Chapter 5

Semiclassical Transport

Transport properties are, in contrast to the level density considered above, readily accessible in experiment. This chapter gives a short introduction to the semiclassical approximation of electrical transport within the linear response formalism. The formulas presented will be used in the subsequent chapters.

Contents

The semiclassical approximation of the level density has been successfully applied to hydrogen as well as to Rydberg states [92, 52] and to neutral helium [28]. In all these cases, the experimental observables are emission or absorption lines. A theoretical description hence has to resolve the individual energy levels of the system. This is feasible in a semiclassical approach, but not the most favorable application of this method. For the required full quantization, many periodic orbits have to be included in the trace formula. The benefit from a semiclassical approach is considerable larger for systems where the line widths exceed the mean level spacing. In these situations only the shell structure is observed, which usually depends only on a few orbits.

Systems in this regime include nuclei, clusters and nanostructured devices – finite fermion systems with particle numbers of some 10 to a few 1000. For all these systems, semiclassical level density calculations have been performed. Such an analysis was presented for the fission barrier of nuclei [19, 118] as well as for the shell structure of metal clusters in magnetic fields [77] and their ground-state deformation [121, 122, 59]. Apart from these examples, the application of the standard trace formula to experimental situations is very limited, as the level density is rarely directly observable. In some cases a close relation to the measured quantity can be assumed. Such an approach was used for the analysis of the mass distribution of sodium clusters [61] or the magnetoconductance of a mesoscopic circular quantum dot [2].

To extend the applicability of semiclassical methods it is desirable to develop descriptions for other physical quantities than the level density. This has been done for example regarding the magnetic susceptibility [96, 78], current oscillations in I-V curves [114] or the conductance [63, 41].

As already pointed out, nanostructured semiconductor devices are extremely versatile systems. Many parameters like size, geometry, electron density or magnetic field can be varied experimentally, some even during measurement. This opens up tremendous new theoretical and experimental opportunities, as many of these parameters are beyond control in more "natural" systems like atoms and nuclei. Most easily accessible to measurement are electrical transport properties. This is also an area of great commercial interest: The rapid developments in semiconductor technology lead to continually decreasing feature sizes on memory or logic circuits. The smallest structures already approach the mesoscopic scale. It is for these reasons, the direct experimental access, the great variability of the device, the large number of controllable parameters, and the commercial relevance that much of the work on nanostructures deals with electrical transport properties.

A quantum mechanical description of these systems is very demanding. The usually large number of electrons involves the calculation of numerous highly excited states. Regarding semiclassics, in contrast, high quantum numbers are especially favorable. As pointed out above, the semiclassical description is further facilitated by the broad line widths of these systems, which generically only allow the observation of the shell structure. All this makes a semiclassical approach to these structures very promising.

The following sections are devoted to the derivation of a semiclassical linear response formula for electrical transport. This will be applied to specific systems in the subsequent chapters.

5.1 Semiclassical linear response

The calculation of transport properties for small external fields is possible within the context of linear response theory. This powerful tool relates the response of a system to a small external excitation to its ground state properties. Richter and Mehlig [58, 120] have derived a general semiclassical treatment of dynamic linear response functions for ballistic quantum systems at finite frequency and finite temperature. Their ansatz is not only applicable to electrical transport, but also to magnetic properties or far-infrared absorption of closed quantum dots. Here, the discussion is restricted to electrical transport in static external fields. Please note that due to the linear response ansatz all nonlinear transport effects are beyond the scope of this work. Those effects can already occur for low-excitation measurements (cf. Ref. [74]).

For absolutely clean systems the conductivity is not finite. In contrast to the level density, which can also be calculated for pure systems, transport properties are inseparably related to the disorder present in the system. The semiclassical approximations therefore depend strongly on the detailed properties of the scatterers in the sample. This is why it is not possible to give a unified approach valid for all situations.

The following section will describe the different transport regimes, before Sec. 5.5 presents a semiclassical approximation for coherent ballistic transport. This is the regime that will be relevant for the specific systems considered later.

5.2 Different transport regimes

The transport properties depend on the microscopic scattering process, the density of the scatterers, their strengths and their distribution. A rough classification of the different transport regimes is possible regarding the typical length scales involved:

The system size a:
This important datum for the discussion of quantum oscillations may be ambivalent for some systems.[1]

The magnetic length ℓ_B:
A magnetic fields introduces an additional length scale $\ell_B = \sqrt{\hbar/(eB)}$, which may replace the system size a in some problems. This complication will not be discussed here.

The Fermi wavelength λ_F:
$\lambda_F = 2\pi\hbar/\sqrt{2m^\star E}$ usually defines the smallest length scale. For two-dimensional systems this is equivalent to $\lambda_F = \sqrt{\pi/n_s}$, where n_s denotes the electron density per spin.

The elastic mean-free path ℓ:
This is a quantum mechanical quantity, generally without classical meaning. It is related to the total amplitude diffracted by disorder [68] and to the single-particle relaxation time [97]. It is often given in terms of the total relaxation time $\tau = \ell/v_F$.

[1] For a long, narrow channel it is *a-priori* not clear whether the length or the width is the characteristic quantity. Something similar holds for antidot lattices, where both the system size and the size of the elementary cell might be relevant.

Here v_F denotes the Fermi velocity $v_F = \hbar k/m^\star$, which in two dimensions can be expressed as $v_F = 2\hbar\sqrt{\pi n_s}/m^\star$.

The transport mean-free path ℓ_T:
This quantity can be interpreted classically, indicating the length scale over which the electron momentum is randomized. It is related to the momentum relaxation time τ_p via $\ell_T = \tau_p v_F$. Short-range impurity potentials lead to isotropic scattering, and $\ell_T \approx \ell$. For long-range impurity potentials the momentum before and after the scattering process are correlated, so that ℓ_T can significantly exceed ℓ.

The phase coherence length ℓ_Φ:
ℓ_ϕ gives the length over which the phase coherence of the wave function is lost. The phase coherence length exceeds the mean-free path, as elastic scattering preserves phase coherence. Only some inelastic scattering processes lead to finite ℓ_ϕ.

Depending on these length scales, transport can roughly be divided into the following regimes:

macroscopic ($a \gg \lambda_F$) or microscopic ($a \gtrsim \lambda_F$):
$a \gg \lambda_F$ is the regime of high quantum numbers, where the levels get closer in energy.[2] Once the line width exceeds the mean level spacing, the quantization information gradually disappears, eventually leading to classically smooth spectra.

classical ($a > \ell_\Phi$) or coherent ($a < \ell_\Phi$):
For $a > \ell_\Phi$, phase coherence is broken between two points in the system. Thus no correlation of the wavefunctions at these points is left, and the two parts of the system add classically (i. e. without interference).

diffusive ($\ell_T \ll a$) or clean ($\ell_T \gg a$):
The regime ($\ell_T > a$) is often referred to as the *ballistic regime*. There particles can traverse the system without randomizing their momentum.

The distinction between diffusive and ballistic systems is easily visualized in the semiclassical picture. Fig. 5.1(A) depicts the diffusive situation, where a trajectory is frequently scattered, and the motion is essentially a random walk. The periodic orbits in this system are depicted in the lower part of Fig. 5.1(B). They depend on the individual locations of the scatterers. The assumption that, in analogy to the level density discussed above, the

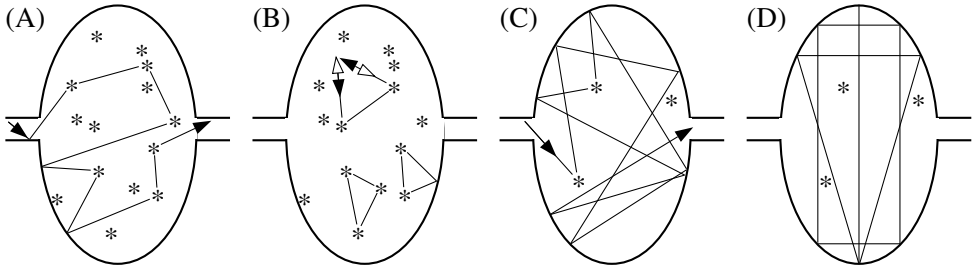

Figure 5.1: *Diffusive (A, B) and ballistic transport regime (C, D). (B) and (D) depict some classical closed orbits. These are relevant for quantum oscillations.*

[2] This holds for systems where the number of degrees of freedom minus the number of constants of motion is larger than one.

system properties depend on the classical periodic orbits already captures the essential physics of these systems. The detailed structure of the magnetoconductance depends on the microscopic distribution of the scatterers, which is unique for each sample. This leads to the "fingerprint" characteristics of the magnetoconductance of disordered samples.

Weak localization, another effect in diffusive samples, can be understood as a consequence of coherent backscattering: The central mechanism is that closed paths as in the upper part of Fig. 5.1(B) can be followed in both directions. Their contributions therefore interfere constructively. This enlarges the return probability of the particle, which is hence weakly localized. A magnetic field breaks the time-reversal symmetry, so that the two orientations are no longer coherent. This explains why a magnetic field destroys weak localization. Detailed information about these and related diffusion-based effects can be found in Refs. [99, 90, 91].

In the following coherent ($a < l_\Phi$), ballistic ($l_T > a$), mesoscopic ($1 \ll \lambda_F/a \ll \infty$) transport is considered. Fig. 5.1(C) sketches the ballistic case, where trajectories are rarely scattered. In this regime the periodic orbits (c.f. Fig. 5.1(D)), and thus the quantum oscillations, mainly depend on the confinement of the system and not on the distribution of the scatterers.

The effects of disorder on the semiclassical approximations have already been listed on page 17. For the low impurity concentrations of ballistic systems, periodic orbits as in Fig. 5.1(B) can be neglected, and the coherence of degenerate families is hardly affected. The orbits which contribute in the ballistic regime are therefore those of the clean system. Disorder induces a finite probability of scattering out of a periodic trajectory. This leads to a reduction of the semiclassical amplitudes.

Note that in the ballistic regime the quantum oscillations are dominated by the confinement potential, i. e. depend on the fact that the system is finite. Therefore quantum mechanical calculations including impurity scattering which rely on the translational invariance of an infinite system cannot be applied here.

5.3 The model for disorder

Scattering is, as already outlined in Sec. 3.1, introduced by appropriate averages. For a single, isolated system this is the average over the impurity constellation. If ensembles of systems, like dot-arrays, are considered, this average also includes system parameters like geometry and Fermi energy.

For an explicit calculation, both the scattering potential and the distribution of scatterers have to be known. The problem of a realistic description of these properties is not completely settled so far. The scattering potential depends strongly on the nature of the scatterer, its distance to the 2DEG, and, for ionized impurities, the screening properties of the 2DEG. Modeling the distribution of scatterers is also non-trivial. For high-mobility 2DEG, scattering at ionized donors is the dominant process. Their distribution does not only depend on the growth process,[3] but also on the cooling scheme. The underlying mechanism is called *coulomb ordering*. It applies to the generic case where only a part of the donors is ionized. While cooling down slowly, an energetically favorable subgroup is getting ionized. The ionized donors are hence preferably equally spaced. This introduces

[3] The growth process is usually, but not generally believed to lead to randomly distributed donors.

correlations in the positions of the scatterers, even if the donors themselves are randomly distributed [110, 113].

The calculation of transport properties, especially of line shapes and amplitudes, from realistic impurity potentials and distributions is currently an area of active research (see, e. g., [60]). As this work is not intended to contribute to this area, impurity correlation effects will be neglected in the following. A wide-spread model for uncorrelated impurities uses random gaussian potentials

$$V(\boldsymbol{r}) = \sum_{i=i} N \frac{V_i}{2\pi\xi^2} \exp\left[-\frac{1}{2}\left(\frac{\boldsymbol{r}-\boldsymbol{R_i}}{\xi}\right)^2\right] , \tag{5.1}$$

characterized by an average strength V_0 and a correlation length ξ. Following this ansatz, Richter [105] derived a semiclassical approximation for the susceptibility. He finds that the impurities can be included in the semiclassical susceptibility by factors $F(L)$ damping the orbit amplitudes. Due to the different averages involved, the results for individual systems differ from those for ensembles. They also depend on the relative size of the correlation length ξ, the system dimension a, and the Fermi wavelength λ_F. In the context of this work isolated systems with finite-range ($\lambda_F < \xi < a$) impurities will be considered. For those systems $F(L)$ is given by

$$F(L) = e^{-L/(2\ell)} , \tag{5.2}$$

with the elastic mean-free path ℓ. For these samples the transport mean-free-path ℓ_T is considerably larger than ℓ [105]. Therefore a ballistic treatment of systems with a size comparable to the elastic mean-free-path is still justified.

Please note that the ansatz of randomly distributed scatterers is restricted to the first repetition of classical orbits. This comes about as the repetition of an orbit sees the same impurity constellation as the primitive orbit. Therefore random impurity positions on the sample are not random along the trajectory. A refined discussion as presented by Richter [105] shows that the higher repetitions of orbits are also damped exponentially, but with an exponent depending quadratically on the repetition number.

5.4 Finite temperature

Just as the inclusion of scattering, the consideration of finite temperatures in semiclassical linear response formulae is not completely settled so far[4]. The intuitive approach to replace the δ functions in the corresponding quantum mechanical expressions by Lorentzians with width γ

$$\delta(E) \to \frac{1}{\pi}\frac{\gamma}{E^2+\gamma^2} \tag{5.3}$$

has been confirmed by more involved calculations [80] and has been established as a quasi-standard [112]. Since a detailed discussion of the microscopic mechanism involved in dissipation is beyond the scope of this work, this heuristic approach will be implemented.

[4] For grand canonical systems, the approach of Sect. 3.1 can shown to be exact [17].

5.5 The semiclassical Kubo formula

In the ballistic regime the quantum oscillations are, as already pointed out, determined by the sample boundaries, not by the impurity constellation. This *geometric* effect is of special interest, as the geometry of the sample can be adapted in a wide range. Two different types of ballistic devices can be distinguished:
The first are small structures coupled to leads, which are completely phase coherent. The current through these systems does not scale with the system size, so that only conductances, but no conductivities can be defined. For the transport through those samples, a semiclassical approximation of the Landauer-Büttiker formalism is appropriate.
The generic example for the second class of devices is a regular array with a lattice constant smaller than the phase coherence length, and a total size exceeding ℓ_Φ. Then quantum oscillations stemming from interference effects within elementary cells can be observed, but the elementary cells themselves add classically. Therefore the definition of specific quantities like conductivities is justified. For those systems, Kubo linear response theory is the adapted description.
For the systems considered in this work, the Kubo formalism will provide the correct framework. Please note that the distinction between Kubo and Landauer does not reflect a physical difference: Quantum mechanically, both approaches have been shown to be equivalent [12].

The general idea how to obtain a semiclassical version of the Kubo conductivity is to express the quantum mechanical Kubo formula in terms of Green's functions. After the inclusion of finite temperature and weak disorder by appropriate averages, the Green's functions are replaced by their semiclassical approximation. Following this line, Richter and Hackenbroich/von Oppen derived a semiclassical expression for the oscillating part of the conductivity tensor.[5] They use approximation Eq. (5.2), which is equivalent to the assumption of an energy-independent scattering time. Temperature is included as indicated in Eq. (5.3). Vertex corrections, which correspond to orbits including scattering events (c.f. Fig. 5.1(B)), are neglected. Under these assumptions they find

$$\begin{aligned}
\delta\sigma_{xx}(E_F,B) &= \frac{2}{V}\frac{e^2}{h}\sum_{\mathrm{ppo},n} \qquad\qquad \mathcal{C}_{xx}\ \ \frac{R_n(\tau_\beta)F_n(\tau_s)}{|\mathrm{Det}(\widetilde{\mathrm{M}}^n-\mathbf{1})|}\cos\left(\frac{nS}{\hbar}-\mu_n\frac{\pi}{2}\right)\\
\delta\sigma_{xy}(E_F,B) &= \frac{2}{V}\frac{e^2}{h}\sum_{\mathrm{ppo},n}\left(\frac{1}{e}\frac{\partial S}{\partial B}+\mathcal{C}_{xy}\right)\frac{R_n(\tau_\beta)F_n(\tau_s)}{|\mathrm{Det}(\widetilde{\mathrm{M}}^n-\mathbf{1})|}\cos\left(\frac{nS}{\hbar}-\mu_n\frac{\pi}{2}\right)\ .
\end{aligned} \tag{5.4}$$

In these formulas the sum over the primitive periodic orbits ppo is separated from the sum over their repetitions n. All quantities except the Maslov indices μ refer to the primitive periodic orbit.[6] The temperature T is included by

$$R_n(\tau_\beta) = \frac{nT_0/\tau_\beta}{\sinh(nT_0/\tau_\beta)}\ , \tag{5.5}$$

with the temperature-related scattering time $\tau_\beta = \hbar/(\pi k_B T)$. The impurities lead to an exponential suppression of longer orbits according to Eq. (5.2). In the following an

[5] The derivations of the authors are virtually identical, and the results were published simultaneously. Please note the (identical!) misprints in the expression for σ_{xy} in Refs. [63, 41]. There, the action of the total orbit instead of the primitive orbit shows up in $\partial S/\partial B$. The formulas in Refs. [105, 42] are correct.

[6] The Maslov index for stable orbits is not proportional to the repetition number.

approximate expression for the damping term which depends on the period of the orbit instead of its lengths will be convenient:

$$F_n(\tau_s) = e^{-n^2 T_0/(2\tau_s)} \; . \tag{5.6}$$

The scattering time $\tau_s = m^*\mu/e$ is extracted from the experimental mobility μ. The velocity-velocity correlation $\mathcal{C}_{ij}$ of a primitive periodic orbit is finally given by

$$\mathcal{C}_{ij} = \int_0^\infty dt\, e^{-t/\tau_s} \int_0^{T_0} d\tau\; v_i(\tau)\, v_j(t+\tau) \; . \tag{5.7}$$

Apart from the prefactors and the velocity correlation function (which replaces the period of the orbit), the structure of the trace formula Eq. (5.7) is identical to the Gutzwiller expression for the level density Eq. (2.14).

The semiclassical approximation of the conductivity tensor will be used to calculate electrical transport properties of the free 2DEG in chapter 6 and of the channel with antidots in chapter 7. Prior to this, the basic formulas connecting σ with the measured voltages and currents will be reviewed.

5.6 Electrical transport

Within linear response, the local electrical field $\vec{E}$ and the local current density $\vec{j}$ are related via the *conductivity tensor* $\underline{\sigma}$ according to

$$\vec{j} = \underline{\sigma}\vec{E} \; . \tag{5.8}$$

The inverse tensor $\underline{\rho} = \underline{\sigma}^{-1}$ is known as the *resistivity*. It connects $\vec{j}$ and $\vec{E}$ by $\vec{E} = \underline{\rho}\vec{j}$, and is explicitly given by

$$\underline{\rho} = \frac{1}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \begin{pmatrix} \sigma_{yy} & -\sigma_{xy} \\ -\sigma_{yx} & \sigma_{xx} \end{pmatrix} \; . \tag{5.9}$$

For isotropic systems $\sigma_{xx} = \sigma_{yy}$ and $\sigma_{yx} = -\sigma_{xy}$, so that Eq. (5.9) simplifies to

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2} \qquad \text{and} \qquad \rho_{xy} = \frac{-\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2} \; . \tag{5.10}$$

For the free electron gas in high magnetic fields $|\sigma_{xy}| \gg \sigma_{xx}$. In this case the hall resistivity and the hall conductivity are, as expected, inverse quantities: $\rho_{xy} \approx 1/\sigma_{xy}$. The longitudinal conductivity, however, is proportional to the longitudinal resistivity: $\rho_{xx} \propto \sigma_{xx}$. This relation is somewhat counterintuitive.

For the usual hall-bar geometry, i. e. a macroscopic, homogeneous, rectangular system with length l and width w where a current I is drawn in x-direction, Eq. (5.10) leads to

$$U_x = R_l I \qquad \text{and} \qquad U_y = R_h I \; , \tag{5.11}$$

with the longitudinal resistance $R_l := \frac{l}{w}\rho_{xx}$ and the hall resistance $R_h := \rho_{xy}$. Please note that for two-dimensional systems the hall resistivity and the hall resistance are identical.