12 Overview of the theory

In this Section, the main results of the theory of quantum transport in quasi-one dimensional electron systems are summarized. As references, with the exception of a few key articles, solely review articles are provided. The number of original papers in this field is so tremendously large that citing even only a selected number of them would certainly exceed the frame of this overview.

In contrast to their higher dimensional counterparts, several aspects of interacting one dimensional (1D) electron systems are exceptional.

1. By removing a single chemical bond between two adjacent atoms in a chain, the system is cut into two independent parts. The transport is completely blocked.

2. One-electron excitations are not well-defined. Landau-quasi-particles do not exist. The energetically lowest excitations are collective charge and spin density modes. In analogy with the higher dimensional Fermi liquid, the interacting one dimensional electron system is called a Tomonaga-Luttinger liquid.

3. Some properties may be treated mathematically rigorously. The most important examples are the scattering by impurities (localization), the flow of electrical current, and low-energy collective low-energy charge and spin modes. Thus, results obtained in the 1D limit may serve as a key for the understanding of the properties of higher dimensional systems.

12.1 Quasi-1D ideal quantum wires

The subject of quantum transport in almost ideal quasi-1D semiconductor systems has been treated exhaustively in a review article by Beenakker and van Houten from both the experimental as well as the theoretical viewpoint.

This includes a survey on the basic material aspects, especially of GaAs/AlGaAs heterostructures, and a description of many of the diffusive and quasi-ballistic transport properties, starting with classical size effects, weak localization, conductance fluctuations, the Aharonov-Bohm effect, certain aspects of electron-electron interaction, quantum size effects and the influence of a periodic potential.

Ballistic transport is discussed including quantum point contacts, electron focusing and collimation as well as scattering in a junction of quantum wires and tunneling effects. Adiabatic transport in smooth point contacts as well as in strong magnetic fields is also discussed [91B5].

12.2 Impurity scattering and localization

Neglecting electron interaction, the standard Hamiltonian has the form [93K]

$$H = H_{\mathrm{kin}} + H_{\mathrm{imp}} \,. \tag{68}$$

Here H_{kin} and H_{imp} are the operators of the kinetic energy and the impurity potential, respectively. Most simple examples of the former are

$$H_{\mathrm{kin}} = \frac{p^2}{2m^*} \tag{69}$$

in the continuum limit, or

$$H_{\mathrm{kin}} = t \sum_{[jk]} |j\rangle\langle k| \tag{70}$$

in the lattice limit, with a complete set of states $|j\rangle$ associated with the sites of a regular lattice (lattice constant a). In the former case, the 1D operator of the momentum is $p = (\hbar/\mathrm{i})(\partial/\partial x)$ and m^* denotes the effective mass of the electron. In the latter case, t is the amplitude for an electron

to be transferred between two neighbouring lattice sites j and k. A relation between the two limits can be established by the effective mass approximation of the Schödinger equation corresponding to (70) which gives

$$m^* = \frac{\hbar^2}{a^2 t} \,. \tag{71}$$

The impurity potential energy is

$$H_{\text{imp}} = \sum_j V_j(x) \tag{72}$$

in the continuum limit, V_j representing the potential energy of the impurity j at space point x, and in the lattice limit

$$H_{\text{imp}} = \sum_j \varepsilon_j |j\rangle\langle j| \tag{73}$$

with ε_j the energies associated with the lattice sites j.

The impurity potential energy (as well as the lattice site energy) is usually assumed to be distributed randomly

according to some probability density distribution $P([V]) = P(V_1 \ldots V_N)$ (N number of impurities, lattice sites). For statistically independently distributed impurities

$$P([V]) = \prod_j P_j(V_j) \,. \tag{74}$$

This is equivalent to replacing the system by a statistical ensemble of macroscopically equivalent systems. The widths of P_j, say W_j, gives the degree of the disorder in the system. In the simplest model, where all lattice sites are assumed to be identical, the disorder is given by $W \equiv W_j = W_k$. A physical quantity A has to be calculated as a statistical average

$$A = \overline{A} \equiv \int \mathrm{D}[V] P([V]) A([V]) \,. \tag{75}$$

where $A([V]) = \langle \Psi[V]|A|\Psi[V]\rangle$ is the quantum mechanical expectation value of the operator corresponding to A in some state $\Psi[V]\rangle$ that depends on the realization V.

Averages are usually assumed to be representative of the experimentally measurable quantities. However, this is only the case if the average is the same as the most probable value in the ensemble, at least in the thermodynamic limit, $L \to \infty$, $N \to \infty$ but $N/\Omega = c \neq 0$ ("central limit theorem", L length of the system). In 1D, this condition is not always fulfilled. Especially the conductance is known to show unusually large statistical but nevertheless reproducible fluctuations when $T \to 0$ [87L2, 98J1].

Given the above model, it is possible to prove mathematically rigorously that all eigenstates of the Hamiltonian are exponentially localized, independent of their energy, and independent of how small the disorder W is [61M, 73I, 74T, 78M, 80K, 83D]. This means that the (randomly fluctuating) wave functions are on the average exponentially decaying when $x \to \infty$, with a characteristic decay length $\lambda(W, E)$. The latter is often called the localization length. For small disorder W, one obtains,

$$\lambda(W, E) = \frac{\lambda_0(E)}{W^2} \,, \tag{76}$$

with the constant $\lambda_0(E = 0) = 105at^2$ at the centre of the band of the above lattice model [74T, 93K]. Physically, the origin of the complete localization is that in one dimension an impurity can

cause only forward and backward scattering, and that eventually with many impurities backward scattering dominates the states.

The consequence of the complete localization in 1D is that the DC-conductance of a very long one dimensional electron system becomes exponentially small at absolute zero of the temperature $T \to 0$ [78A, 93K, 98J1],

$$G \propto \frac{e^2}{h} \left(\frac{\lambda}{L}\right)^{3/2} e^{-L/4\lambda} . \tag{77}$$

In the limit $L \to \infty$, the conductance vanishes exponentially with a characteristic length scale 4λ. As a consequence, the zero-temperature DC-conductivity vanishes

$$\lim_{L\to\infty} \sigma(L) = G \cdot L = 0 . \tag{78}$$

In 1D, there are no true metallic conductors. Near the absolute zero of temperature, the transport is dominated by hopping processes between the localized states [61M, 82G].

There are also important relations between the localization phenomenon and the statistical properties of the spectrum of eigenvalues of the Hamiltonian, which is known to be singularly continuous in the energy regions that correspond to localization [73I]. Another important topic is the statistical behaviour of the wave functions associated with localization [98J1]. Important cross-relations exist also with the spectral statistics of classically chaotic systems [96D2].

12.3 Electrical Transport and quantum transmission

As the DC-conductivity vanishes, alternatives of the conventional theories of electrical transport have to be explored in the quantum regime. Mainly, three approaches have been persued.

12.3.1 Recursive Green function method

Starting from linear response theory, the conductivity of a 1D disordered system at frequency ω and temperature T without interaction can be written in terms of products of one-electron Green functions [93K]

$$\begin{aligned} \sigma(\omega, T) &= \lim_{\epsilon\to 0} \lim_{L\to\infty} \frac{\hbar e^2}{\pi \Omega m^2} \int_{\infty}^{\infty} \mathrm{d}E \, \mathrm{Tr} \left[p \, \mathrm{Im} G^+(E) \, p \, \mathrm{Im} G^+(E+\hbar\omega) \right] \times \\ &\quad \times \frac{f(E+\hbar\omega, T) - f(E, T)}{\hbar\omega} . \end{aligned} \tag{79}$$

Here,

$$G^{\pm}(E \pm \mathrm{i}\epsilon) = \frac{1}{E \pm \mathrm{i}\epsilon - H} \tag{80}$$

is the one-electron resolvent at energy E with an infinitesimally small imaginary part $\pm\epsilon$ in order to avoid the singularities at the real energy axis when integrating over the energy, p is the operator of the momentum, Ω the volume of the system, and $f(E, T)$ the Fermi distribution function at temperature T and energy E. By expanding in powers of the disordered part of the Hamiltonian Eq. (68) one obtains the recursive equation

$$G^{\pm}(E) = G_0^{\pm}(E) + G_0^{\pm}(E) H_{\mathrm{imp}} G^{\pm}(E) \tag{81}$$

with $G_0^{\pm}(E) = (E \pm \mathrm{i}\epsilon - H_{\mathrm{kin}})^{-1}$ the resolvent of the ordered part of the Hamiltonian.

From Eq. (79) and Eq. (81), recursive algorithms have been derived which permit the microscopic calculation of the conductance of quasi-one dimensional, bar-shaped disordered systems of finite length L with semi-infinite ideal leads attached at the left and right ends [80M, 85M, 88M3]. For the DC-conductivity tensor $\sigma_{jk}(0, 0)$ of a quasi-1D bar of cross-sectional area M^{d-1} and length

L at $T = 0$ at with the Fermi energy E_F, a convenient set of starting equations are, in lattice representation,

$$\sigma_{xx}(0,0) = \lim_{\epsilon\to 0}\lim_{L\to\infty}\frac{e^2}{h}\frac{4}{LM^{(d-1)}}\mathrm{Tr}\left[\epsilon^2\sum_{i,j}^{L}\boldsymbol{G}^{+}_{ij}(E_\mathrm{F})x_j\boldsymbol{G}^{-}_{ji}(E_\mathrm{F})x_i - \epsilon\sum_{i=1}^{L}\mathrm{Im}\,\boldsymbol{G}^{+}_{ii}(E_\mathrm{F})x_i^2\right], \quad (82)$$

$$\sigma_{xy}(0,0) = \lim_{\epsilon\to 0}\lim_{L\to\infty}\frac{e^2}{h}\frac{4}{LM^{(d-1)}}\mathrm{Tr}\left[\epsilon^2\sum_{i,j}^{L}\boldsymbol{G}^{+}_{ij}(E_\mathrm{F})\boldsymbol{y}\boldsymbol{G}^{-}_{ji}(E_\mathrm{F})x_i - \epsilon\sum_{i=1}^{L}\mathrm{Im}\,\boldsymbol{G}^{+}_{ii}(E_\mathrm{F})x_i\boldsymbol{y}\right], \quad (83)$$

where $\boldsymbol{G}$ is the matrix of the resolvent associated with the slice of cross-sectional area M^{d-1} at position i, and $\boldsymbol{y}$ the position vector in this area. The quantum transport properties of disordered systems (including also a magnetic field) of arbitrary shapes can be computed microscopically at finite frequencies and temperatures. A summary of the relevant non-linear equations is given in [85M].

12.3.2 Conductance and quantum transmission

Linear response theory, when applied to a system attached via quasi-one dimensional ideal leads to reserviors, has been shown to yield a relation between the conductance of a system and its quantum transmission properties [80A, 81E1, 81E2, 81F, 82E, 85B, 86P2, 94P]. The ideal leads serve to define transport channels, which correspond to the transversely confined modes and can propagate freely in both positive and negative directions. The result can be written as

$$G = \frac{e^2}{h}\mathrm{Tr}\left(tt^\dagger\right) \quad (84)$$

where t is the matrix of the transmission probability amplitudes. For a system with M channels, t is a $2M \times 2M$ dimensional scattering matrix, since a single channel has to be represented by a 2×2-scattering matrix. This accounts for the scattering of two incoming waves, one incident from the left and one from the right, into two outgoing waves in each of the channels. The off-diagonal matrix elements of t describe scattering between different channels. The total probability for transmission is $T = \mathrm{Tr}\left(tt^\dagger\right)$.

A formula which is similar in spirit, has been suggested earlier for the conductance of a 1D conductor of finite length L, namely

$$G = \frac{e^2}{h}\frac{T}{R} \quad (85)$$

with the transmission probability

$$T = |t|^2 \quad (86)$$

and the reflection probability [57L, 70L, 85B, 85B]

$$R = 1 - T\,. \quad (87)$$

One can prove, also for quasi-1D systems with a finite cross-section, that for $L \to \infty$, the transmission probability vanishes exponentially, $T = \exp -L/\lambda_\mathrm{t}$, even for vanishingly small disorder. Thus, power expansion of Eq. (85) yields to first order the result Eq. (84). The latter seems to be consistent with all of the presently available experiments. This establishes yet another proof that all of the quantum states in an infinitely long one-dimensional disordered system are exponentially localized.

Quantum transport is apparently closely connected with pure quantum mechanical wave functions with dissipative processes completely excluded. This immediately implies that the microscopic local currents and fields near impurities are purely of quantum nature [88L2]. On the other

hand dissipation is unavoidable, and a thorough understanding of transport in the quantum systems must include this phenomenon [93W3]. Due to the stiffness of quantum mechanical wave functions, quantum transport is in general non-local [89V].

The above so-called Landauer formula, Eq. (84), is frequently used to discuss quantum transport properties of ultra-small electronic devices [90D].

12.3.3 The Thouless conjecture

The so-called Thouless conjecture relates the shifts of eigenenergies as a function of the boundary conditions with the DC-quantum conductance of a system [72E, 78T],

$$G = \frac{e^2}{h} \frac{\langle \delta E \rangle}{\langle \Delta E \rangle} \,. \tag{88}$$

Here, $\langle \delta E \rangle$ is the geometric mean of the energy level shifts caused by a reversal of the phase of the boundary conditions for the wave functions from periodic to anti-periodic, and $\langle \Delta E \rangle$ is the mean energy level spacing.

This relation was originally suggested on the basis of the Kubo formula [72E] and by using a heuristic argument based on the uncertainty principle [78T]. In addition, the theory of quantum transport as quantum transmission in one dimension has been used in order to derive Eq. (88) more rigorously [80A]. Strictly speaking, all of these derivations are only qualitalively correct. The Thouless conjecture has been the starting point of very important developments in the theory of quantum phase transitions. It has been a basic ingredient of the one-parameter scaling theory of the disorder-induced metal-insulator transition in which a localized system ($\sigma = 0$) is transformed into a delocalized one ($\sigma \neq 0$) [76W, 79A].

The calculation of transport properties of systems with reduced dimensionality in the presence of disorder has been performed [87K2] up to the level of device engineering [93B3].

12.4 Conductance fluctuations

Since the DC-conductance at absolute zero depends exponentially on the length of a system one expects unusually large statistical but reproducible fluctuations, when some parameter is changed for a *given* sample. Theoretically, for many macroscopically identical samples, it is then expected that the conductance will exhibit also unusally large flucutations within a statistical ensemble. This has been suggested by several groups [79L2, 81S2, 83A, 84A2, 85A2, 85L3, 86I, 87L2], and it was therefore a major breakthrough in the field, when the reproducible conductance fluctuations were experimentally discovered. Several reviews which cover exhaustively most of the subject are given in [91A1].

One consequence of the conductance fluctuations is the lack of usual self-averaging. The absence of self-averaging implies that the statistical average of a physical quantity is *not* equal to the most probable value in the statistical ensemble

$$\overline{A} \neq A_{\max} \tag{89}$$

where the most probable value of A, $A_{\max}$, is defined by

$$P(A_{\max}) = \mathrm{Max}_A\{P(A)\} \,. \tag{90}$$

In classical statistical systems, the relative fluctuations of a quantity decay with increasing system size Ω as $\Omega^{-1/2}$ such that self-averaging is always guaranteed. To see this for a classical conductor, one can consider a 1D chain of (random) resistances R_i ($i = 1 \ldots N$). The total resistance is

$$R = \sum_{i=1}^{N} R_i \,, \tag{91}$$

and its variance, by the central limit theorem,

$$\frac{\mathrm{Var}(R)}{\overline{R}^2} \propto \frac{\mathrm{Var}(R_i)}{N\overline{R_i}^2} \tag{92}$$

with $\mathrm{Var(x)} = \overline{(x-\overline{x})^2}$. The relative variance of the resistance is proportional to L^{-1}. For a hypercube in d dimensions, one can show that the relative variance is $L^{-d/2}$, as expected.

In the present situation of a quantum conductor, this argument breaks down due to quantum coherence. This can be seen by using perturbation theory in the metallic regime, but including weak localization vertex corrections [85A2, 87L2], by applying the theory of random matrices to the quantum transmission problem described above [86I, 88M4, 90P4, 95M3] and by the supersymmetric method [90I2, 97E]. In 1D, the result is (in units of e^2/h)

$$\sqrt{\mathrm{Var}(G)} \approx 0.75\,. \tag{93}$$

In particular, the unusally large fluctuations imply that the averages of conductance $\langle G\rangle$ (in units of e^2/h) and inverse of the average resistance $\langle R\rangle$ (in units of h/e^2) are not identical [81S2, 93K]. In 1D

$$\ln\langle G\rangle = -\frac{1}{8}\ln\langle R\rangle \tag{94}$$

and

$$\ln\langle G\rangle = \frac{1}{4}\langle \ln G\rangle\,. \tag{95}$$

The right hand side of the latter is nothing but the inverse localization length.

12.5 Persistent currents

The magnetic properties of ring structures have been investigated in the early days of quantum physics [37L, 38H]. The existence of persistent currents has been discussed for superconducting rings enlcosing a magnetic flux [61B, 65B, 68B, 70B, 68S, 69G] and for normal metallic loops [83B].

The basic phenomenon can be understood by considering the simplest model of an ideal 1D ring threaded by a magnetic flux ϕ [88C6]. In this model, the energy levels and corresponding currents are

$$\varepsilon_n = \frac{1}{2m}\left[\frac{2\pi}{L}\left(n+\frac{\phi}{\phi_0}\right)\right]^2 \tag{96}$$

and

$$i_n = \frac{4\pi e}{mL^2}\left(n+\frac{\phi}{\phi_0}\right)\,, \tag{97}$$

respectively, with $n = 0, \pm1, \pm2, \ldots$. The total current $I(\phi)$ at $T = 0$ is obtained by adding all currents of levels lower than the chemical potential $\mu = N_e^2\pi^2/2mL^2$, with $2N_e$ the total number of electrons in the ring,

$$I(\phi) = -I_0\left[\frac{4\phi}{\phi_0} - 1 + (-1)^{N_e})\right]\,. \tag{98}$$

with the amplitude of the current

$$I_0 = |e|\frac{v_\mathrm{F}}{L}\,, \tag{99}$$

the Fermi velocity

$$v_\mathrm{F} = \frac{\pi N_e}{mL} \tag{100}$$

and with

$$-\frac{1}{2} \le \frac{\phi}{\phi_0} < \frac{1}{2} \quad \text{and} \quad 0 \le \frac{\phi}{\phi_0} < 1 \tag{101}$$

for N_e odd and even, respectively. The current is periodic in applied flux with period $\phi_0 = h/e$.

From this, one obtains several important results. For an ensemble of rings where the number of rings with odd and even N_e are equal, the periodicity of the ensemble-averaged persistent current is $\phi_0/2$. This holds quite generally, also when averaging over disorder configurations. Furthermore, the maximum of the average current is I_0 while the current of a level at the Fermi energy is $4I_0$. The total current is thus obtained as a result of a rather subtle cancellation of microscopic one-level currents. This shows that the assumptions used when calculating persistent currents influence the results. Different experimental situations are expected to require different averaging procedures, and different averages of the current. For instance, when considering a single ring, it is believed that the so-called typical current

$$I_{\mathrm{typ}} = \sqrt{\overline{I^2}} \tag{102}$$

has to be considered, instead of the ensemble-averaged current. Also, the choice of the statistical ensemble — canonical versus grand canonical — might be crucial [91S2, 91A4]. In addition, it is generally accepted that disorder is important and interaction effects such as Coulomb repulsion between electrons, and spin cannot be neglected, in order to understand the contradictory experiments. The present status of the theory can be extracted from several reviews [88C4, 91B3, 91I3, 91R3, 93W2, 94K3, 95E2, 96K4, 97E].

12.6 Electron-electron interaction

Electron-electron scattering in low dimensions is a very important subject which has been pursued intensively during the past decades in connection with electrical transport [84K1].

Interacting electrons in 1D constitute a very important paradigm in condensed matter physics, since within the Tomonaga-Luttinger liquid model the problem can be solved exactly [56T, 63L, 80H, 81H]. The Tomonaga-Luttinger liquid is also a counter example of what is usually assumed to be a good description of electrons in metals, the Fermi liquid. While quasi-particles, with all effects of the interaction incorporated in some parameters like an effective mass and a finite lifetime, are the essential feature of the Fermi liquid, the main property of the Tomonaga-Luttinger liquid is that the excitations with the lowest energies are *collective* charge and spin modes, and quasi-particles do not exist.

The basic assumption of the model is that the energy spectrum of the non-interacting electrons can be approximated by a linear dispersion around the two Fermi wave numbers $\pm k_{\mathrm{F}}$ which represent the Fermi surface in 1D,

$$\varepsilon(k) \approx \hbar v_{\mathrm{F}}(\lambda k - \lambda k_{\mathrm{F}})\,. \tag{103}$$

This defines two branches $\lambda = \pm$ of the spectrum which correspond to right- and left-moving plane waves. This approximation is justified since one expects that for the energetically lowest excitations only the states near the Fermi energy contribute. A second assumption is that only forward scattering processes are induced by the interaction. Generally, this is not allowed. However, when only the excitations with small wave numbers q are of interest, interaction processes involving wave numbers of the order $2k_{\mathrm{F}}$ are not important. A third assumption is that extending the dispersion relation to negative energies is merely a technicality and helps to simplify the mathematics.

The Hamiltonian of the interacting system can be written in terms of Boson operators b_q, $b_q^\dagger$

$$[b_q, b_{q'}^\dagger] = \delta_{q,q'}\,. \tag{104}$$

It is given by

$$H = \sum_{q\neq 0} \hbar\omega(q) b_q^\dagger b_q + \frac{\pi\hbar}{2L}\left[v_N N^2 + v_J J^2\right] \tag{105}$$

with

$$\omega(q) = v(q)|q| \tag{106}$$

$$v(q) = v_{\mathrm{F}}/K(q) \tag{107}$$

$$K(q) = \left[1 + \frac{V(q)}{\pi\hbar v_{\mathrm{F}}}\right]^{-1/2} \tag{108}$$

where $V(q)$ is the Fourier transform of the repulsive interaction between the electrons. Thus, the dispersion law of the Bosonic excitations directly reflects the interaction. The operators $N = N_+ + N_-$ and $J = N_+ - N_-$ correspond to the total number of particles in the left and right moving branches and the difference of the numbers of the particles in right and left moving branches, respectively. The corresponding velocities are $v_N = v(0)^2/v_{\mathrm{F}}$ and $v_J = v_{\mathrm{F}}$. By taking into account the electron spin, one arrives at a contribution to the Hamiltonian similar to the first term of the above one but with the repulsive interaction replaced by the exchange interaction. Spin and charge modes are thus completely decoupled in the Tomonaga-Luttinger liquid model.

Standard reviews which provide a broad overview over the present status of the field are [79E, 79S, 91B6, 94G5, 95V, 96S3, 96S5, 98W2].

The above model is only the simplest possible system. Corrections have to be treated within renormalization group schemes [91B6, 96S3, 96S5, 98W2].

In addition to the diagonalization of the Hamiltonian one can calculate exactly also several correlation functions which are of importantance for understanding experiments, as for instance the one electron Green function [95V, 96S3, 96S5]. Linear transport properties may be calculated exactly [95P3, 96S6, 98C2]. The differential cross-section for Raman scattering may be determined [98S2, 98S3, 98S4].

The case of an impurity embedded in a Tomonaga-Luttinger liquid can be treated with the renormalization group [92K5, 92K6]. The current-voltage characteristic becomes non-linear, with a vanishing DC-conductance when the interaction is repulsive. The non-linear current-voltage characteristic gives rise to non-linear AC-phenomena, such as frequency mixing and harmonic generation [99F3].

The study of the interplay of disorder and interaction in 1D is presently only in its infancy [88G2].

12.7 Monographs and edited volumes

A number of very useful monographs and edited volumes exist which describe aspects of quantum transport in quantum wires. As the field is still rapidly developing, they are not exhaustive [90B4, 91K1, 92F3, 95C, 95D, 96K1, 98S5]. The localization problem in 1D is treated in [78B, 88L3]. Aspects of the Bosonization method for interacting electrons in 1D are described in [94S, 97K2].

12.8 References for Section 12

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