Charge and energy transport in the presence of disorder and interactions

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DECLARATION

I hereby declare that this thesis is composed independently by me at the Raman research Institute, Bangalore, under the supervision of Dr. Abhishek Dhar. The subject matter presented in this thesis has not previously formed the basis of the award of any degree, diploma, associateship, fellowship or any similar title in any other University.

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CERTIFICATE

This is to certify that the thesis entitled **Charge and energy transport in the presence of disorder and interactions** submitted by Dibyendu Roy for the degree of DOCTOR OF PHILOSOPHY of Jawarharlal Nehru University, is based upon his original work and that neither this thesis nor any part of its has been submitted for any degree / diploma or any other academic award anywhere before.

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List of Publications

I. articles in journals:

[1] Dibyendu Roy and N. Kumar, *Langevin dynamics in crossed magnetic and electric fields: Hall and diamagnetic Fluctuations.*, Phys. Rev. E 78, 052102 (2008).

[2] Dibyendu Roy and Abhishek Dhar, *Role of pinning potentials in heat transport through disordered harmonic chain*, Phys. Rev. E 78, 051112 (2008).

[3] Dibyendu Roy, *Crossover from ballistic to diffusive thermal transport in quantum Langevin dynamics study of a harmonic chain connected to self-consistent reservoirs* , Phys. Rev. E **77**, 062102 (2008).

[4] Abhishek Dhar, Diptiman Sen and Dibyendu Roy *Scattering of electrons from an interacting region*, Phys. Rev. Lett. **101**, 066805 (2008).

[5] Dibyendu Roy and Abhishek Dhar, *Heat transport in ordered harmonic lattices*, Journal of Statistical Physics **131**, 535 (2008).

[6] Dibyendu Roy and N. Kumar, *Decohering d-dimensional quantum resistance*, Phys. Rev. B **77**, 064201 (2008).

[7] Dibyendu Roy, *Electron transport in an open mesoscopic metallic ring*, J.Phys.: Condens. Matter **20**, 025206 (2008).

[8] Dibyendu Roy and N. Kumar, *Random-phase reservoir and a quantum resistor: The Lloyd model* , Phys. Rev. B **76**, 092202 (2007).

[9] Dibyendu Roy and Abhishek Dhar, *Electron transport in a one dimensional conductor with inelastic scattering self-consistent reservoirs* , Phys. Rev. B **75**,195110 (2007).

[10] Abhishek Dhar and Dibyendu Roy, *Heat transport in harmonic lattices* , Journal of Statistical Physics **125**, 801 (2006).

Abstract

This thesis deals with different perspectives on charge and heat energy transport in one, two and three dimensions from the context of disorder, decoherence and interaction between carriers. A complete theory of transport should not only take account of the system, but also consider the reservoirs and system-reservoir couplings. This is referred as open-system description of transport. This thesis mostly comprises of the developement and applications of a recent transport approach employing Langevin equations and Green's function (LEGF) within the framework of open-system description of transport. We have extensively applied this method to study both thermal and electrical transport phenomena in non-interacting systems. We also include our studies employing the invariant embedding technique for disordered electronic systems and applying the Lippmann-Schwinger scattering theory for transport in mesoscopic models with electron-electron interactions. 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. Below we briefly present the details of the problems studied and results obtained in this thesis.

Chapter (1) is an introduction to the thesis. Here we first describe five traditional transport approaches in the context of charge and energy transport in solids and compare different approaches. Next part of the chapter is devoted to the essential and important ideas directly related to our work and the problems investigated in the thesis. We introduce some interesting models of electrical and thermal disordered systems, voltage probes and electron-electron interactions in mesoscopic systems. Later, we discuss three more transport approaches which we apply in this thesis.

In Chapter (2), we introduce the LEGF transport approach in detail to study heat conduction in harmonic lattices. By solving generalised quantum Langevin equations of motion of harmonic lattices using Fourier transform method, we evaluate the steady state heat current through finite systems coupled with infinitely extended reservoirs. Our reservoirs are also modeled by harmonic lattices. The resulting expressions for the steady state current is similar in form to those obtained from the nonequilibrium Green's function (NEGF) method. Then we employ this LEGF method to calculate steady state 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 derive an expression for the temperature-dependent thermal conductivity which, in the high temperature classical limit, matches with the 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 regime of thermal transport in the finite chain. We end 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. We discuss the later results in the context of higher dimensions and quantum regime.

Chapter (3) reports four different problems on electrical transport in the presence of various type 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 modeled by self-consistent stochastic reservoirs or voltage probes which act as sources of inelastic scatterings (hence, one has decoherence and dissipation in the systems). 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. Next part of this Chapter deals with the invariant embedding technique. Here, we demonstrate the comparison between phase randomisation and decoherence, responsible for localization phenomenon and classical nature, respectively. For this purpose, we introduce phase disorder in a one dimensional quantum resistor through the formal device of 'fake channels' distributed uniformly over its length L such that the out-coupled wave amplitude is re-injected back into the system, but with a phase which is random between 0 and 2π. The associated scattering problem is treated via invariant embedding in the continuum limit, and the resulting transport equation for the transmission amplitude $T(L)$ 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 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 decoherence in two and three dimensions.

Chapter (4) gives detail of the implementation of LEGF method to study heat transport in disordered harmonic lattices. We find an interesting universality in the length dependence of the

thermal conductivity of the disordered chain coupled with different thermal baths such as Rubin's model 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 imposed by the quadratic pinning potentials. We also address the effects of finite number of quadratic pinning potentials in the disordered chain. Finally, we comment on the above results in the quantum regime of thermal energy transport.

Finally, in Chapter (5), we turn our attention to a microscopic model with electron-electron interactions. Here we employ 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 and 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 detail yielding exact expressions for the S-matrix. We also compare our scattering theory results with numerics from time evolution of a two-particle wave-packet and find 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 in the dot. We also extend our technique to study non-equilibrium phenomena of more general interacting electronic systems such as parallel and series double dots or interacting parallel conductors in proximity to each other. We discuss how the presence of the onsite energy in the interacting localized regime modifies the change in the Landauer current; the later part has been evaluated numerically.

Contents