Quantum Transport in Mesoscopic Systems

Coulomb Blockade and Kondo Effect

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A short introduction to the quantum transport in mesoscopic systems is given, and various regimes of quantum transport such as diffusive, ballistic, and adiabatic are explained. The effect of interactions and inelastic scattering along with the characteristic coherent effects of mesoscopic systems give interesting new mesoscopic effects, such as Coulomb Blockade and Kondo Resonance. The basic physics of these phenomena is explained in simple language. In the end, some current research problems in this field are discussed.

Keywords
Quantum transport, mesoscopic systems, Coulomb blockade, Kondo effect.

1. Introduction to Electronic Transport in Mesoscopic Systems

It is well known that the conductance G of a macroscopic conductor is given as $G = \sigma A/L$, where σ is the conductivity (the intrinsic property of the conducting material), A is the area of cross-section of the conductor, and L is its length. So the conductance decreases as the cross-sectional area is reduced and it increases as the length of the conductor is reduced. One may suspect that the conductance goes to infinitely large values as the length of the conductor is made extremely small. But this is not true. The above mentioned simple scaling law (or the so-called ohmic behavior) breaks down at mesoscopic length scales (sub-micrometer length scales) to be defined precisely later. It does not become infinite, but it reaches a limiting value G_c. To understand the cause of the breakdown of this simple scaling law, one has to take into account the quantum nature of the electrons, according to which, the electron is not a classical tiny charged particle, but a quantum

mechanical wave-particle. This wave character of the electron is responsible for many analogies in the field of Anderson localization, propagation of light through a random medium, and mescoscopic conduction through a disordered sample with static disorder. The mesoscopic length scales (usually submicrons) are defined as length scales at which the wave character of electrons has definite effect on the measurable physical properties, such as conductance. The conductance no longer monotonically varies but it shows 'jumps' or 'steps' in units of $G_c = 2e^2/h$. This is a universal character independent of the material of the sample.

Box 1. Glossary

***Aharanov–Bohm oscillation*:** When an electron moves in a magnetic field, its wave function picks up an additional phase, called the Aharanov–Bohm phase. In a ring with a threaded magnetic field, the phase difference between the two alternate paths for an electron to go from one point of the ring to a point across is proportional to the magnetic flux through the ring. Hence in mesoscopic rings with tunable threaded magnetic fields the current across the ring oscillates as a function of the magnetic field due to the tunable interference effects that result.

***Anderson localization*:** In a sufficiently strong disorder, due to back scattering and quantum interference effects, electronic wave functions get localized (with exponentially decaying amplitude from a localization site). The typical length scale over which one such wave function is localized is called its localization length, and this phenomenon is called Anderson localization.

***Coulomb blockade*:** If the tunneling energy of the electron is much less than the thermal energy and applied voltage bias, the tunneling of the electron from the lead to the dot and vice versa will happen very rarely. Then two successive tunneling events will not be phase coherent, and the charge on the dot itself is nearly quantized, and changes in easily seen-steps of unit charge. This is called the sequential tunneling and the regime of Coulomb blockade.

***Equation-of-motion theory*:** From the Heisenberg (picture) equations for the time evolution of the field operators, if one differentiates a one-particle Green's function with respect to one of its time arguments one obtains the first of an infinite hierarchy of 'equations of motion' involving successively higher order Green's functions. One has to truncate this hierarchy by invoking some physical arguments, i.e., mean field approximation or neglect of higher order correlations to obtain a closed set of differential equations that can be solved for the Green's functions.

Continued...

Box 1. Continued

***Green's function*:** In condensed matter systems, Green's function refers to space and time-dependent correlation functions of field operators (creation or destructions operators that can add or remove electrons). Many observable properties of the system (for example spectral function) are directly expressible in terms of the simplest, 'one-particle' Green's functions which involve one creation and one destruction operator.

***Keldysh's non-equilibrium Green's functions method*:** It is a mathematical technique to extend the Green's function method to non-equilibrium or time-dependent situations. Perturbation expansion is made on an imaginary contour (called Keldysh contour). This also called contour perturbation theory.

***Kondo effect*:** If the dot–lead coupling is strong (i.e., greater than the thermal energy and applied voltage bias), then the electron tunneling events will be frequent. A very interesting case emerges when the coulomb interaction effects on the quantum dot are sizable, whence two successive tunneling events can cause the spin of a single unpaired electron on the dot to flip. As a consequence, at sufficiently low temperatures a local 'spin screening cloud' or a subtle 'correlated many-body state' called Kondo resonance is formed between the unpaired dot electron and the lead electrons. This effect, called the Kondo effect, enhances the conductance of the quantum dot and lifts the Coulomb blockade.

***Linear response theory*:** It is the formal theory that describes the response of quantum systems to external perturbations that are small enough in size that the response of the system is linearly related to the perturbing field. It establishes the fundamental connection between fluctuations and dissipation, leading to transport coefficients being expressible as integrals of time correlation functions.

***Spectral function*:** Related to the imaginary part of the Fourier transform of the Green's function, it defines the spectrum of possible excitation energies for adding or removing a particle.

***Quantum dots and metallic quantum dots*:** A quantum dot can be thought of as an artificial atom, or a small droplet of electrons. In such low dimensionality systems, electron–electron interactions are very important, and Fermi Liquid theory breaks down; the low energy excitations of such systems with a few interacting electrons can no longer be mapped to those of a system of nearly non-interacting quasi-particles, as can be done in extended systems. In a quantum dot the electrons have a discrete energy spectrum, and in a large dot the spacing between the energy levels can become small enough for the energy spectrum to be regarded as quasi-continuous. Then it is referred to as a metallic quantum dot.

The physics of electron transport is called mesoscopic transport physics when (i) the de-Broglie wavelength associated with the electrons, (ii) the mean free path, which is the distance traveled by the electron before its initial momentum is destroyed, and (iii) the phase relaxation length, which is the distance traveled by the electron before its initial phase is destroyed, become of

the order of the sample size. In this regime all our classical intuition about electron transport breaks down. New interesting effects appear, such as the above mentioned conductance quantization, universal conductance fluctuations, interference effects in mesoscopic rings and their tuning by threaded magnetic fields (Aharonov–Bohm oscillations), interesting phenomena in driven quantum dots such as Coulomb blockade, Kondo effect, non-equilibrium Kondo effect, quantum dynamics of the Kondo cloud, etc.

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Roughly speaking, these mesoscopic effects can be divided into two parts: (1) equilibrium or static properties (such as interference effects in mesoscopic rings and their tuning by threaded magnetic fields) which are by now quite well understood and (2) non-equilibrium problems (such as in driven quantum dot systems, Coulomb blockade, non-equilibrium Kondo effect, quantum dynamics of the Kondo cloud), which are not yet well understood (see the discussion on open problems at the end of Section 2).

Early quantum theories of electron transport in bulk metals were semi-classical in nature, and consisted of two steps: (1) The electrons were accelerated by external forces across Bloch states, and then scattered between Bloch states by impurities or phonons. (2) In the second step, balancing processes were treated using simple occupation probabilities, which do not consider any coherent processes (for a review of semi-classical (incoherent) transport in metals based upon the Bloch–Boltzmann–Peierls kinetic equation, see [1]). All the phase information was considered to be lost in scattering. This semi-classical approach completely fails in electron transport in mesoscopic conductors, where the phase relaxation length of electrons becomes of the order of the size of the sample or device. A radically new approach was needed to understand coherent transport in mesoscopic conductors. The first steps in this direction were taken

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by Landauer [2], Buttiker [3], and refined and clarified further by Imry [4]. The theme of their theory of quantum transport can be summed as 'conductance viewed as transmission'.

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1.1 *Diffusive Regime*

The mesoscopic sample here is the usual experimental sample: the two-dimensional electron gas (2-DEG), formed at the interface of a heterojunction usually of GaAs/GaAlAs. This 2-DEG has many desirable features as compared to thin metallic films. It has very low electron density ($\sim 10^{12}/\text{cm}^2$) which can be externally controlled by using gate electrodes. This implies large Fermi wavelength ($\sim$ 40nm) comparable to the nanosample and very large electron mean free path ($\sim 10\mu$m) at low temperatures ($\sim$ 1K), and the quantum interference effects extend over the length of the sample. In this regime phonon generation and inelastic scattering are not there and elastic scattering processes do not destroy phase coherence.

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As static disorder leads to elastic scattering, the presence of it does not destroy phase coherence and the conductance of a disordered sample is very much affected by the way in which the impurities are distributed in the sample. Conductivity changes from sample to sample. This is the regime of diffusive transport in which the sample is much bigger than the electron average mean free path, i.e., $L \gg l$. There is another important length scale known as localization length l_{loc}. In a sufficiently strong disorder (in 3D case), due to back scattering and quantum interference effects, electrons form localized states (with exponentially decaying wave packet from a localization site). The typical length scale over which

the wave packet is localized is called the localization length ($l_{\rm loc}$). This phenomenon was first pointed out by Anderson [5]. In the regime where $L \gg l_{\rm loc} \gg l$, and at zero temperature, the sample behaves as an insulator. But at a finite temperature transport can be subdiffusive. In this regime transport is dominated by thermal activation mechanisms such as hopping to a nearby localized state. Dimensionality plays a crucial role in this localization regime. In 1D all the states are localized even for a vanishingly small disorder. But in 2D, states are only marginally localized for weak disorder and a small magnetic field or spin-orbit coupling can lead to the existence of extended states that leads to transport.

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1.2 *Ballistic Regime*

Now if the sample size is very small ($L \sim l$), the elastic scattering of electrons by the impurities can be neglected as there will be very few impurities in the path of the electron, and we enter into a regime called ballistic transport. It is very helpful, conceptually and computationally, to view conductance as an average transmission of the sample. The transmission properties of the sample depend strongly on the shape of the sample, very much like in a wave-guide in radar electronics, where the geometry of the wave-guide affects its transmission properties. The quantum transport in this regime can be very well understood by using the Landauer formalism. The conductance of a ballistic conductor is given by the Landauer formula,

$$G = \frac{2e^2}{h} \sum_{m,n=1}^{N} |t_{mn}|^2 = \frac{2e^2}{h} {\rm Tr} T T^{\dagger} \ . \qquad (1)$$

Here T is the transmission matrix and t_{mn} is an element of it, which gives the transmission probability amplitude from mode n to mode m. The generalization of this two-terminal Landauer formula to multi-terminal samples is

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due to Buttiker [3]. Here the T-matrix describes the elastic scattering only. One may ask the question (based on the experience with macroscopic conductors, heating resistors, light bulbs, etc.): Where is the dissipation happening because inside the conductor we have only elastic processes? The answer lies in the mechanisms that occur inside the reservoirs used to drive current through the mesoscopic sample – inelastic scattering processes in the reservoirs cause dissipation.

1.3 *Adiabatic Regime*

The third kind of quantum transport called adiabatic transport happens in 2D systems in the presence of a strong perpendicular magnetic field. In this case, a fine shell of electrons around the Fermi energy splits to form levels called Landau levels. The magnetic length of the electron ($\sqrt{\frac{\hbar}{eB}} \sim 10\,\text{nm}$) is the characteristic wavelength of the electron in the problem. If the magnetic length is of the order of the sample size, then inter-Landau level scattering of the electrons is suppressed and they flow without scattering. This is called the adiabatic transport regime.

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The above three situations are idealistic (although experimentally realizable) in the sense that we have neglected all the electron–electron and electron–phonon interactions. In quantum dots or so-called artificial atoms, electron–electron interactions are important, as the Fermi liquid theory breaks down in such low-dimensionality systems. We cannot replace a few interacting electrons by almost non-interacting quasi-particles, as one can do in extended systems. So a new formalism or methodology is required. Also in most of the situations of quantum transport experiments we have a non-equilibrium situation. Thus a different microscopic theory called non-equilibrium Green's function formalism (NEGF) is required to describe the interacting non-equilibrium mesoscopic systems. The semi-classical kinetic transport

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2. Non-Equilibrium Transport Phenomena in Quantum Dot Systems: Coulomb Blockade and Kondo Effect

A typical mesoscopic quantum dot system (a small droplet of electrons) is shown in *Figure* 1. It consists of a quantum dot with discrete energy spectrum, whose mean energy level spacing is δE (in some cases, one has a metallic dot with quasi-continuous energy spectrum). The dot is connected with two metallic leads through tunnel couplings ($H_{\rm TL}$ for left lead and $H_{\rm TR}$ for right lead). The gate electrode with voltage $V_{\rm g}$ is used to control the number of electrons on the quantum dot. A voltage bias is applied between the right and the left leads to drive a tunneling current through the system [6,7]. The conductance or V/I characteristics of the system shows a very rich behavior with subtle many-body effects.

The general system Hamiltonian consists of the following parts,

$$H = H_{\rm D} + H_{\rm L} + H_{\rm R} + H_{\rm T} \ . \qquad (2)$$

Here $H_{\rm D}$ is the dot Hamiltonian which further consists of two parts: (i) the non-interacting part $H_{\rm D}^0 = \sum_{\nu_{\rm D}} \xi_{\nu_{\rm D}} C_{\nu_{\rm D}}^\dagger C_{\nu_{\rm D}}$, (here $\nu_{\rm D}$ represents different levels in the dot) and (ii) the interaction between the dot electrons $H_{\rm D}^{\rm int}$. It could be either constant interaction model ($H_{\rm D}^{\rm int} = \frac{e^2}{2C}(\sum_\nu n_\nu)^2, C \equiv$ dot capacitance) or Anderson type model of the total Hamiltonian ($H_{\rm D} = \sum_{\sigma=\uparrow\downarrow} \xi_{d\sigma} C_{d\sigma}^\dagger C_{d\sigma} + U n_{d\downarrow} n_{d\uparrow}$). Here U is the Coulomb interaction energy

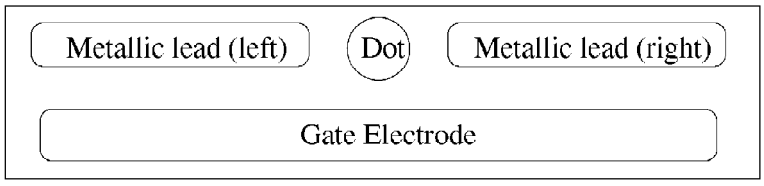

Figure 1. Mesoscopic quantum dot system.

If the tunneling energy is much less than the thermal energy and applied voltage bias, the tunneling of the electron from the lead to the dot and vice versa will happen very rarely.

among the electrons which is of the order of charging energy Δ of the dot. The left and right metallic lead Hamiltonians are as usual ($H_\alpha = \sum_{k,\alpha=\mathrm{L,R}} \epsilon_{k\alpha} C^\dagger_{k\alpha} C_{k\alpha}$, $\alpha = \mathrm{L,R}$). H_T represents the tunneling Hamiltonian which further consists of two parts, (i) tunneling from the left side ($H_\mathrm{TL} = \sum_{\nu_\mathrm{L}\nu_\mathrm{D}} t^\mathrm{L}_{\nu_\mathrm{L}\nu_\mathrm{D}} C^\dagger_{\nu_\mathrm{L}} C_{\nu_\mathrm{D}} + hc$) and (ii) tunneling from the right side ($H_\mathrm{TR} = \sum_{\nu_\mathrm{R}\nu_\mathrm{D}} t^\mathrm{R}_{\nu_\mathrm{R}\nu_\mathrm{D}} C^\dagger_{\nu_\mathrm{R}} C_{\nu_\mathrm{D}} + hc$). In the Anderson model only one level is assumed in the dot.

Now if the tunneling energy is much less than the thermal energy and applied voltage bias, the tunneling of the electron from the lead to the dot and vice versa will happen very rarely (this timescale is the largest timescale in the problem). Two successive tunneling events will not be phase coherent and charge is quantized in the sense that electron as a whole will be transferred. This is called 'sequential tunneling' and we are in the regime of Coulomb blockade. The phenomenon of Coulomb blockade occurs at sufficiently low temperatures where Coulomb charging energy (energy required to put one electron in the dot) $\Delta = \frac{e^2}{2C}$ is much greater than thermal activation energy (thermal energy). That is, $k_\mathrm{B}T$ ($\mathrm{T} \sim 1$Kelvin) $\ll \frac{e^2}{2C}$($C \sim 0.1$ femto farad). High temperatures ($k_\mathrm{B}T \gg \frac{e^2}{2C}$) destroy Coulomb blockade. For some values of the gate voltage V_g, there exists a finite Coulomb charging energy; thus the electron transfer through the dot is not very easy and the conduction is low. But for some typical values of the gate voltage, charging energy is very small, and electrons flow through the dot very easily. It is called the activationless transfer. Thus the conductance of the quantum dot system shows regularly spaced peaks and valleys as a function of the gate voltage and the average charge on the dot increases or decreases in steps (see *Figure* 2a) or in units of an elementary charge known as 'Coulomb Staircase' – a hallmark of Coulomb blockade phenomena.

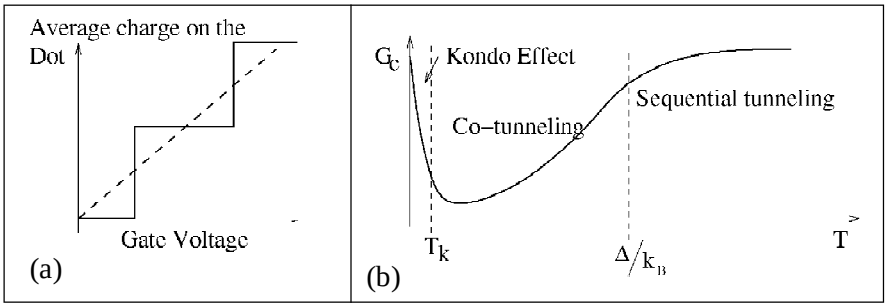

Figure 2. (a) Coulomb Staircase showing the single electron transfer; at high temperatures $k_BT \gg e^2/2C$, this Coulomb blocking vanishes and the average charge on the dot varies linearly with the applied gate voltage (dotted line). (b) Conductance vs temperature for the quantum dot; $\Delta = e^2/2C$ is the electron charging energy (adding or removing of one electron), and C is the dot capacitance.

Because the coupling strength is small, one can use the Fermi golden rule (lowest order in perturbation theory) to get the tunneling rates. Then one can solve for the dynamical behavior of the distribution function of the dot states by setting up a rate equation or master equation [8].

But if the dot–lead coupling is strong (i.e., greater than the thermal energy and applied voltage bias) we cannot use lowest order perturbation theory – the Fermi golden rule. Instead we have to use the generalized Fermi golden rule, i.e., T-matrix. The tunneling events will be frequent, and higher order virtual processes will contribute to tunneling. This is called co-tunneling. There will be a 'leakage' current even in the Coulomb blockade case. The co-tunneling process can be either elastic (no change in the electron energy in the leads) or inelastic (change in the electron energy in the leads due to the formation of electron-hole pair). A very interesting case emerges when co-tunneling involves a spin flip of a single unpaired electron on the dot; at sufficiently low temperatures a local 'spin screening cloud' or a subtle 'correlated many-body state' called Kondo resonance is formed. This enhances the conductance of the quantum dot and lifts the Coulomb blockade – it is called Kondo effect (see *Figure* 2b).

A very interesting case emerges when co-tunneling involves a spin flip of a single unpaired electron on the dot; at sufficiently low temperatures a local 'spin screening cloud' or a subtle 'correlated many-body state' called Kondo resonance is formed. This enhances the conductance of the quantum dot and lifts the Coulomb blockade – it is called Kondo effect.

For non-perturbative treatments when dot–lead coupling is strong, one has to use the Green's function apparatus. For example, in the Anderson-type model discussed above one can calculate the conductance for small applied bias by using the linear response theory, but coupling can be treated to any desired order. One first does a rotation in left lead and right lead electron operators and then uses the linear response theory result (for details, see [6]) and expresses the conductance as a function of retarded current–current correlation function – the Kubo formula,

$$G = \lim_{\omega \to 0} \mathrm{Re}[\frac{ie^2}{\omega} C^{\mathrm{R}}_{II}(\omega)], \qquad (3)$$

to arrive at the conductance

$$G = -e^2 \sum_{\sigma} \int \frac{\mathrm{d}\xi}{2\pi} \frac{\Gamma^{\mathrm{L}}\Gamma^{\mathrm{R}}}{\Gamma^{\mathrm{R}} + \Gamma^{\mathrm{L}}} A(d\sigma, \xi)(\frac{\partial n_{\mathrm{F}}(\xi)}{\partial \xi}), \qquad (4)$$

where n_{F} is the Fermi distribution function. The spectral function $A(d\sigma, \xi)$ is the central quantity. It is calculated from the retarded Green's function ($A(d\sigma, \xi) = -2\mathrm{Im}G^{\mathrm{R}}(d\sigma, \omega)$) to any order in perturbation of tunneling.

The retarded Green's function is computed using the equation-of-motion theory, in which one differentiates $G^{\mathrm{R}}(d\sigma, \xi) = -i\theta(t)\langle\{C_{d\sigma}(t), C^{\dagger}_{d\sigma}(t')\}\rangle$ with respect to time, and one gets equations of motion involving higher order Green's functions. One has to truncate this recursive procedure by invoking some physical arguments, i.e., mean field approximation or neglect of higher order correlations. For Coulomb blockade problem it is not necessary to take into account the higher order processes involving spin flip; by neglecting the higher order correlations one closes the hierarchy, and Coulomb blockade physics can be explained. But for Kondo effect one has to take into account these higher order spin-flip processes. Finally by the knowledge of Green's function

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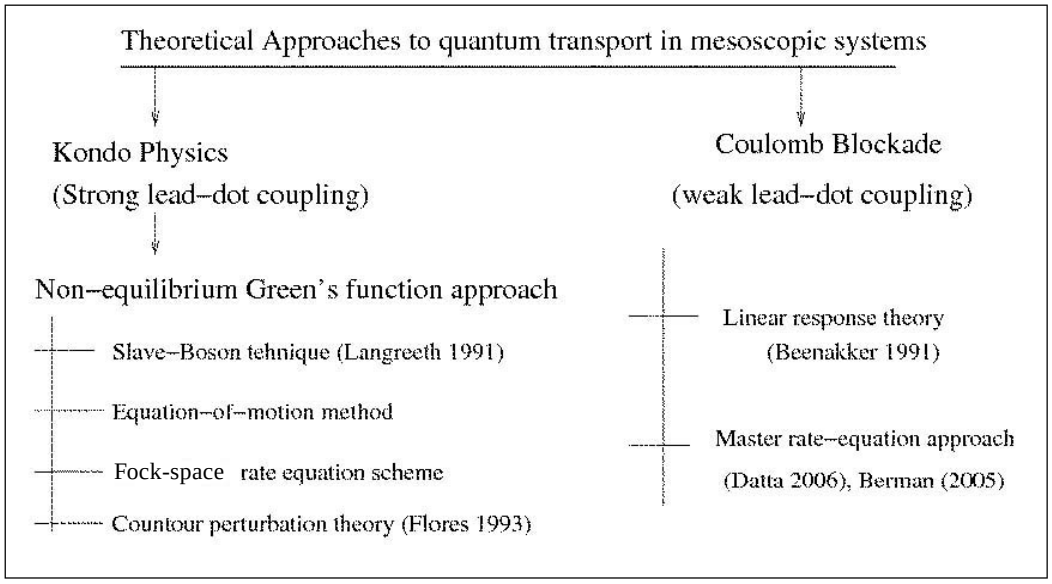

Figure 3. Various theoretical approaches.

and spectral function one calculates the conductance. The very interesting behavior of conductance as a function of temperature is shown in *Figure* 2b. Beyond linear response, i.e., finite voltage bias, one can calculate the conductance using Keldysh's non-equilibrium Green's function method [9]. The present status of various theoretical approaches to quantum transport through mesoscopic systems is summarized in *Figure* 3.

One research problem of current interest is the inelastic scattering effects due to large applied bias on the Kondo physics. The equilibrium properties of the Kondo effect are well understood and it is quite a mature field now. The methods used to treat the equilibrium problems are also understood; equilibrium Bethe ansatz, renomalization group, conformal field theory, bosonization, equilibrium slave-boson technique, etc., are now textbook material [11–14]. However, in out-of-equilibrium cases, many of the above methods fail. One has to generalize these for out-of-equilibrium situations – a wide open domain. Recently, there has been progress, like non-equilibrium generalization of equilibrium Bethe ansatz [15]. On the experimental front considerable progress is

going on in the out-of-equilibrium regime [16]. One reason is that the biases applied in nano-electronic devices are sufficiently large that steady-state transport cannot be described as a perturbation about the equilibrium state.

2.1 *Some Open Problems*

Although out-of-equilibrium physics of mesoscopic systems is largely unexplored, for definiteness or to be specific, we consider a recent ongoing controversy about splitting the Kondo peak and its disappearance at large applied bias.

It is well known that at equilibrium, Kondo correlations due to spin flip processes give rise to a sharp resonance in the density of states (DOS) at the chemical potential of the leads (in equilibrium both leads are at the same potential). For a finite bias the resonance was predicted to split [17]. The two peaks are now at the different chemical potentials of the leads. As the applied bias is increased further, the peaks become progressively smaller and smaller due to decoherence introduced by the inelastic scattering of the electrons from the two leads [17,18].

The question whether Kondo correlations survive at voltage larger than Kondo temperature at equilibrium has raised a considerable debate [18,19]. In other words, what is the governing energy scale in out-of-equilibrium Kondo effect? How and by what rate do inelastic channels open up as the bias is increased? These are some of the questions that are open. The treatment of the inelastic effects is a major open problem now.

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Another problem is about Kondo splitting in magnetic fields. Theoretical investigations [17] point out that the Kondo peak in the differential conductance measurements as a function of applied bias across the leads should split in the presence of a parallel magnetic field. Instead of one peak at the origin in zero B case, two

peaks appear at $eV = \pm 2\Delta$, where $\Delta = |g|\mu_B B$ is the Zeeman energy for the spin splitting, in finite B case. This prediction was experimentally verified by Cronenwell *et al* [20]. But later on, theoretical investigations by Costi [21] predicted that due to the screening of the Kondo spin by the conduction electrons of the leads, spin splitting should occur only above some critical magnetic field B_c which is a function of Kondo temperature T_k. Experiments [22] agree with the theory on the value of critical magnetic field but are in disagreement with theory on the position of the peaks, *peak distance is more than* 2Δ. Also the theoretically predicted critical magnetic field B_c as a function of T_k is larger than what is experimentally measured in [22].

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