# 1 Introduction

In this thesis, we have studied different aspects of charge and energy transport in the presence of disorder and interactions. The theory of transport is now almost a century old and still today this field is one of the most active area of physics research. In this Introductory chapter, we first give a brief commentary on the main approaches of transport developed in the last century. Next part of the chapter is devoted to the essential and important ideas directly related to our work and the problems studied in the thesis. Here we have developed and extensively used a method based on Langevin equations and Green's function (LEGF) to study transport phenomena in different thermal and electrical systems. The problems addressed here can be divided in to two relevant classes. (i) In the first class we have studied charge and energy transport in one, two and three dimensional non-interacting systems (quadratic Hamiltonians). Apart from studying ordered systems, we have studied the effect of disorder, and that of decoherence due to interactions with other degrees of freedom. (ii) Next we have considered electron transport in mesoscopic systems with electron-electron Coulomb interactions. Decoherence is a physical phenomenon in which quantum mechanical interference effects get suppressed due to interactions between system and its environment. The sections of this chapter are organised as following. We describe five traditional transport approaches in Sec.(1.1). In Sec.(1.2) we introduce some interesting models which have been studied here in the context of transport. Then in Sec.(1.3) we discuss three more transport approaches which we employ in this thesis. In the final Sec.(1.4) we state the problems, investigated in the rest of the chapters.

## 1.1 Commentary on transport approaches

Here we try to capture the essence of our understanding of electron and phonon transport in solids through some popular transport approaches. The selection of approaches are based on our understanding and the relevance to the problems studied in this thesis. So, we have left out other important transport approches like random matrix theory (RMT) of quantum transport or methods based on Feynman-Veron influence functionals. Physics in the second half of the last century was controlled by the advancement of semiconductors and its applications to every parts of modern life, including computers and tele-communications. Understanding of both electron and phonon transport in these materials has significant contributions in that fantastic progress.

### 1.1.1 Drude-Sommerfeld model of transport

One of the first model for charge and energy transport by electrons in metals was proposed by Paul Drude in 1900 [1]. He applied the kinetic theory of gas to the mobile conduction electrons wandering through the heavier almost stationary ions forming the underlying lattice. In the course of their motion, electrons collide with the ions and get deflected. These instaneous collisions are phenomenologically modelled by constant damping or relaxation time $(\tau)$. The crucial assumption here is that the electrons are in local thermal equilibrium with their surroundings due to these collisions. The last point has been critically re-examined in this thesis. We have provided simple models which show local thermal equilibrium and studied the consequences of it on thermoelectric transport. One main drawback of the Drude model is that here both electron-ion and electron-electron Coulomb interactions are neglected. Yet the simple Drude model was quite successful to explain Ohmic behavior of metallic conductor, nature of charge carriers in the classical Hall experiment and phenomenological Wiedemann and Franz rule. Ohm's law states that the charge current density $(\mathbf{j}_{el})$ is linearly proportional to the applied weak electric field $(\mathbf{E})$. The Drude model gives an explicit form of this proportionality constant $\sigma$ (called electrical conductivity or inverse of resistivity).

$$\mathbf{j}_{el} = \sigma \mathbf{E}, \quad \text{with} \quad \sigma = \frac{ne^2\tau}{m} \ , \tag{1.1}$$

where $e, m, n$ are, respectively, the charge, mass and density of electrons. If local thermal equilibration is assumed to be achieved in collisions, then one can find an expression for thermal conductivity $(\kappa^e)$ due to electrons. It is given as

$$\mathbf{j}_{th} = -\kappa^e \nabla T, \quad \text{with} \quad \kappa^e = \frac{1}{3} v^2 \tau c_v^e \ , \tag{1.2}$$

where $\mathbf{j}_{th}$ is the thermal current, $\nabla T$ is the temperature gradient across the sample. Here, $v$ and $c_v^e$ are, respectively, the mean electron velocity and electronic specific heat. Drude applied classical ideal gas laws to evaluate $v$ and $c_v^e$. But this gives incorrect values of these parameters as it ignores quantum statistics for electrons. Sommerfeld re-examined conduction in metals in the Drude model using Fermi-Dirac statistics for the velocity distribution of electrons. The main idea of Sommerfeld's theory was to treat the electrons' motion between collisions classically, with various input parameters calculated from quantum theory of free electron gas. Some ingenious thought will convince that classical dynamics of $N$ noninteracting metallic electrons will not be drastically affected by quantum postulates; so as long electronic velocity distribution does not play a significant role, the predictions of the Drude theory are correct, such as for those DC or AC electrical conductivities, but for thermal conductivity would be incorrect.

### 1.1.2 Semiclassical Boltzmann transport theory

Electrons in metals are not completely free, but subjected to interactions due to ions making the band structure, though we still do not consider electron-electron interactions. The semiclassical transport theory of solids treats the dynamics of electron classically, with inputs taken from the quantum mechanically calculated band structure using Bloch theory. Validity of the semiclassical treatment strongly relies on the assumption that the external applied field varies on length scale longer than the underlying periodic potential of the lattice. In the Boltzmann transport theory of electrons [2], one starts with finding $g(\mathbf{r},\mathbf{k},t)$, a non-equilibrium analog of equilibrium electronic distribution function, where $g(\mathbf{r},\mathbf{k},t)d\mathbf{r}d\mathbf{k}/4\pi^3$ is the number of electrons in the phase space volume $d\mathbf{r}d\mathbf{k}$ around $(\mathbf{r},\mathbf{k})$ at time $t$. One can determine $g(\mathbf{r},\mathbf{k},t)$ using relaxation time approximation, where it is assumed that (a) the distribution of electrons after collision is independent of $g(\mathbf{r},\mathbf{k},t)$ just before the collision and (b) collisions do not change the form of the equilibrium distribution of $g(\mathbf{r},\mathbf{k},t)$ at local temperature. Both the assumtions are over estimation of the efficiency of collisions. On the other hand in the kinetic theory of Boltzmann, one evaluates $g(\mathbf{r},\mathbf{k},t)$ from the differential Eq.(1.3) derived without the above assumptions.

$$\frac{\partial g}{\partial t} + \mathbf{v}.\frac{\partial}{\partial \mathbf{r}}g + \mathbf{F}.\frac{1}{\hbar}\frac{\partial}{\partial \mathbf{k}}g = \left(\frac{\partial g}{\partial t}\right)_{coll}, \tag{1.3}$$

where $\mathbf{F}(\mathbf{r},\mathbf{k}) = \hbar\dot{\mathbf{k}}$ is the external applied force and $\mathbf{v}(\mathbf{k}) = \dot{\mathbf{r}}$. The collision term in the right side of the equation is usually calculated using quantum theory like Fermi golden rule. At high temperatures the main source of collision or scattering is intrinsic deviations from the crystal periodicity, i.e., thermal lattice vibrations, whereas impurities, crystal defects are dominant sources of collisions at low temperatures. Surface (or boundary) scattering is an important collision mechanism in nanostructures, such as quantum dots, nanowires and graphene.

In solids, ions are arranged in a regular periodic array or lattice which themselves act as dynamical entities. The quanta of lattice vibrations is known as phonon which carries heat energy in metals as well as in electrical insulators. Similar to Drude model Debye first applied kinetic theory for phonon gas. He expressed the phonon thermal conductivity $(\kappa^{\mathrm{ph}})$ as proportional to $c_v^{\mathrm{ph}} v\ell$ where $c_v^{\mathrm{ph}}$,$v$,$\ell$ are, respectively, the phonon specific heat, velocity and mean free path. Peierls formulated above Boltzmann type transport for heat conduction by phonons. Now, in case of phonons, the main sources of scattering are impurities and phonon-phonon interactions. Impurity scattering can arise because of randomness in the masses of the particles or in the spring constants. In this case, the phonons still do not interact with each other and one can think of the phonons of the original pure crystal getting elastically scattered by impurities. Alternatively, since the system is still harmonic, one can think of heat transmission by the new normal modes of the disordered system. The second mechanism for scattering is through phonon-phonon interactions and this occurs if we include the higher order nonlinear terms (*i.e*, beyond quadratic order) of

the inter-particle potential. Phonon-phonon interactions are usually classified into those which conserve momentum and those which do not (Umklapp processes). Anharmonicity or phonon-phonon interaction is necessary to get diffusion of energy through the momentum non-conserving Umklapp processes. The Boltzmann-Peierls approach has become one the cornerstones in the theory of lattice thermal conductivity. One can compute $(\kappa^{\rm ph})$ using this approach with different approximations, like the relaxation-time approximation similar to electron case.

### 1.1.3 Kubo linear response theory

Until now, we have discussed approaches of transport based on either classical or semi-classical dynamics, where accelerated electrons are balanced by scattering due to phonons and lattice defects. Also, in the above theories, scattering events from different points in the phase space are assumed to act incoherently. A full fledged quantum transport theory for weak external perturbation can be developed applying the Kubo linear response theory [3]. Linear response theory is a widely used concept in all branches of physics but we discuss here in the context of transport only. Linear response theory implies that the effective motion (or velocity) of the carriers is proportional to the external perturbation and one needs to find the proportionality constant to quantify the transport behavior. It has been used both for mechanical perturbations (perturbation of Hamiltonian) and thermal perturbations (perturbation of boundary conditions).

We now briefly describe linear response theory for mechanical perturbations. Let us start with a quantum system in thermodynamic equilibrium, described by the time-independent Hamailtonian $\hat{H}_0$. The expectation value of any physical observable $\hat{A}$ in equilibrium (at temperature $T$) is given by

$$\langle \hat{A} \rangle_0 = \frac{\mathrm{Tr}[\hat{\rho}_0 \hat{A}]}{\mathrm{Tr}\hat{\rho}_0} \quad \text{with} \quad \hat{\rho}_0 = e^{-\beta \hat{H}_0} \ . \tag{1.4}$$

Here $\hat{\rho}_0$ is the equilibrium density operator and $\beta = 1/k_B T$, with $k_B$ being the Boltzmann constant. Then, at some instant, $t = t_0$, an external weak perturbation is applied to the system to drive the system out of equilibrium. The full Hamiltonian at time $t > t_0$ is given by

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t)\theta(t - t_0) \ . \tag{1.5}$$

We are interested to get the expectation value of $\hat{A}(t)$,

$$\langle \hat{A}(t) \rangle = \frac{\mathrm{Tr}[\hat{\rho}(t) \hat{A}]}{\mathrm{Tr}\hat{\rho}(t)} \tag{1.6}$$

The time evolution of the density operator $\hat{\rho}(t)$ can be determined in the interaction picture using Bloch equation, $\partial_\beta \hat{\rho} = -\hat{H}\hat{\rho}$. Then one finds the response to linear order in the external

perturbation $\hat{V}(t)$ as

$$\begin{aligned} \delta\langle\hat{A}(t)\rangle &= \langle\hat{A}(t)\rangle - \langle\hat{A}\rangle_0 = \int_{t_0}^{\infty} dt' C^R_{AV}(t,t') \ , \qquad (1.7) \\ \text{with } C^R_{AV}(t,t') &= -i\theta(t-t')\big\langle\big[\hat{A}_I(t), \hat{V}_I(t')\big]\big\rangle_0 \ . \end{aligned}$$

The previous equation is the famous Kubo formula where the response has been expressed through equilibrium time-correlation function. In Eq.(1.7), $I$ indicates that operators are given in interaction picture representation. Linear response theory has typically viewed the electric field as a cause and the current flow as a response. We sketch here a derivation of a relation in the frequency $(\omega)$ domain for electrical conductivity $\sigma(\mathbf{r},\mathbf{r}',\omega)$, with the equilibrium time autocorrelation function of the current density operator for small applied electric field $\mathbf{E}(\mathbf{r},\omega)$. One starts with

$$\begin{aligned} \hat{V}(\omega) &= \frac{e}{i\omega}\int d\mathbf{r}\ \hat{\mathbf{J}}(\mathbf{r}).\mathbf{E}(\mathbf{r},\omega) \ , \qquad (1.8) \\ \text{where } \hat{\mathbf{J}}(\mathbf{r}) &= \hat{\mathbf{J}}_p(\mathbf{r}) + \frac{e}{m}(\mathbf{A}_0 + \mathbf{A}_{ext})\hat{\rho}(\mathbf{r}) \ , \qquad (1.9) \end{aligned}$$

where $\mathbf{A}_0$ denotes vector potential in equilibrium before the external perturbation, $\mathbf{E}(\mathbf{r},\omega) = i\omega A_{ext}(\mathbf{r},\omega)$, is applied. In Eq.(1.9), the first term $\hat{\mathbf{J}}_p(\mathbf{r})$ is the paramagnetic current operator while the second term is the diamagnetic contribution. $\hat{\rho}$ is the particle density operator. Then non-local electrical conductivity tensor $\sigma^{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)$ is defined as

$$\hat{J}^{\alpha}_e(\mathbf{r},\omega) = -e\langle\hat{J}^{\alpha}\rangle = \int d\mathbf{r}' \sum_{\beta}\sigma^{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)E^{\beta}(\mathbf{r}',\omega) \ . \qquad (1.10)$$

After some calculation using the Kubo formula Eq.(1.7) one finds an expression for the conductivity tensor.

$$\sigma^{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = \frac{ie^2}{\omega}C^R_{J^{\alpha}_0(\mathbf{r})J^{\alpha}_0(\mathbf{r}')}(\omega) + \frac{e^2\langle\rho(\mathbf{r})\rangle}{i\omega m}\delta(\mathbf{r}-\mathbf{r}')\delta_{\alpha\beta} \ , \qquad (1.11)$$

where $\hat{\mathbf{J}}_0(\mathbf{r}) = \hat{\mathbf{J}}_p(\mathbf{r}) + e\mathbf{A}_0\hat{\rho}(\mathbf{r})/m$. The expression of Eq.(1.7) is exact and is given in terms of microscopic quantities only.

A number of attempts (see Ref.[4]) have been made to formulate general linear transport coefficients in the form of Eqs.(1.7,1.11). The viscosity coefficients, thermal conductivity are some of the examples of linear coefficients arising in reponse to inhomogenieties which are not generally expressible as mechanical perturbations of the form of Eq.(1.8). These are generally known as thermal transport coefficients and the derivation of exact formulas for these coefficients are more involved.

### 1.1.4 Conductance viewed as transmission: Landauer formalism

All three previous transport approaches deal only with the sample through which charge or energy is being transported. But transport is a dissipative phenomenon where charge or energy is exchanged either with the reservoirs at the ends of sample or with the environment at the bulk of the sample. So, for a complete understanding of transport phenomena, one should consider all parts of the full system. Landauer formalism is based on this principle. Here, one assumes that the system in question is connected to large reservoirs, where all inelastic scattering processes take place. Consequently, transport through the system can be formulated as a quantum mechanical scattering problem. Thus, one can reduce the nonequilibrium transport problem to a quantum mechanical one. Landauer [5] derived a formula which connects the resistance or conductance of a sample with the reflection or transmission coefficient of the carrier through the sample. Of course, the value of the resistance or conductance depends on the way one probes the system. In the thesis we have used the Landauer two-probe and four-probe resistance formule. We briefly discuss the formulae here.

$Four\text{-}probe\ formula$ : In a four-probe measurement, current is sent through the two outer probes, and one measures the voltage across the two inner probes. It can be proved that the resistance ($\rho = g^{-1}$) of a 1D (single channel) conductor in units of $\pi\hbar/e^2$ is

$$\rho(L) = \frac{1 - t(L)}{t(L)} \ , \tag{1.12}$$

where $t(L)$ is the transmission coefficient of the sample of length $L$. It gives correct zero resistance of a perfect metal with unit transmission.

$Two\text{-}probe\ formula$ : A two-probe measurement is done with same voltage and current probes and it can be shown that the two-probe resistance of a single channel is

$$\rho(L) = \frac{1}{t(L)} \tag{1.13}$$

In the absence of scatterer, the four-probe formula gives zero resistance; but the two-probe resistance is unity (in the unit of $\pi\hbar/e^2$). This is to maintain the contact potential difference in the two-probe measurement, as the voltage and the current probes are the same and the particles have to work to transmit ballistically from one lead to other. This constant resistance is known as the Sharvin contact resistance. One of the earliest and important experimental verification of the Landauer formalism came from the celebrated studies of conductance of narrow two dimensional channels, called quantum point contacts (QPC) connecting wide reservoirs [6, 7]. The channel width can be controlled by externally applied gate voltage. As the conducting channel is widened, the number of transverse conducting eigenstates $N$ in the conductance, $g = Ne^2/\pi\hbar$, of perfectly conducting channel, increases. Conductance steps corresponding to increasing values of N are clearly observed in experiments. Today, the Landauer formalism is the most widely used approach for electron and heat transport in nanostructures.

### 1.1.5 Non-equlibrium Green's function formalism (NEGF)

The non-equilibrium Green's function formalism is a highly developed technique to investigate quantum transport in coherent mesoscopic systems far away from equilibrium [8]. It is also a complete transport theory (like the Landauer approach) as it describes time evolution of any observable with the full Hamiltonian of the system and the resrvoirs. The main advantage of NEGF over the Landauer approach is that weak interaction between carriers like electron-electron (e-e), phonon-phonon (ph-ph) or electron-phonon (e-ph) can be studied here. This technique has been developed to the present stage by several physicists including Kadanoff, Baym, Schwinger, Keldysh, Meir and Wingreen. NEGF has been formulated in structurally equivalent fashion following equilibrium Green's function of many body quantum theory. It relies on Wick's theorem and perturbation technique using Feynmann diagrams. But the crucial difference here from the equilibrium case, is that finite bias in non-equilibrium problem breaks down the time reversal symmetry between the initial and final states, which has been exploited heavily to construct perturbation theory in equilibrium. In NEGF, one can tackle the problem by allowing the system to evolve from time $t = -\infty$ (if one is not interested in transient behaviour) to a time $t = t_i$ when one is interested to study the system (or in general, after steady state has been reached), and then to continue the time evolution from $t = t_i$ back to $t = -\infty$. In this scheme, all the expectation values are defined with respect to a well-defined initial state at $t = -\infty$. But one should treat both the time braches on equal footing. Now, we ouline the scheme of constructing perturbation theory in NEGF.

Consider the Hamiltonian

$$\hat{\mathcal{H}} = \hat{H}_0^S + \hat{H}_I^S + \hat{H}^R + \hat{V}^C \tag{1.14}$$

where $\hat{H}_0^S, \hat{H}_I^S$ are, respectively, the noninteracting and the interacting part of the system Hamiltonian and $\hat{H}^R$ defines Hamiltonian of the reservoirs. The system is coupled to the reservoirs by the coupling $V^C$ at time $t = -\infty$. Before the coupling is turned on, the full system is described by the equlibrium density matrix

$$\hat{\rho}(\hat{H}) = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}[e^{-\beta\hat{H}}]}\ , \tag{1.15}$$

where $\hat{H} = \hat{H}_0^S + \hat{H}_I^S + \hat{H}^R$. Now, the expectation value of any operator $A(t)$ corresponding to a physical observable (like steady state current) at time $t$ is given by

$$\langle \hat{A}(t) \rangle = \mathrm{Tr}[\hat{\rho}(\hat{H})\hat{A}_{\hat{\mathcal{H}}}(t)] \tag{1.16}$$

Here, $\hat{A}_{\hat{\mathcal{H}}}(t)$ is written in Heisenberg picture. Also, note that we have used equilibrium density matrix in Eq.(1.16). One can even use time evolution of the density matrix instead of $\hat{A}$ as we

have done in case of linear response theory. Now, one needs to apply perturbation technique to find the time evolution of $\hat{A}_{\hat{\mathcal{H}}}(t)$. In most of the cases, we can find exactly the propagator for noninteracting part of the Hamiltonian $\hat{\mathcal{H}}_0 = \hat{H}_0^S + \hat{H}^R$, we need to apply the perturbation to it twice with respect to $\hat{H}_I^S$ and $\hat{V}^C$ using Wick's theorem to determine the full propagator. Also, one should be careful in defining time ordered Green's functions in different branches of the full time contour, and it is carried out using Langreth theorem. In this thesis, we have developed a simpler approach based on Langevin equations where it is possible to derive NEGF-like expressions for the steady state quantities for noninteracting systems.

## 1.2 Some models of interest

In this section, we describe the models which have been studied in this thesis. We also briefly summarize previous important results related to these models. Resistance against transport arises due to elastic or inelastic scattering of carriers. Scattering of electrons or phonons from quenched disorder such as static random potential, is elastic and energy of scattered electrons or phonons remains the same. Inelastic scattering caused by dynamical interactions, where carriers exchange energy with other degrees of freedom. For electrons, electron-phonon interactions and electron-magnetic impurity interactions are some important sources of inelastic scattering. Usually in solids, inelastic scattering due to electron-phonon interactions dominates in high temperature transport and the transport follows classical Drude-like behaviour due to lack of phase coherence. In the absence of magnetic impurity, low temperature electrical transports in a noninteracting disordered medium is dominated by interference of the electron waves along the alternative time-reversed paths, which leads to quantum correction to the classical Drude conductivity. This phenomenon, known as coherent back-scattering, causes weak localization correction which, under certain circumstances, leads to localization in disordered conductor, and metallic conductor becomes insulator [9]. In Sec.(1.2.1) we also discuss models of disordered phononic systems. In our work we have introduced inelastic scattering in the transport channels phenomenologically through voltage probes as in Sec.(1.2.2).

In real systems, long range Coulomb interaction between electrons or phonon-phonon interactions due to anharmonic lattice vibrations at finite temperature are always present. Still, in many cases, for extended syatems (such as good metals or electron gases), it is valid to investigate at low temperatures in the almost non-interacting limit as long range interactions effectively get screened. But this is not true when charge tends to be localized on the nanostructures and the flow of electrons become correlated due to Coulomb interactions [10]. We study a simple model of strongly interacting electrons in the last chapter of this thesis. We have chosen to study simple but nontrivial models, since this enables us to derive many exact and accurate results. We believe that the models still keep basic essential features of real systems and our analytical studies enable

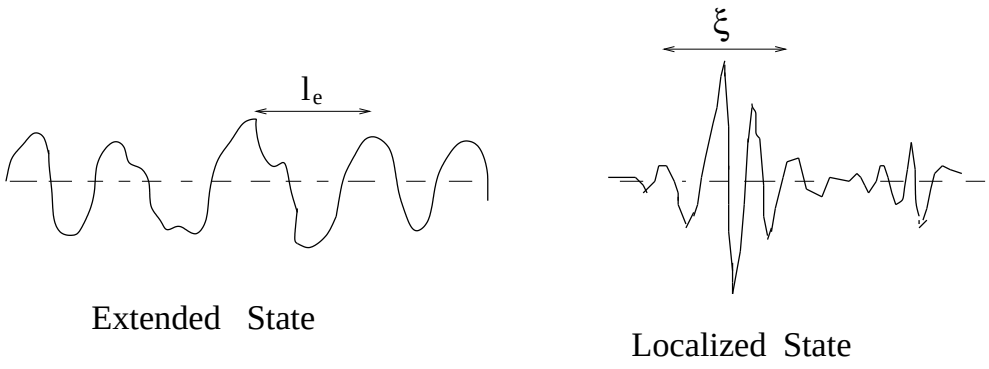


Figure 1.1: Plot of a typical wave function of an extended state with mean free path $l_e$ and a localized state with localization length $\xi$.

one to understand underlying physical mechanisms of system of practical interests.

### 1.2.1 Disordered systems

Quatification of disordered samples is done by specifying some macroscopic properties of the system, such as the concentration of the impurities (like doping atoms in semiconductors). Now, one can have many different microscopic realisations of the disordered samples, keeping the average macroscopic characters fixed. A model of disordered system is constructed by an ensemble of such different microscopic realisations together with the information of occurance of the sample system in the ensemble. In short, models of disordered systems are described by a Hamiltonian with the distribution of the disorder. We include here models of disordered systems both for electron and phonon.

*Model* 1. *Anderson Model* :

Consider a disordered noninteracting electronic system of tight-binding Hamiltonian [11] on a $d$-dimensional lattice,

$$\hat{\mathcal{H}} = -\sum_{\mathbf{l}\neq\mathbf{m}} t_{\mathbf{lm}}|\mathbf{l}\rangle\langle\mathbf{m}| + \sum_{\mathbf{l}} \epsilon_{\mathbf{l}}|\mathbf{l}\rangle\langle\mathbf{l}| \ , \tag{1.17}$$

where $\mathbf{l}$ is a $d$-dimensional vector. Disorder can be realized by making on-site potential $\epsilon_{\mathbf{l}}$ random from site to site (site-diagonal disorder), or, by inserting random tunneling matrix element $t_{\mathbf{lm}}$ (off-diagonal disorder). For the case of site-diagonal disorder with disorder distributed uniformly over a band of site energies over $\pm\Delta/2$ (i.e., width $\Delta$) and a tunneling bandwidth $W = 2Zt_0$ (where $t_0$ is nearest-neighbour tunneling and $Z$ is co-ordination number), the Anderson theorem predicts that for $\eta = (\Delta/W) \geq (\Delta/W)_{\text{critical}}$, all states are localized.

All states of 1D Anderson model are localized for any finite fraction of disorder potentials of any strength [12]. For 3D Anderson model, all eigenstates get localized with sufficient strength of disorder potential for a given ordered band width. The disorder induced transition from

conducting to insulating phase is known as Anderson transition which is a mechanical or quantum phase transition. For highly disordered media, waves undergo multiple coherent scatterings and produce localised states due to interference effects. In FIG.(1.1) we have shown typical examples of localised and extended states. The wavefunction for a localised state has an envelope which decays exponentially from the peak point with a characteristic length called the localisation length, $\xi$. Extended states are described by the typical length scale called the coherence length, $l_e$, over which phase coherence is retained. $l_e$ is generally the elastic mean free path in a good metal. In Chapter (3), we will have more discussion on the different regimes of disorder and scaling theory of localization.

*Model 2. Lloyd Model* :

In the one dimensional tight-binding Hamiltonian of the form of Eq.(1.17), if the site energies $\epsilon_l$ are chosen to be distributed randomly with a Cauchy probability distribution

$$P(\epsilon_l) = \frac{1}{\pi}\frac{\Gamma}{(\epsilon_l - \epsilon_0)^2 + \Gamma^2} \ , \tag{1.18}$$

and only nearest-neighbour hopping elements $t_{l,l+1} = 1$ are present, then the disordered electronic model is called the Lloyd model. Here, $\epsilon_0$ and $\Gamma$ are, respectively, the mean value and width of the distribution. This is an exactly solvable model of disordered electronic system, where one can calculate the localization length $\xi(E)$ and the average density of state $\rho(E)$ as a function of the energy $E$ [13].

*Model 3. Isotopically disordered harmonic lattices* :

This model has been nvestigated in this thesis extensively. The Hamiltonian of a disordered d-dimensional harmonic lattice is given by

$$H = \sum_{\mathbf{l}} \left( \frac{p_{\mathbf{l}}^2}{2m_{\mathbf{l}}} + \frac{1}{2}k_0 x_{\mathbf{l}}^2 \right) + \sum_{\mathbf{l}\neq\mathbf{n}} \frac{1}{2}k_{\mathbf{ln}}(x_{\mathbf{l}} - x_{\mathbf{n}})^2 \tag{1.19}$$

where $\mathbf{l}$ is again a d-dimensional vector. Here, $\{x_{\mathbf{l}}, p_{\mathbf{l}}, m_{\mathbf{l}}\}$ denote the scalar displacements about equilibrium positions, momentum, and mass of a particle at the site $\mathbf{l}$. The mass $\{m_{\mathbf{l}}\}$ in Eq.(1.19) is random and usually chosen from a uniform distribution. Similar to Anderson model, one can have random spring constant $\{k_{\mathbf{ln}}\}$ also. We need to specify boundary conditions for $x_{\mathbf{l}}$. We use either fixed or free boundaries in Chapter (4). For the case $k_0 = 0$, the total momentum is conserved and thus, there exists a zero frequency translational (Goldstone) mode; then the Hamiltonian in Eq.(1.19) has at least one phonon branch whose frequency vanishes for vanishing wave number and this model (i.e., the case $k_0 = 0$) is known as acoustic model. In the presence of finite $k_0$, the total momentum is no longer a constant of motion and all branches of the dispersion relation have a gap at zero wavenumber. Then it is referred to as the optical model [14].

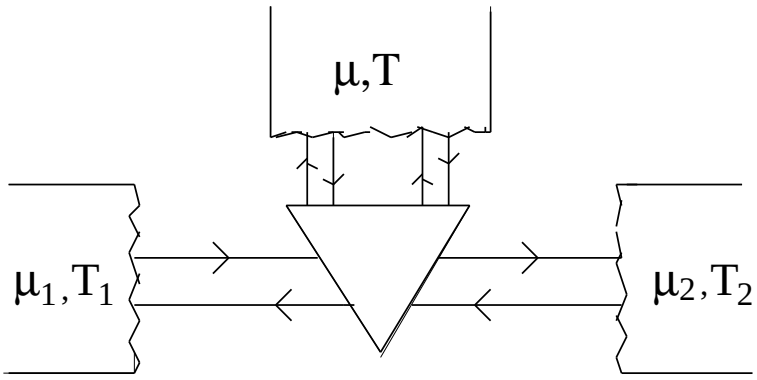


Figure 1.2: Plot of a two-channel voltage probes coupled in between two reservoirs at different chemical potentials and temperatures.

In Chapter (4), we study the random mass disordered harmonic chain with constant nearest neighbour elastic couplings in case of the acoustic model, with a few on site quadratic pinning potentials. In contrast to Anderson model, all states of the acoustic model, even in one dimension, are not localised and low frequency modes are extended, which can conduct significantly [15–18]. It has been shown [19], using field theoretic treatment for the disordered harmonic lattices with vector displacement, that all finite-frequency phonon-modes in one and two dimensions are localised with low-frequency $(\omega)$ localization lengths diverging as $1/\omega^2$ and $e^{1/\omega^2}$ respectively, and there exists Anderson like transition from extended to localised modes at finite frequency in three dimensions. In Chapter (4), we study the scalar displacement model analytically as well as numerically and obtain many interesting results.

### 1.2.2 Self-consistent reservoirs or voltage probes

In most of the transport theories like the Drude model or the semiclassical Boltzmann transport theory with relaxation time approximation, one attributes all the efficacy of collisions to the phenomenological parameter, namely, the relaxation time $\tau$, without bothering much about the scattering mechanism closely. Though in modern perturbation theory and numerical studies, it is possible to take into account the microscopic Hamiltonian causing scatterings, still it is hard in many cases to have a simple understanding of the role of inelastic and quasi-elastic scattering mechanisms in transport behavior. Self-consistent reservoirs (SCR) or voltage probes are introduced phenomenologically in microscopic theory of transport to have a better understanding of the role of scatterings in transport with less complication. The SCR model was introduced in the early seventies of the last century by Bolsterli, Rich and Visscher [20–22] to study heat conduction in ordered and disordered harmonic lattices. The SCRs incorporate phenomenologically interactions of phonons with other degrees of freedom such as electron's charge and spin present in the physical system. The temperature of the SCR, connected to the transport channel

of phonons, is determined self-consistently by the condition of net zero heat current from the SCR to the transport channel. The SCR of thermal transport matches in many sense to the dephasing probes (of electrical transport) which introduce incoherent quasi-elastic scattering into a mesoscopic conductor.

Engquist and Anderson [23] introduced the concept of potentiometer probes in transport channel to have a physical understanding of the Landauer four probe formula and removed the paradox arising from the derivation of Landauer-like formula from the Green-Kubo formula. But the present form of voltage probes was originated by M. Büttiker [24, 25] to study dephasing in persistent current in a metallic ring. Voltage probes coupled to a coherent conductor permit incoherent inelastic scattering processes. A particle entering the probe is thermalized by dissipation and, later on, fed back into the system to conserve the number of particles in transport channel. Voltage probe models are widely used to address mostly the disappearance of quantum coherent nature in transport, such as to show the transition from quantum combination of scatterers to the series addition of resistances, the transition from the quantum Hall effect to the classical Hall effect or to incorporate the effect of inelastic effects on quantum pumping. In FIG.(1.2.2), we show a double-channel voltage probe (with chemical potential $\mu$ and temperature $T$) coupled to a transport channel which conducts between two reservoirs at different chemical potentials and temperatures. Here, $\mu$ and $T$ will be determined by the net zero particle and heat current respectively, but it also depends on the coupling matrix between the voltage probe and transport channel. In Chapter (3), we present some example of coupling matrices and calculate the potential of the voltage probe.

### 1.2.3 Electron-electron interactions in mesoscopic systems

Until now our discussion has been confined to the single particle picture. Here, we briefly review some mesoscopic models with electron-electron Coulomb interactions. The main focus here is to find how does the transport behavior modify in the presence of many-body effects. We study electron transport through an interacting region (such as quantum dot) connected to two non-interacting leads at finite potential difference. Quantum transport through quantum dots with Coulomb interactions has been extensively investigated for many years, but most of the studies are either perturbative for weak interactions or within linear response regime. Many popular methods like NEGF, numerical renormalisation group or functional Bosonisation have been employed for these studies [26]. Recently, Bethe ansatz technique has been extended to study nonequilibrium transport through interacting resonance level model for arbitrary interaction. We have studied a very simplified model of interacting electrons in Chapter (5), and our scope of discussions here is also limited. We briefly introduce two popular models of correlated electron transport through quantum dots.

Our first example of Hamiltonian comprises metallic quantum dot, where many energy levels are present near the Fermi energy (i.e., internal dimensionless conductance $g >> 1$). Using RMT, one can express the universal quantum dot Hamiltonian [27] in terms of single particle energy level $\alpha$ as

$$\hat{H}_D = \sum_{\alpha\sigma} \epsilon_\alpha \hat{a}^\dagger_{\alpha\sigma}\hat{a}_{\alpha\sigma} + E_c\big(\sum_{\alpha\sigma} \hat{a}^\dagger_{\alpha\sigma}\hat{a}_{\alpha\sigma} - N_0\big)^2 + J_s\big(\frac{1}{2}\sum_{\alpha\sigma_1\sigma_2} \hat{a}^\dagger_{\alpha\sigma_1}\vec{\sigma}_{\sigma_1\sigma_2}\hat{a}_{\alpha\sigma_2}\big)^2 \ . \qquad (1.20)$$

Here Coulomb interaction between electrons is included through the charging energy $E_c = e^2/C$, with $C$ being the effective capacitance of the dot. $J_s$ is the strength of exchange spin interactions between electrons. $\sigma$ denotes spin level and $\vec{\sigma}$ is the Pauli spin operator. We have discarded Cooper and spin-orbit interaction channels. Many of the earlier important results like Coulomb blockade have been studied with this form of Hamiltonian. This model is also known as constant interaction model or capacitor model.

The second model is similar to the popular Anderson impurity model which was originally proposed by P.W. Anderson [28] to study the well-known Kondo problem, the behavior of single magnetic impurity coupled to a conduction band of electrons. Now, for the case of quantum transport through dot, the conduction band acts as the two leads and the magnetic impurity is replaced by the quantum dot. The full Hamiltonian of the dot, leads and dot-lead couplings is given by

$$\hat{H}_D = \sum_{\sigma=\uparrow\downarrow} \epsilon_d \hat{a}^\dagger_{d\sigma}\hat{a}_{d\sigma} + U\hat{a}^\dagger_{d\downarrow}\hat{a}_{d\downarrow}\hat{a}^\dagger_{d\uparrow}\hat{a}_{d\uparrow} + \sum_{k,\sigma=\uparrow\downarrow} \epsilon_k \hat{a}^\dagger_{k\sigma}\hat{a}_{k\sigma} + \sum_{k,\sigma=\uparrow\downarrow} V_k(\hat{a}^\dagger_{k\sigma}\hat{a}_{d\sigma} + \hat{a}^\dagger_{d\sigma}\hat{a}_{k\sigma}) \ , \ (1.21)$$

where $d$ denotes dot level. Here, $U$ is the Coulomb interaction energy and $V_k$ is the coupling between dot level and leads' levels denoted by the subscript $k$. In the case of linear dispersion relation for the band and $V_k = V$ =constant, the equilibrium problem of this model was solved using a Bethe-ansatz method. Recently, Bethe-ansatz technique has been extended to study the nonequilibrium transport in a similar model called interacting resonance level model for arbitrary interaction exactly [29]. In the final chapter of this thesis, we study the transport problem with a simple model of quantum dot for spinless interacting electrons, similar to the Anderson model.

## 1.3 Approaches applied in the thesis

In Sec.(1.1), we discuss about five transport theories. These are indirectly related to the work in the present thesis. Here, we illuminate three different approaches which have been employed to study heat and charge transport problems in this thesis. We have developed and applied a formalism based on Langevin equations and Green's function [4] to most of the problems here. For noninteracting thermal and electrical systems, this formalism is quite easy to implement

analytically as well as numerically. Invariant embedding technique (see Sec.(1.3.2)) suits better to investigate weakly disordered electronic systems analytically. Our study of electrical transport in the presence of strong Coulomb interaction is based on the Lippmann-Schwinger scattering theory. We briefly illustrate the Lippmann-Schwinger scattering theory at the end of this section in Sec.(1.3.3).

### 1.3.1 Langevin equations and Green's function (LEGF)

The LEGF approach allows to study systems in steady state arbitrarily away from the linear response regime and includes the system, reservoirs and system-reservoir couplings explicitly. This method, based on Langevin equations and Green's functions was first applied by Ford, Kac and Mazur [30] to the case of coupled oscillators. Recently, this method has been extended to study quantum and classical transport in noninteracting systems by Dhar and co-workers [31–33]. Idealized reservoirs act as perfect blackbody with zero reflection. The LEGF has been devised to elucidate the role of reservoirs and system-reservoir couplings in electrical and thermal transport in [31]. It was also shown that ideal Landauer result for a disordered 1D conductor could be obtained with special choice of reservoir. A nice analogy between NEGF and LEGF has been drawn in [32]. This approach has been rigorously applied in next three chapters to deal with various types of open quantum systems. We briefly summarise the basic steps of this formalism here.

We start with the full Hamiltonian of system, reservoirs and system-reservoir couplings. Usually, we take the reservoirs to be modeled by non-interacting electron gas for electrical transport study, and harmonic lattices for thermal transport. Then, we write down equations of motion for the system and reservoirs degrees of freedom. The reservoir degrees of freedom are eliminated to get effective Langevin equations for the system alone. The reservoirs are serving as effective sources of noise and dissipation. Finally, the Langevin equations, which are linear for the case of non-interacting system are solved by Fourier transformations to obtain the steady state properties such as current, local chemical potentials or temperatures. The most appealing character of LEGF is its transparency and direct connections with other popular transport approaches such as Keldysh NEGF, Caldeira-Leggett, Landauer and scattering theory methods. It is possible to study interacting systems in LEGF approach using perturbation technique as NEGF, or, applying self-consistent mean field theory like Hatree-Fock approximation. Still the implementation of LEGF for interacting systems requires further careful studies.

### 1.3.2 Invariant embedding technique

The main idea of the invariant embedding approach is to deal directly with the outer emergent characteristics, like complex reflection amplitude $R(L)$ and transmission amplitude $T(L)$ of a

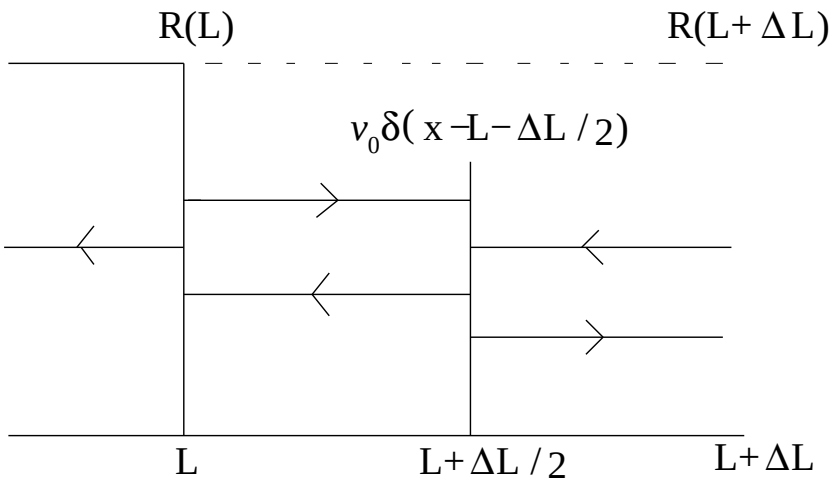


FIGURE 1.3: A schematic diagram of a scatterer of length $L$ having reflection amplitude $R(L)$; an added length $\Delta L$ makes the length of the scatterer $L + \Delta L$. The effective potential of the length $\Delta L$ is given by a delta-function potential of strength $v_0$.

sample of length $L$. In this approach, one first derives non-linear Langevin equations for $R(L)$ and $T(L)$, which vary with the length of the sample and then, calculates the electronic transport phenomena using the Landauer formula. One can study $1D$ disordered syatems analytically and non-perturbatively using invariant embedding [34–37]. In Chapter (3), we have applied this technique to investigate electrical transport in disordered conductors with external probes. Now, we briefy outline a derivation of the invariant embedding equations for $R(L)$ and $T(L)$, following Kumar [38].

Consider a disordered 1D conductor with $N$ random scatterers of length $L$ with the reflection amplitude $R(L)$, and $N+1$ scatterers of length $L+\Delta L$ with the reflection amplitude $R(L+\Delta L)$. Here, $L = N\Delta L$, where $\Delta L$ can be thought as lattice spacing. In the continuum limit, we use $\Delta L \to 0, N \to \infty$ keeping $N\Delta L = L$ fixed. We wish to find a relation between $R(L)$ and $R(L + \Delta L)$. Let there be a delta-function potential scatterer of strength $v(L)$ at length $L + \Delta L/2$, which acts as an effective scatterer due to length $\Delta L$ added with $L$. In the limit $\Delta L \to 0$ (i.e., $k_F \Delta L \ll 1$, with $k_F$ being the Fermi wave vector), we can treat the extra scatterer as an effective delta potential $v_0(L)\delta(x - L - \Delta L/2)$ with $v_0(L) = v(L)\Delta L$. One can easily evaluate reflection amplitude $r$ and transmission amplitude $t$ for an electron plane wave (with energy $\hbar^2 k_F^2/2m$) incident on a delta-function scatterer of strength $v_0(L)$. We expand $r$ and $t$ to first order in $\Delta L$ for the present problem.

$$r(L) = \frac{2mv(L)\Delta L}{2i\hbar^2 k_F}, \quad t(L) = 1 + \frac{2mv(L)\Delta L}{2i\hbar^2 k_F} \ . \tag{1.22}$$

Now, consider an electron wave of unit amplitude incident at Fermi energy ($E_F = \hbar^2 k_F^2/2m$) on the right side of the sample length $L + \Delta L$ as shown in FIG.(1.3). Summing all the process of

direct and multiple reflections and transmissions on the right side of the sample of length $L$ with the effective delta potential at $L+\Delta L/2$, one finds the geometric series for reflection amplitude.

$$R(L+\Delta L) = r(L)e^{ik_F\Delta L} + e^{ik_F\Delta L/2}t(L)e^{ik_F\Delta L/2}R(L)e^{ik_F\Delta L/2}t(L)e^{ik_F\Delta L/2} + ... \quad (1.23)$$

Substituting for the values of $r(L)$ and $t(L)$ from Eq.(1.22) in Eq.(1.23), and taking continuum limit for $k_F\Delta L \ll 1$, one determines the Langevin equation for $R(L)$

$$\frac{dR(L)}{dL} = i\frac{k_F}{2}\xi(L)(1+R(L))^2 + 2ik_FR(L) \quad \text{with} \quad \xi(L) = -\frac{2mV(L)}{\hbar^2k_F^2} \ , \quad (1.24)$$

and the initial condition $R(L=0)=0$. Similarly, one can show, for the transmission amplitude $T(L)$,

$$\frac{dT(L)}{dL} = ik_FT(L) + i\frac{k_F}{2}\xi(L)(1+R(L))T(L), \quad (1.25)$$

with the initial condition $T(L=0)=1$. In Chapter (3), we elucidate on how to solve the non-linear Langevin equations for weakly disordered systems within random phase approximation.

### 1.3.3 Lippmann-Schwinger scattering theory

The Landauer approach (also known as the Landauer-Büttiker formalism in mesoscopic physics) relies on determination of transmission coefficient in scattering theory. For disordered systems, one can use RMT. In the last chapter of this thesis, we have reported our results on transport through interacting mesoscopic systems, based on the Lippmann-Schwinger scattering theory. The Lippmann-Schwinger theory [39] is a time-independent formulation of elastic scattering processes. The simplest model of scattering experiment is given by solving the Schrödinger equation for a plane wave impinging on a localised potential (or scatterer) $\hat{V}$. A potential $\hat{V}$ might represent what an electron shooted from a metallic lead experiences in a quantum dot or an alpha particle from a nucleus in high energy experiments. The total Hamiltonian of the open system (with continuous energy spectra) can be written as

$$\hat{\mathcal{H}} = \hat{H}_0 + \hat{V} \ , \quad (1.26)$$

where $\hat{H}_0$ stands for the kinetic energy operator with plane wave energy eigenket $|\phi_{\mathbf{k}}\rangle$ satisfying

$$\hat{H}_0|\phi_{\mathbf{k}}\rangle = E_{\mathbf{k}}|\phi_{\mathbf{k}}\rangle \ . \quad (1.27)$$

Now we wish to find the eigenket $|\psi_{\mathbf{k}}\rangle$ of $\hat{\mathcal{H}}$ for the same energy eigenvalue $E_{\mathbf{k}}$, i.e.,

$$(\hat{H}_0+\hat{V})|\psi_{\mathbf{k}}\rangle = E_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle \ . \quad (1.28)$$

Next transforming the differential Eq.(1.28) to an integral equation in the bra-ket language, we get

$$|\psi_{\mathbf{k}}\rangle = |\phi_{\mathbf{k}}\rangle + \frac{1}{E_{\mathbf{k}} - \hat{H}_0}\hat{V}|\psi_{\mathbf{k}}\rangle \ . \tag{1.29}$$

$|\psi_{\mathbf{k}}\rangle$ correctly gives the undisturbed incoming wave $|\phi_{\mathbf{k}}\rangle$ for $\hat{V} = 0$. But complication arises from the singular nature of the operator $1/(E_{\mathbf{k}} - \hat{H}_0)$, which we encounter by the transformation from the differential Eq.(1.28) to the integral Eq.(1.29). To overcome the problem, one can add an infinitesimal imaginary part to the denominator of the singular operator. One needs to be careful about the sign of the imaginary part from the physical point of view since the solution (1.29) has a single incoming plane wave, and outgoing waves in all directions, generated by the interaction of the incoming wave with the scatterer $\hat{V}$. But the Schrödinger equation Eq.(1.28) could equally describe ingoing waves in other directions. So the physical solution is

$$|\psi_{\mathbf{k}}\rangle = |\phi_{\mathbf{k}}\rangle + \hat{G}_0^+\hat{V}|\psi_{\mathbf{k}}\rangle \ , \ \text{with} \ \ \hat{G}_0^+ = \frac{1}{E_{\mathbf{k}} - \hat{H}_0 + i\epsilon} \ . \tag{1.30}$$

The last equation Eq.(1.30), is known as the Lippmann-Schwinger equation. We use Eq.(1.30) to determine exact two particle scattering states for the problem of electron transport through a one dimensional tight binding chain with e-e interaction in a bond of the chain. As we will see in Chapter (5), this problem can be mapped to a problem of calculating the eigenstates of an impurity in two dimensions.

## 1.4 Problems studied in this thesis

Finally in this section, we introduce the problems studied in the following four chapters. This thesis mostly comprises of the developement and applications of the recent transport approach employing Langevin equations and Green's functions. We have extensively used this method to investigate both thermal and electrical transport phenomena in non-interacting systems. Later, in the thesis, we also discuss our studies with the invariant embedding technique for disordered electronic systems and with the Lippmann-Schwinger equations for one dimensional models with electron-electron interactions.

In Chapter (2), we elaborate the LEGF transport approach to study heat transport in harmonic lattices. By solving generalised quantum Langevin equations of motion of harmonic lattices using Fourier transform method, we derive NEGF-like expressions for the steady state heat current through finite systems coupled to infinitely extended reservoirs. Our reservoirs are also modeled by harmonic lattices. Then, we employ this LEGF method to evaluate heat current through quantum harmonic chain with each site connected to self-consistent reservoirs. For infinite chain with finite coupling with the interior reservoirs, heat conduction is diffusive, satisfying Fourier's

law. We calculate a temperature-dependent thermal conductivity which, for high temperature classical limit matches with previous result obtained for classical model using different method. We also show that by tuning the strength of the coupling with self-consistent reservoirs, one can crossover from ballistic to diffusive thermal transport for finite chain length. We complete this chapter with another application of LEGF to derive asymptotic expressions for steady state heat current in ordered harmonic lattices with different boundary conditions implied by on-site pinning potentials.

Chapter (3), is the longest chapter of this thesis; here we report four different problems on electrical transport in the presence of external probes. In the first part here, we apply LEGF to investigate electron transport through one (or quasi one) dimensional systems in the presence of the dissipative environment (present in the real experimental set-up due to interactions of electrons with other degrees of freedom), modeled by the self-consistent stochastic reservoirs which act as a source of inelastic scatterings. As expected, depending on the strength of inelastic scattering, transport through the one-dimensional wire crosses over from ballistic to Ohmic region above some critical size of the wire. We show how dissipation from the wire gets equally distributed from end contacts to bulk of the wire as the transport character shifts from ballistic to Ohmic behaviour. We also extend the phenomenology for uniform dephasing to mesoscopic metallic rings. The next part of this chapter deals with the invariant embedding technique. We demonstrate the comparison between phase randomisation and decoherence responsible, respectively, for localization phenomenon and classical nature. For this purpose, we introduce phase disorder in a 1D quantum resistor through the formal device of 'fake channels' distributed uniformly over its length such that the out-coupled wave amplitude is re-injected back into the system, but with a phase which is random. The associated scattering problem is treated via invariant embedding in the continuum limit, and the resulting transport equation is found to correspond exactly to the Lloyd model of disordered system. It is further argued that our phase-randomizing reservoir, distinct from the well known phase-breaking reservoirs, induces no decoherence, but essentially destroys all interference effects other than the coherent back scattering. Using Migdal-Kadanoff scaling theory, we extend the phenomenology of decoherence via external reservoirs (phase-breaking reservoirs) to higher dimensional disordered quantum resistance. We find that there is no metal-insulator Anderson transition on minute introduction of decoherence in three dimensional disordered systems. We also compute the corrections to the conductance due to the decoherence in two and three dimensions.

In Chapter (4), we consider the implementation of LEGF method to study heat transport in disordered harmonic lattices. Some years back, it was shown in an important paper [18] on heat conduction in the mass-disordered harmonic chain that the thermal conductivity depends not just on the system itself but also on the spectral properties of the heat baths. Now, we find an interesting universality in the length dependence of the thermal conductivity of the disordered

chain coupled to different thermal baths such as Rubin's model of baths and Langevin white noise baths. We yield analytical expressions for the disorder-averaged steady state thermal current through the disordered chain for fixed and free boundary conditions. We also address the effects of finite number of quadratic pinning potentials in the disordered chain. Finally we discuss these results in the quantum regime of heat transport.

Next, in Chapter (5), we turn our attention to a model with electron-electron interactions. Here, we employ the Lippmann-Schwinger scattering theory to address the problem of transmission of electrons between two noninteracting leads through a region where they interact. We consider a model of spinless electrons hopping on a one-dimensional lattice with electron-electron interactions on a single bond. We show that all two-particle states in this model can be found exactly. The scattering states are analysed in details to get exact expressions for the S-matrix. Comparisons are made with numerical results from time evolution of a two-particle wave-packet, which reveal several interesting and subtle features. For $N$ particles the scattering state is obtained within a two-particle scattering approximation. For a dot connected to Fermi sea at different chemical potentials, we find an expression for the change in the Landauer current resulting from the interactions on the dot. We also extend our technique to study nonequilibrium phenomena of more general interacting electronic systems such as parallel and series double dots or interacting parallel conductors in proximity to one another.