neq 0$ and also $n_0(E) \neq 0$. Also, all the singularities of $G_{aa}(E)$ and $\Sigma_0(E \pm is)$ lie on the real axis and are either simple poles, corresponding to localized states or branch-cuts corresponding to extended states.

5.7 Confluence states

Thus in terms of Green's function the regime of extended states, (E_c, E_c'), is represented by a branch cut and the regime of localized states consists of a dense set of poles. In the Mott-CFO model the branch-cut and the poles are sharply separated from one another at E_c and E_c'. We suggest a new possibility wherein one could analytically continue the Green's function into the branch-cut

and study the poles if any appearing in the higher Riemann sheet. In other words if we view the branch-cut as Riemann manifold, then some poles may be found on the so-called 'unphysical' sheets lying below the top (or the physical) sheet. The overlapping regions in fig.(5.1b) correspond to such a situation.

Such poles which lie inside the branch-cut are found to behave differently from the poles that exist outside the cut [100]. These poles represent extended states with a difference in the sense that the stay-put probability, $\lim P_i(t)$, for them goes to zero as $t \to \infty$ so slowly that its time integral I diverges. Thus these states share properties of both, the extended states ($\lim_{t\to\infty} P_i(t) = 0$) and the localized states ($I = \infty$) and they may be classified as neither localized nor extended. Thus the spectrum can be recharacterized as shown in the table below. This

$\lim_{t\to\infty} P_i(t)$	$I = \int_0^\infty P_i(t)dt$	$Nature\,of\,states$
0	$finite$	$extended$
0	∞	$'confluence'$
> 0	∞	$localized$

Table 5.1: Energy spectrum in terms of stay-put probability and its time integral.

intermediate state is termed as confluence states because they correspond to poles linked with branch-cut or in other words to a localized state coupled to degenerate extended states. It has been found that if a localized state (represented by a pole) happens to be degenerate with the extended state (represented by the cut) then the localized state will lose its pure-point nature and such a confluence of localized and extended states will eventually, in the limit $t \to \infty$, evolve into a conducting extended state which is confirmed by the fact that the stay-put probability for such a state will approach zero for $t \to \infty$. The manner of formation of the confluence state indicates that the wave function would have a very ramified

shape with isolated and very pronounced bumps of amplitude. The property of the divergence of the time integral for this bumpy extended state indicates that the diffusion should be sluggish for electrons having energy in this part of the spectrum since $P_i(t)$ goes to zero in the limit $t \to \infty$ sufficiently slowly.

This sluggish diffusion in the confluence state regime can be comprehended in terms of a bumpy wave function, i.e. there are a series of connected bumps and an electron spends considerable time in a bump (or an isolated region) and then eventually diffuses into the neighbouring one to conduct through the system. Using a wave function of this kind the conductivity in the region close to E_c can be found.

5.8 Kubo-Greenwood and confluence states

The confluence states possessing the bumpy character discussed in sec.(5.7) meet the requirements of the issues (i) and (iii) raised in sec.(5.5). The extent of each bump can be assumed for convenience to be the same, say ξ_a, and the phase coherence may be taken to last over ξ_a. The average separation between the two bumps can be taken as R. The fractal nature of the wave function as proposed in (iv) of sec.(5.5) can be taken care into account by assuming between two bumps a hierarchy of smaller bumps of successively reducing height and width, the phase being coherent in each bump. For our calculation here we shall not use the details of the fractal nature of the wave function apart from the fact that (a) the phase is coherent over length ξ_a, so the Ioffe-Regel limit [5], $l \sim a$, shall have to be replaced by $l \sim \xi_a$ and (b) the magnitude of the fluctuation in the phase diminishes for distances $\frac{1}{2}\xi_a < r < \frac{1}{2}R$.

The schematic forms of the wave function in different regions of the spectrum are shown in figs.(5.4, 5.5). The localized wave function below E_c has the form,

$$\psi_{loc} = \sum_n A_n \phi_n \exp(-r/\xi_b), \tag{5.15}$$

where A_n, ϕ_n, ξ_b are respectively the co-efficients with random phases, the atomic wave functions and the extent of localization. The wave function just above E_c

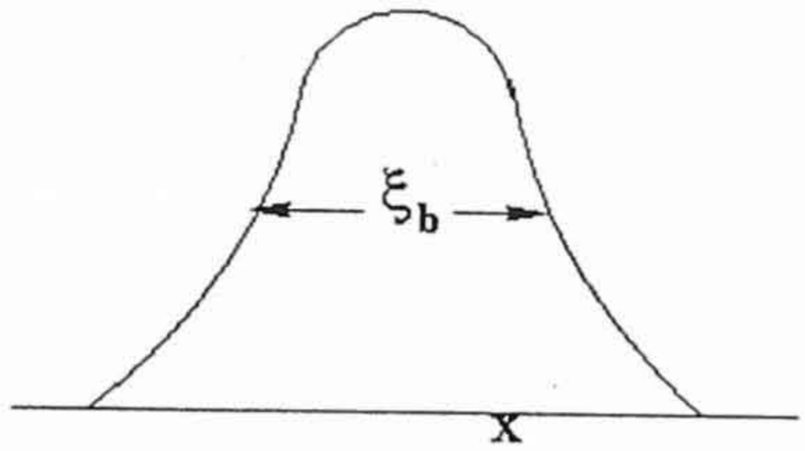


Figure 5.4: Schematic wave function of a localized state below E_c

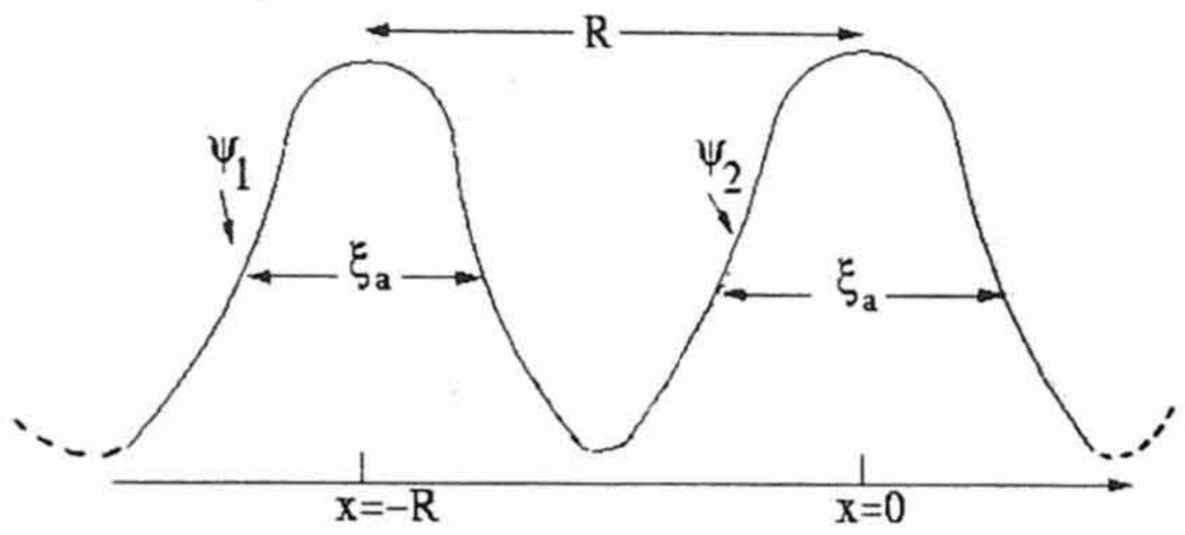


Figure 5.5: Schematic wave function of an extended state above E_c

is constructed by taking a phase-correlated combination of wave functions like

$$\psi_{1,2} \quad = \quad Re\ \psi_{ext} \exp\left(-r/\xi_a\right), \tag{5.16}$$

where the subscripts $1, 2$ represent two neighbouring wave functions that overlap and the subscripts a and b on ξ in eqn.(5.15) and eqn.(5.16) indicates the regime 'above' and 'below' E_c. The relevant length-scales on two sides of E_c are the following:

Below E_c, the localization length ξ_b behaves as

$$\xi_b \sim a \left[\frac{E_c}{E_c - E}\right]^s \tag{5.17}$$

with the exponent $s \sim 1/2$ for 3d systems and a is the mean free path. The phase fluctuates from site to site. Above E_c, the mean free path is ξ_a and the length-scale that diverges as $E \rightarrow E_c$ from above is the separation R, between the bumps. So we propose,

$$R \sim \xi_a \left[\frac{E_c}{E_c - E}\right]^s . \tag{5.18}$$

Above E_c the extent of the states is infinite with finite ξ_a and R. As the E_c is approached, ξ_a remains finite but the density of the bump reduces thereby increasing R. At E_c the bumps are infinitely separated, the overlap reduces to zero and each isolated bump represents a localized state – at this stage ξ_a gets redefined as ξ_b.

Above E_c, the overlap integral for two neighbouring wave functions ψ_1 and ψ_2 differing in energy by $(E - E_c)$ is taken as

$$I = I_o \exp\left(-R/\xi_a\right) \tag{5.19}$$

I_0 represents complete overlap corresponding to $R = 0$, $\xi_a = infinite$. For ψ_1 and ψ_2 to overlap, I should be $\leq (E - E_c)$ and the separation between ψ_1 and ψ_2 should satisfy

$$R \geq \xi_a \ln\left(I_0/(E - E_c)\right) \tag{5.20}$$

i.e. the closer is E to E_c the larger will the separation R have to be which provides a justification for the proposal of eqn.(5.18). Thus our model seems to be suitable for handling a second-order phase transition across the E_c as was required in (ii) of sec.(5.5). The implication of eqn.(5.20) will be dealt with a little later.

5.9 New calculation of σ

We use the form of eqn.(5.16) to calculate δ^2 of eqn.(5.4).

$$\begin{aligned}
\delta^2 &= \left| \int_{R^3} \psi^*_{ext\,1} \exp\left(-(x+R)/a\right) \left(\frac{\partial}{\partial x}\right) \psi_{ext\,2} \exp\left(-(x/\xi_a)\right) \frac{d^3x}{\Omega} \right|^2 \\
&= \exp\left(-2R/\xi_a\right) \left| \int_{R^3} \psi^*_{ext\,1}\, \psi_{ext\,2}\, \frac{d^3x}{\Omega} \right|^2 \\
&= \exp\left(-2R/\xi_a\right) \delta^2_{pl\,wave} \qquad (5.21)
\end{aligned}$$

The $|D|^2$ is thus reduced by a factor, $\exp\left(-2R/\xi_a\right)$, given as,

$$\exp\left(-2R/\xi_a\right) \sim \left(\xi_a/R\right)^2 \sim \left[(E-E_c)/E_c\right]^{2s} \qquad (5.22)$$

with the help of eqn.(5.20) for $I_0 \sim E_c$.

We can now insert corrections to the formula (eqn.(5.6)) obtained by Mott [100]:

- Since we are well above the Ioffe-Regel limit, we must multiply σ by Ω/l to undo the l/Ω that has gone into it through the expression in eqn.(5.6) for $|D|^2$,
- Since $l \sim \xi_a$, we must multiply σ by ξ_a/Ω; and
- Multiply σ by $\left[(E-E_c)/E_c\right]^{2s}$ in accordance with eqns.(5.21) and (5.22). Consequently the $\sigma(E)$ becomes

$$\begin{aligned}
\sigma(E) &\sim 0.03 \frac{e^2}{\hbar a} \frac{\Omega}{l} \frac{\xi_a}{\Omega} \left[\frac{(E-E_c)}{E_c}\right]^{2s} \\
&\propto (E-E_c)^{2s} \simeq (E-E_c) \quad \text{for} \qquad s \simeq 1/2 \qquad (5.23)
\end{aligned}$$

i.e. the σ goes to zero almost linearly in energy as E approaches the E_c from the extended side.

5.10 Conclusions

The calculation of σ taking into account the confluence states shows that σ_{min} ought to be zero in general. There are still some loose ends in the above calculation that need to be tied up.

For the specific case of MIT at very low electron densities one can in fact deduce from Mott's simple calculation itself that σ_{min} should be very small if not exactly zero. Note the presence of l and Ω in eqn.(5.6). Since we now know that the phase coherence length l remains finite even at $T = 0$, $|D|^2$ will always be finite. With decreasing electron density, Ω grows rapidly. This should make $|D|^2$ small, which will make σ_{min} very small. Thus without invoking Ioffe-Regel limit one can account for diminishing σ_{min} and see that the new density-driven MIT in 2D should be of second order.

Finally we will see how the confluence states picture can account for the non-zero σ_{min} in the presence of a magnetic field.The magnetic field will shift the degeneracy between the localized and the extended states that constitute the confluence states. The coupling between them is thus broken and they assume their individual identities as localized and extended states. The regime of slow diffusion is no longer expected to exist and consequently the transition from the extended regime to the localized regime is now expected to be sharp with $\sigma_{min} > 0$.

Thus we conclude that the experimental observation that $\sigma(E) \sim (E - E_c)$ near E_c and that $\sigma_{min} = 0$ is in conformity with the proposal that the states in the neighbourhood of E_c (on the extended side) are somewhat special in the sense that they posses the features of both the extended as well as the localized states, the latter contributing to their being slowing the diffusion rates.

Chapter 6

SUMMARY AND SCOPE FOR FUTURE WORK

6.1 Summary

The work in this thesis involves study of the role of disorder in the electrical properties of low dimensional systems. Our arguments mainly embark upon the random distribution of substitutional and topological defects, the latter being exemplified by two level systems or tunneling states.

The first problem that we have studied involves a calculation of the ratio of the increase in resistance to the metallic resistance, $\Delta R/R_0$, with the lowering of temperature for a quasi-1D wire. Here we mainly stress upon the role of the TLS in causing the inelastic scattering of the electrons. The ideas that have gone into this result includes the concept of variable-range hopping as well as the exponential length dependence of R got from the scaling theory of localization. The dependence of our result on various parameters, namely area A, temperature T and resistivity ρ_e, is in conformity with the experimental results. There is a tally with regard to the order of magnitude as well. From this work we understand that the electrical resistance in the quasi-1D wires is sensitive to the frequency of inelastic scattering events. Our results and their analysis call for new experiments to be done under controlled conditions of disorder and temperature to study in detail the roles of inelastic scatterings from TSs, electrons and phonons separately in the electrical transport in quasi-1D system. This should give more insight into the microscopic details of electron diffusion in the backdrop of localization. Also, the experiments at very low temperatures should possibly reveal something new arising from the interaction between TS which can change the nature of tunneling

from coherent to incoherent.

Our work on the intrinsic phase decoherence in mesoscopic system, raises some fundamental issues in this very new result still being debated in the literature. We have explained the saturation of the phase decoherence time $\tau_\phi(T)$ by taking into account the interaction between the tunneling states, which occurs at lower temperatures and/or a dense concentration of them, and makes the tunneling in the TLSs incoherent. A good amount of further experimentation is needed to ascertain a number of finer points, the first and foremost being to check for the existence of TLS in the systems that show τ_ϕ saturation. It also has to be ascertained if the e-e interactions in dilute electron systems indeed involve sufficient energy to be classified as inelastic at low temperatures. We also speculate as suggested by Imry et al. that there may be a temperature range over which τ_ϕ remains saturated, but at $T << \hbar/\tau_0$, τ_0 being the saturation value, the τ_ϕ may diverge. Only careful experimentation can resolve these issues.

Our work on the MIT in 2D systems is basically centered on the experimental results of Kravchenko et al. which showed the existence of an unexpected metallic phase in these systems. We have attempted to piece together a good cross-section of available experimental information and some of the existing theoretical ideas to understand how the insulating state at the high electron concentration end changes into a metallic state as the density reduces and eventually how the system enters again into an insulating state at the low end of the density. Our arguments are based on a novel possibility of delocalization caused by the interactions between the localized electrons, below a concentration at which V_{ee}, the e-e interaction energy exceeds the E_F, the Fermi energy. This gives rise to the new metallic phase. In other words, delocalization in a system consisting predominantly of localized states can happen if they are connected by hopping events provoked by e-e interactions and form a percolative network whose nodes

are the localized states. With the decrease in concentration and temperature, there will be a transition from one electron to many-electron hopping and the concentration for the onset of many-electron quantum correlation effects in 2D turns out to be less than $10^{15} cm^{-2}$, in agreement with the threshold value below which V_{ee} exceeds E_F. This metallic state turns into an insulating state at a very low density of electrons. This insulating state is a Wigner insulator and not an Anderson insulator; the electrons are pinned in their random positions by long range e-e interactions.

Thus by interpolating between the recent and the earlier regimes of concentration we are of the view that we have an Anderson insulator at the high concentration end and a Wigner glass at the lower end with an intermediate metallic phase. We are of the opinion that many experiments have to be done at the higher concentration end around $10^{15} cm^{-2}$ to check how the metallic state evolves from the Anderson insulator.

Next we have calculated an expression for the minimum metallic conductivity, σ_{min} by modifying Mott's calculation. Some loop holes in Mott's calculation has been plugged. Here we have discussed the existence of an intermediate singularly continuous spectrum, comprising confluence states, that separate the localized and the extended states. We have reviewed the basic definiton of localization in terms of Green's function. The confluence states share the properties of both localized and extended states. The existence of these states leads to the vanishing of σ_{min} making any MIT a continuous one, in general. This calculation needs to be polished further.

6.2 Scope for future work

Our work quasi-1D wires can have some interesting extensions. Herzog et al.'s result [118] on granular metal wires requires special attention in this context.

They find a large discontinuous drop in resistance exhibited in terms of a gap in the resistance which is found to gradually decrease and eventually close up as the continuous 2D limit is approached. It is speculated that this is a first order electronic phase transition in granular 1D system. This correspondence of the granularity with the order of the transition requires more investigation. We suspect that a uniform wire with TS scatterings acting as short-range local events connected with other such events located in far off regions of the system by non-local long-ranged variable-range hopping may mimic the granular scenario.

It should also be interesting to investigate the conditions under which the τ_{ee} takes over from τ_{TS}, and also the nature of this transition. This transition is expected to be different from the weak [93] to strong localization cross-over.

Our work on the intrinsic decoherence in mesoscopic systems is yet to be developed further. Our proposal that it is the TS-TS interaction that is causing the saturation of decoherence time is to be substantiated quantitativey. But with the available literature in the experimental results and theories our work seems to be a plausible one.

The area of metal-insulator transitions in 2D has extensions to other branches like quantum Hall effect [168, 166]. Curious observations have been made about the similiarities in the nature of MIT at low n_s in the absence of magnetic field and that of the MIT in QHE setting when there is a strong magnetic field perpendicular to the 2DHG systems which indicates some common underlying physics for the MIT in $B = 0$ and $B \neq 0$ situations.

In connection with our work on 2D MIT we would suggest experiments to be done to ascertain the existence of TS or TLS in the system. For this we suggest measurements of specific heat and ultrasonic attenuation on the 2DESs as well as the mesoscopic systems which show the saturation of decoherence time. The excess specific heat as well as the linear dependence of this excess specific

heat on temperature below 1K in the disordered electron systems as compared with the crystalline ones had led to the development of the phenomenological model of tunneling states. A linear temperature dependence of specific heat and an increased ultrasonic attenuation would suggest the existence of TLS in these systems.

Our calculation of the minimum metallic conductivity σ_{min} taking into account the existence of confluence states needs to be extended further.

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