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Response of an inhomogeneous electron gas to an external electric field

Diplomová práca

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Anotácia

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Abstrakt

Táto práca sa zaoberá problematikou kvantového transportu cez nanoskopický kontakt. Modelovým systémom je nekonečný jednorozmerný elektrónový plyn s poruchou, ktorá je simulovaná delta-potenciálom. Pomocou teórie lineárnej odozvy v neinteragujúcom priblížení sme spočítali odozvu elektrónovej hustoty v čase i priestore na priložené napätie. Ukázali sme na možný nedostatok tohto modelu (existencia ustáleného stavu je problematická) a navrhli jeho príčinu i spôsob odstránenia.

Annotation

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Title of the diploma thesis Response of an inhomogeneous electron gas to an external electric field

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Abstract

This work deals with quantum transport through nanowire. The model system that has been used is an electron gas with a disorder. The disorder is modeled by a delta function potential. Electron density response to an external potential bias has been calculated in the linear regime. We have noted that the onset of steady state is doubtful when one considers the electron-electron interaction.

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List of symbols

$[\ ,\ ]$	Commutator
$\sum_{k!}$	Sum up to Fermi energy
c	Magnitude of a delta-function potential
$\delta(t)$	Dirac delta-function
E_j	Eigen-energy
E_F	Fermi-energy
erf(z)	Complex error function
erfc(z)	Complementary error function
$\|\Phi_0\rangle$	Many-particle ground state in the Heisenberg picture
$\|\phi_j\rangle$	One-particle energy eigenstate
$\phi_j(x)$	One-particle wave-function of an energy eigenstate
G^r	Retarded Green's function
G^a	Advanced Green's function
χ	Density response function
χ_0	Density response function of a homogeneous electron gas
i	Imaginary unit
$\mathfrak{Im}\{\}$	Imaginary part of a complex number
$\mathbf{H}$	One-particle Hamiltonian
$\mathcal{H}$	Many-particle Hamiltonian
$\mathcal{H}_0$	Unperturbed many-particle Hamiltonian
k_F	Fermi momentum
$\mathbf{n}(x,t)$	Electron density operator in the interaction picture
$\mathbf{n}_F$	Zero-temperature density matrix
$\mathcal{P}$	Principal value of an improper integral
$\mathfrak{Re}\{\}$	Real part of a complex number
$\theta(t)$	Heaviside step-function
Tr	Trace
$V(x,t)$	Potential energy
$\mathcal{V}$	Potential energy operator
$\mathcal{V}_I$	Potential energy operator in the interaction picture

Contents

Introduction

It's well known that the successful story of quantum mechanics was ushered mainly by the invention of a Schrödinger equation. This equation described the quantum dynamics of a single electron in few significant cases by giving analytical results.
Unfortunately the number of such cases is very limited. Soon the main scope of interest in the nonrelativistic physics became the systems of larger complexity (eg. condensed matter). These systems are described by a large set of coupled equations in the formalism of quantum mechanics. Manyfold sophisticated approaches have been devised in order to solve them approximately. In the light of electronic structure theories it has been shown that under certain circumstances electron dynamics can be mapped to a single electron case governed by the Schrödinger equation. For instance this *non-interacting* regime has been shown to be a good approximation in metals and doped semiconductors at low temperatures where the electron motion in a conduction band becomes phase coherent at distances that are much larger than Fermi wave-length. Moreover, the two dimensional and one dimensional variants of the Schrödinger equation were employed successively in systems which restricted the motion of an electron by transverse fields.
The present work arose in this context. Although there's no explicit reference to the famous equation (we use a formally more comfortable Green's function formalism) the essence of the Shrödinger equation, the unitary time-evolution, persists.
We focus on the problem of non-equilibrium quantum transport through nanoscopic junction. Of particular interest is the onset of a steady current through the junction as a consequence of a transient state caused by switching on an external potential in the leads that connect the junction.
Another strong motivation for the study of non-interacting system is understanding of non-equilibrium electronic processes. After a remarkable success of *ab-initio* ground state electronic calculations a major effort is placed on a study of time-dependent processes. Transport phenomena of electrons at nanoscale [7] form a significant part of this effort nowadays.
The results presented here refer neither to a particular material nor geometry, our simple model of a non-interacting electron gas is a space for

understanding basic phenomena that occur in the system driven from equilibrium.
These topics are discussed in the framework of a quantum theory of many particles. The essential result that we have employed in this work comes with the name Kubo's formula.
We give an example of how does this device work. The classical picture of the electric conduction in an isotropic medium is represented by phenomenological relations of the type

$$\vec{i}(\vec{r},t) = \sigma(\vec{r})\vec{E}(\vec{r},t). \tag{1}$$

This is the *local* Ohm's law which relates the electric current density to the intensity of the electric field in the same point and time by the conductivity σ. This paradigm is in contrast with the *non-local* nature of quantum mechanics where the expectation value of the electric current density is given in the linear regime by Kubo's formula

$$\vec{i}(\vec{r},t) = \int\int_0^t \sigma(\vec{r},t,\vec{r}',t')\vec{E}(\vec{r}',t')\mathrm{d}t'\mathrm{d}\vec{r}'. \tag{2}$$

Thus the current density is influenced by the value of intensity in the whole space and by the "history" of the system.
The objective of this work is the calculation of the electron density of system with disorder driven from equillibrium by an external potential. The particular shape of the potential represents a nanojunction attached to a pair of leads. Our own contributions involve

- Eq. 3.8 which expresses the density response function through one-particle Green's functions.
- The detailed derivation of the constituents that enter the Eq. 3.8, especially the Green's function in a direct space and time of an electron with delta-potential.
- The implementation of Eq. 3.5 in a computer program for an arbitrary potential.
- Analysis of the relaxation time dependence on the parameters of the external potential and a disorder.
- Study of space-time dependence of the response function.

In Chapter 1 we describe our model system in detail. Chapter 2 summarizes the essentials of one-particle Green's functions. The theory of linear response is tackled in Chapter 3 where we obtain a relation for the density response of the same form as the Eq. 2. The response function is expressed through Green's functions and this is the starting point of a numerical calculation. Some lengthy but necessary analytic calculations are postponed to the appendices.

Chapter 1

Model system

The system of our interest is a *nanowire* - an extremely thin metallic conductor attached to a pair of bulk metals (*leads, electrodes*). The dimensionality of such systems reduces to one effectively.
We note that there might be conceptual problems with one dimensional systems. The argument that favors this model is that in reality every wire is connected with a couple of massive electrodes. Thus the infinite part of the studied system is formed by three-dimensional bulk leads.
The main focus is placed on a nanowire with a scattering center. This is considered as non-magnetic, represented by a potential. If the range of this potential is much smaller than the Fermi wave-length of the electron system, we can assume that the potential has the form of a delta-function

$$V_d(x) = c\ \delta(x). \tag{1.1}$$

In the limit $c \to \infty$ one obtains two systems isolated with an impenetrable barrier.
When applying an external potential drop the delta-function potential provides an obstacle for the electric current, reflecting part of the flux backwards.
This scattering picture of electron transport was emphasized by Landauer and further developed by Büttiker [3] who obtained a formula which directly relates the applied potential bias ΔV to the electric current I in a stationary state by

$$I = 2 \times \frac{e^2}{\hbar 2\pi} T(E_F)\ \Delta V \tag{1.2}$$

where e is the effective charge of the electron and $T(E_F)$ is a transmission coefficient on a Fermi sphere. The factor two in front of the fraction is due to the spin degeneration. It's worth noting that the above formula for the electric current does not depend on the shape of the potential, it is only the overall potential drop that matters.

As has been announced already, we deal with non-stationary system. The transient state is caused by switching on an external potential at $t = 0$. The potential is depicted in the Fig. 1. It represents the electric field that

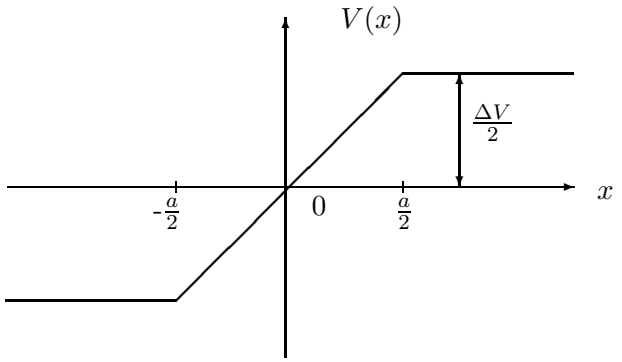

Figure 1.1: External potential

is constant in the region $\langle -\frac{a}{2}, \frac{a}{2} \rangle$ and zero otherwise. This is the region of the junction. It is quite straightforward, as we suppose that the junction is attached to the electrodes. On applying a potential drop (for instance by using a battery) the electric field is screened by the electrons in the bulk area of the electrodes. On the other hand, there's no screening between the electrodes as there's just the thin wire. The potential must be linear there. This shape of the potential is customarily used [6].

We assume that the influence of individual atomic nuclei is only that of providing a positive background of charge, as described by the *jellium* model [1]. Non-interacting point of view is used throughout this work. It is a good approximation in systems where high density of electrons dwells. With the advent of time-dependent density functional theory a new argument for the validity of this approach came out. It can be argued that the dynamics of an interacting system can be described by the evolution of a non-interacting system with a time-dependent Kohn-Sham potential [4].

To attain simplicity we omit the twofold spin degeneration of states. It's inclusion leaves a factor of two for the calculated electron density and the electric current.

In the course of this work atomic units have been used. This choice involves for the electron mass, charge and modified Planck's constant that

$$\frac{e^2}{4\pi\epsilon} = 1,\ m_e = 1 \text{ and } \hbar = 1.$$

The numerical values of energy are in the units of Hartree (1 Ha = 27.2 eV) and lengths in the multiples of Bohr radius ($1a_B = 0.527$ øA).

Chapter 2

One-particle Green's functions

2.1 Introduction

In this chapter we deal with a single-electron quantum system governed by a time-independent Hamilton operator $\mathbf{H}$. As a motivation to the concept of Green's functions [1] consider the dynamic quantity

$$G(x', t'|x, t) = -i\theta(t' - t) \left\langle x' \right| e^{-i\mathbf{H}(t'-t)} \left| x \right\rangle . \tag{2.1}$$

The exponential in Eq. 2.1 is a unitary evolution operator for a time-independent system. The matrix element is taken between localized electron states. Clearly, the physical meaning of the latter expression can be conveyed as a probability amplitude of finding an electron at the time t' and location x', if the electron was created at the $t < t'$ in a localized state $|x\rangle$.
Now consider the effect of a time derivative

$$\begin{aligned} i\frac{\partial}{\partial t'} G(x', t'|x, t) \; &= \\ &= \; \delta(t' - t) \left\langle x' \right| e^{-i\mathbf{H}(t'-t)} \left| x \right\rangle \; + \; i\theta(t' - t) \left\langle x' \right| \mathbf{H} e^{-i\mathbf{H}(t'-t)} \left| x \right\rangle \end{aligned} \tag{2.2}$$

where the orthonormality implies that

$$\lim_{t' \to t} \left\langle x' \right| e^{-i\mathbf{H}(t'-t)} \left| x \right\rangle = \delta(x' - x).$$

Expressing the Hamiltonian in a coordinate representation in turn gives

$$i\frac{\partial}{\partial t'} G(x't'|xt) = \delta(t' - t)\delta(x' - x) + H(x', \frac{\partial}{\partial x'}) G(x't'|xt), \tag{2.3}$$

[1] For a more pedagogic approach see [2]

what is known as a Green's function equation to the Shrödinger equation. For remote distances the probability amplitude must approach zero, hence we are left with the boundary condition

$$\lim_{|x-x'|\to\infty} G(x't'|xt) \;=\; 0. \tag{2.4}$$

2.2 Free electron

As an example we calculate one-electron Green's function for an infinite one-dimensional system with a constant potential. Since the effect of such potential is the shift of all energy levels, we consider only the kinetic energy term of the Hamiltonian. In view of the space-time symmetry the Green's function must have the functional form $G^r(x-x', t-t')$. We proceed to the Fourier representation by the transformations

$$G(q,\omega) = \int \mathrm{d}x \int \mathrm{d}t\; G(x-x', t-t') e^{i\omega(t-t')-iq(x-x')}. \tag{2.5}$$

The Green's function equation (Eq. 2.3) reduces to an algebraic task

$$G(q,\omega)(\omega - \frac{1}{2}q^2) = 1, \tag{2.6}$$

which can be inverted only if a small imaginary part $i\delta$ is added to the frequency ω

$$G^r(q,\omega) = \frac{1}{\omega - \frac{1}{2}q^2 + i\delta} \tag{2.7}$$

so that the poles do not lie on a real frequency axis. The superscript r indicates that the imaginary infinitesimal is positive anticipating the retarded behavior of Eq. 2.1. This is demonstrated by the inverse transformation

$$G^r(q,t) = \frac{1}{2\pi} \int \mathrm{d}\omega e^{-i\omega t} \frac{1}{\omega - \frac{1}{2}q^2 + i\delta} = \theta(t) i(-1) e^{-i\frac{1}{2}q^2 t - \delta t}. \tag{2.8}$$

For any positive time an infinite semicircle in the lower half-plane can be appended to the integration path, as it's contribution vanishes due to the exponential. The contour integration is facilitated by Cauchy's theorem. For $t < 0$ we enclose the contour with a semicircle in the upper half plane, obtaining $G^r(q,t) = 0$. Obviously the choice $-i\delta$ instead of $+i\delta$ in the denominator of Eq. 2.7 leads to the function

$$G^a(q,t) = \theta(-t) i e^{-i\frac{1}{2}q^2 t + \delta t}, \tag{2.9}$$

which is nonzero for negative times. Analyticity is thus an immediate consequence of the required time behavior. We say that the function G^r propagates a particle forwards in time while G^a backwards. The G^r (G^a) is called

retarded (advanced) Green's function.
We accomplish this subsection by calculating the functions

$$G^r(x,t) = \frac{1}{2\pi}\int e^{iqx}G^r(q,t)\mathrm{d}q \quad \text{and} \quad G^r(x,\omega) = \int e^{i\omega t}G^r(x,t)\mathrm{d}t \quad (2.10)$$

which will be important in the remaining part of this work.
On deriving $G^r(x,t)$ we arrive at a Gaussian integral

$$\frac{1}{2\pi}(-i\theta(t))\int e^{iqx-i\frac{1}{2}q^2t-\delta t}\mathrm{d}q \;=\; -i\theta(t)\frac{1}{2\pi}e^{i\frac{x^2}{2t}}\int e^{-i\frac{1}{2}tq'^2}\mathrm{d}q'$$

with the result

$$G^r(x,t) \;=\; -i\theta(t)\frac{1}{\sqrt{2\pi it}}e^{i\frac{x^2}{2t}}. \quad (2.11)$$

We have already taken the limit $\delta \to 0^+$. The latter expression reminds a delta-function representation if $t \to 0^+$.
The spectral representation $G^r(x,\omega)$ will be calculated by transforming Eq. 2.7

$$G^r(x,\omega) = \frac{1}{2\pi}\int e^{iqx}[\omega - \frac{1}{2}q^2 + i\delta]^{-1}\mathrm{d}q.$$

Now the integrand has two poles $q_{1,2} = \pm\sqrt{2(\omega+i\delta)}$ which allow us to employ contour integration as follows: for $x > 0$ the integrand vanishes for q's with large positive imaginary part. Hence $G^r(x>0,\omega)$ is given by the residuum at q_1. Similar reasoning is applied in the case $x < 0$. We have

$$x > 0 \quad G^r(x,\omega) = -ie^{iq_1x}\frac{1}{q_1}$$
$$x < 0 \quad G^r(x,\omega) = +ie^{iq_2x}\frac{1}{q_2},$$

or

$$G^r(x,\omega) = \frac{e^{i\sqrt{2(\omega+i\delta)}|x|}}{\sqrt{2(\omega+i\delta)}}. \quad (2.12)$$

2.3 General solution

Suppose there is a complete set of energy eigenstates $\{|\phi_j\rangle\}$ with eigenvalues $\{E_j\}$ so that

$$\mathbf{H}\,|\phi_j\rangle = E_j\,|\phi_j\rangle\,. \quad (2.13)$$

On inserting the unity $\sum_j |\phi_j\rangle\langle\phi_j|$ twice to Eq. 2.1 we encounter

$$G^r(x't'|xt) \;=\; -i\theta(t'-t)\sum_{k,j}\langle x'|\phi_k\rangle\langle\phi_j|x\rangle\langle\phi_k|\,e^{-i\mathbf{H}(t'-t)}\,|\phi_j\rangle \;=$$
$$=\; -i\theta(t'-t)\sum_k \phi_k(x')\phi_k^*(x)e^{-iE_k(t'-t)}. \quad (2.14)$$

The function $G^r(x', x, \omega)$ can be expressed through eigenstates, too. We can achieve this form by either Fourier - transforming the latter result for $G^r(x't'|xt)$ or by noting that $G^r(x', x, \omega)$ is a matrix element of an operator $\langle x'| \mathbf{G}^r(\omega) |x\rangle$ for which an equation can be derived

$$(\omega - \mathbf{H})\mathbf{G}^r(\omega) = \mathbf{1}. \tag{2.15}$$

The formal solution reads

$$\mathbf{G}^r(\omega) = \frac{\mathbf{1}}{\omega - \mathbf{H} + i\delta}. \tag{2.16}$$

Here we have already shifted the pole away from the real axes according to what we have learned in the previous chapter. Eq. 2.16 can be recast to a coordinate form by inserting unity and sandwiching between $|x\rangle$ and $\langle x'|$ as follows

$$\begin{aligned} G^r(x', x, \omega) = & \sum_j \langle x'| \frac{|\phi_j\rangle \langle\phi_j|}{\omega - \mathbf{H} + i\delta} |x\rangle \; = \\ = & \sum_j \langle x'| \frac{|\phi_j\rangle \langle\phi_j|}{\omega - E_j + i\delta} |x\rangle \; = \\ = & \sum_j \frac{\phi_j(x')\phi_j^*(x)}{\omega - E_j + i\delta}. \end{aligned} \tag{2.17}$$

2.4 Dyson equation with an application

Consider an *ad-hoc* splitting of the Hamiltonian $\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1$. In a typical case one knows the eigenstates of H_0 readily. The total Green's function $G^r(x', t'|x, t)$ to the Hamiltonian $\mathbf{H}$ can be related to the Green's function of $\mathbf{H}_0$ by a Dyson equation, which can be derived starting from the operator form of Eq. 2.16

$$\mathbf{G}^r(\omega) \; = \; \frac{\mathbf{1}}{\omega + i\delta - \mathbf{H}_0 - \mathbf{H}_1} \; = \; \frac{\frac{1}{\omega + i\delta - \mathbf{H}_0}}{1 - \frac{\mathbf{H}_1}{\omega + i\delta - \mathbf{H}_0}} \; = \; \frac{\mathbf{G}_0^r(\omega)}{1 - \mathbf{G}_0^r(\omega)\mathbf{H}_1}, \tag{2.18}$$

where $\mathbf{G}_0^r(\omega) = [\omega + i\delta - \mathbf{H}_0]^{-1}$. We can rewrite Eq. 2.18 to the form

$$\mathbf{G}^r(\omega) - \mathbf{G}_0^r(\omega)\mathbf{H}_1\mathbf{G}^r(\omega) = \mathbf{G}_0^r(\omega). \tag{2.19}$$

On insertion of the unity twice

$$\mathbf{1} = \int \mathrm{d}\bar{x} \, |\bar{x}\rangle \langle\bar{x}|$$

and sandwiching we obtain in turn the Dyson equation in a coordinate representation

$$G^r(x',x,\omega) = G_0^r(x',x,\omega) + \int\int G_0^r(x',\bar{x},\omega)H_1(\bar{x},\bar{\bar{x}})G^r(\bar{\bar{x}},x,\omega)\ \mathrm{d}\bar{x}\mathrm{d}\bar{\bar{x}}. \tag{2.20}$$

We apply this powerful tool to the case of an electron struggling with a delta-function potential, ie $V_d(x) = c\delta(x), \quad c > 0$. Since

$$H_1(x,x') = c\delta(x)\delta(x-x') \tag{2.21}$$

the Dyson equation simplifies to

$$G^r(x',x,\omega) = G_0^r(x',x,\omega) + cG_0^r(x',0,\omega)G^r(0,x,\omega).$$

It can be solved for G^r easily. Specialization to $x' = 0$ yields

$$G^r(0,x) = \frac{G_0^r(0,x)}{1 - cG_0^r(0,0)}.$$

The solution

$$G^r(x',x,\omega) = G_0^r(x',x,\omega) + \frac{cG_0^r(x',0,\omega)G_0^r(0,x)}{1 - cG_0^r(0,0)}$$

converts to

$$G^r(x',x,\omega) = \frac{e^{ik|x-x'|}}{ik} + \frac{c}{ik-c}\frac{e^{ik|x|+ik|x'|}}{ik}, \quad k = \sqrt{2\omega + i\delta} \tag{2.22}$$

on employing the results for G_0^r of Eq. 2.12.

Also the "time" Green's function $G^r(x't'|xt)$ for a delta-barrier can be written as a sum of a "homogeneous" term given by Eq. 2.11 and an inhomogeneous one

$$\begin{aligned} G^r(x't'|xt) \ &= \ G_0^r(x-x',t'-t) \ + \\ &+ \ \int_{-\infty}^{\infty} \frac{c}{i\sqrt{2\omega+i\delta}-c}\frac{e^{i\sqrt{2\omega+i\delta}|x|+i\sqrt{2\omega+i\delta}|x'|}}{i\sqrt{2\omega+i\delta}}e^{-i\omega(t'-t)}\mathrm{d}\omega. \end{aligned} \tag{2.23}$$

The rest of the calculation is postponed to Appendix A. Here we mention only the limit $c \to \infty$ of a strong barrier. This limit affects the fraction

$$\frac{c}{ik-c} = -\frac{ik-c}{ik-c} + \frac{ik}{ik-c}$$

where only the first term contributes in the zeroth order of $1/c$. We are left with

$$G^r(x',x,\omega) = \frac{e^{ik|x-x'|}}{ik} - \frac{e^{ik|x|+ik|x'|}}{ik} \tag{2.24}$$

and

$$G^r(x',t'|x,0) = \frac{-i}{\sqrt{2\pi i t'}}\ \left[e^{i\frac{(x'-x)^2}{2t'}} - e^{i\frac{(|x'|+|x|)^2}{2t'}}\right]\theta(t'). \tag{2.25}$$

Chapter 3

Linear response theory

3.1 Introduction

Now we would like to develop a general tool for studying non-interacting electron systems that are driven away from equilibrium by an external potential. We achieve a formulation which relates directly observable quantities – the electron density and the applied potential.

We adopt the assumption that magnetic effects connected with variation of a scalar potential are negligible. Hence in the gauge we use the vector potential $\mathbf{A}(x,t)$ is zero identically. Instead of using an electric potential we use the potential energy $V(x,t)$ that will be a function of space and time. The time dependence is here only due to a specific way of switching on. As we study the departure from equilibrium, we put $V(x,t)$ zero for $t < 0$.

In this chapter we treat electron gas in the framework of a many-body theory (cf. the reference [1]). It has been stated in the Introduction that the quantum non-locality replaces phenomenological local relations like the Ohm's law with non-local ones. This is an essential result of the Kubo-Greenwood theorem which we derive here for electron density of a non-interacting electron system at zero temperature.

3.2 Ground state electron density

Before we start dealing with linear response we want to show that equilibrium density can be written using one-particle Green's function. It is not surprising, as we deal with a non-interacting system.
We begin by noting that the expectation values for a *non-interacting* electron gas can be shown to reduce to a sum over one-particle basis states. Schematically

$$\langle \text{many-electron state}|\ (\cdots)\ |\text{many-electron state}\rangle\ =\ \mathrm{Tr}\ \{\mathbf{n}_F\ (\cdots)\} \tag{3.1}$$

for an arbitrary one-particle operator; the projector $\mathbf{n}_F$ discards [1] states with energy greater than the Fermi energy E_F In the equilibrium the system is in a stationary state as given by the Hamilton operator $\mathcal{H}_0$ which encompasses kinetic terms and arbitrary potentials representing disorders in the electron gas. The equilibrium expectation value of electron density can be written with the aid of a number density operator

$$n_0(x) = \langle \Phi_0 | \, e^{+i\mathcal{H}_0 t} \mathbf{n}(x,0) e^{-i\mathcal{H}_0 t} \, | \Phi_0 \rangle \,,$$

where $|\Phi_0\rangle$ is a ground state in the Heisenberg picture. In virtue of Eq. 3.1 the density reduces to a sum over one-particle basis states $|\phi_j\rangle$ as follows

$$n_0(x) \;=\; \sum_j \theta(E_F - E_j) \;\; \langle \phi_j | x \rangle \langle x | \phi_j \rangle \;=\; \sum_j \theta(E_F - E_j) \;\; \phi_j(x) \phi_j^*(x).$$

We remind the principal value theorem $(z + i\delta)^{-1} = \mathcal{P}\frac{1}{z} - i\pi\delta(z)$ which enables us further rearrangement

$$\begin{aligned} n_0(x) = \int_0^{E_F} \sum_j \delta(\omega - E_j) \;\; \phi_j(x) \phi_j^*(x) \mathrm{d}\omega = \\ = \frac{-1}{\pi} \int_0^{E_F} \sum_j \mathfrak{Im} \left\{ \frac{\phi_j(x) \phi_j^*(x)}{\omega - E_j + i\delta} \right\} \mathrm{d}\omega = \\ = \frac{-1}{\pi} \int_0^{E_F} \mathfrak{Im} \left\{ G^r(x,x,\omega) \right\} \;\; \mathrm{d}\omega. \end{aligned} \quad (3.2)$$

We have employed the Eq. 2.17 which expresses the Green's function through eigenstates.

3.3 First order

Now imagine that at $t = 0$ we turn on the external potential $V(x,t)$. A considerable information can be obtained from the perturbation theory assuming that the potential is weak. The many-body Hamiltonian $\mathcal{H}$ has the form

$$\begin{aligned} \mathcal{H} = \mathcal{H}_0 \quad \text{for } t < 0 \\ \mathcal{H} = \mathcal{H}_0 + \mathcal{V}(t) \quad \text{for } t > 0. \end{aligned}$$

The potential energy $\mathcal{V}$ is simply an integral of $V(x,t)$ times electron density operator. For positive times the expectation value of electron density reads

$$\begin{aligned} n(x,t) \;&=\; \langle \Phi_0 | \, e^{+i\int_0^t \mathcal{H}(t')\mathrm{d}t'} \mathbf{n}(x,0) e^{-i\int_0^t \mathcal{H}(t')\mathrm{d}t'} \, | \Phi_0 \rangle \;= \\ &=\; \langle \Phi_0 | \, e^{+i\int_0^t \mathcal{H}(t')\mathrm{d}t'} e^{-i\mathcal{H}_0 t} \mathbf{n}(x,t) e^{+i\mathcal{H}_0 t} e^{-i\int_0^t \mathcal{H}(t')\mathrm{d}t'} \, | \Phi_0 \rangle \;= \\ &=\; \langle \Phi_0 | \, U^\dagger(t,0) \mathbf{n}(x,t) U(t,0) \, | \Phi_0 \rangle \,. \end{aligned} \quad (3.3)$$

[1] $\mathbf{n}_F$ is the zero-temperature density matrix

The time evolution of $\mathbf{n}(x,t) = e^{+i\mathcal{H}_0 t}\mathbf{n}(x,0)e^{-i\mathcal{H}_0 t}$ is governed by $\mathcal{H}_0$ only, it's the interaction representation of the density operator.
For the unitary operator $U(t,0)$ a Schrödinger-like equation of motion can be written

$$\begin{aligned} i\frac{\partial}{\partial t}U(t,0) &= e^{+i\mathcal{H}_0 t}(\mathcal{H}-\mathcal{H}_0)e^{-i\int_0^t \mathcal{H}(t')\mathrm{d}t'} = \\ &= \mathcal{V}_I U(t,0), \end{aligned}$$

where

$$\mathcal{V}_I = e^{+i\mathcal{H}_0 t}\mathcal{V}e^{-i\mathcal{H}_0 t}.$$

The solution can be constructed by the means of an integral equation

$$U(t,0) = 1 - i\int_0^t \mathcal{V}_I(t')U(t',0)\mathrm{d}t' \tag{3.4}$$

along with the initial condition $U(0,0) = 1$. A chain of approximations can be written by successive insertions of the left side of Eq. 3.4 to the integrand on the right hand. Since we are interested in the linear regime only, the density (Eq. 3.3) must include the potential to the first order. Hence we take

$$U(t,0) \approx 1 - i\int_0^t \mathcal{V}_I(t')\mathrm{d}t'$$

and recast the Eq. 3.3 to the form

$$\begin{aligned} n(x,t) = \\ &= \langle\Phi_0|\left(1+i\int_0^t \mathcal{V}_I(t')\mathrm{d}t'\right)\mathbf{n}(x,t)\left(1-i\int_0^t \mathcal{V}_I(t')\mathrm{d}t'\right)|\Phi_0\rangle = \\ &= n_0(x) + i\langle\Phi_0|\int_0^t [\mathcal{V}_I(t'),\ \mathbf{n}(x,t)]\ \mathrm{d}t'\,|\Phi_0\rangle\,,\ t>0, \end{aligned}$$

where the second-order term has been dropped and the equilibrium density $n_0(x)$ has emerged. Now we realize that

$$\mathcal{V}_I(t) = \int V(x',t)\mathbf{n}(x',t)\mathrm{d}x'$$

so that for the change of density that stems from the application of external field we have

$$\begin{aligned} \delta n(x,t) = \\ &= i\int_0^t\int \langle\Phi_0|\,[\mathbf{n}(x',t'),\ \mathbf{n}(x,t)]\,|\Phi_0\rangle\ V(x',t')\ \mathrm{d}t'\mathrm{d}x' = \\ &= \int_0^t\int \chi(x,t|x',t')V(x',t')\ \mathrm{d}t'\mathrm{d}x' \end{aligned} \tag{3.5}$$

where

$$\chi(x,t|x',t') = -i \langle \Phi_0 | \left[\mathbf{n}(x,t),\ \mathbf{n}(x',t') \right] | \Phi_0 \rangle$$

is response function that involves equilibrium quantities only. The formulation that we have just attained is quite general and could be applied to systems with arbitrary many-body interactions. We resort to the study of non-interacting systems and utilize the Eq. 3.1. The response function simplifies to

$$\chi(x,t|x',t') = -i \ \mathrm{Tr}\ \mathbf{n}_F \ [\mathbf{n}(x,t),\ \mathbf{n}(x',t')]. \tag{3.6}$$

3.4 Response function

In the last section we have formulated the Eq. 3.5 which relates density change to an external driving potential. Since we treat the potential as a small perturbation, this relation is linear, though non-local in space and time. It is a powerful tool for investigation of transient states in the electron gas. The response function (Eq. 3.6) is written in terms of equilibrium density-density correlations, hence we say that in the first order the equilibrium density fluctuations determine the behavior of a system out of equilibrium.
It is now our task to calculate the response function. The method we have chosen employs one-particle Green's functions. We shall see how do they emerge in the subsequent calculation [9]. Let's start with the prescription of Eq.(3.6) and use the cyclic property of trace to obtain

$$\begin{aligned} \chi(x,t|x',t') = &-i\mathrm{Tr}\ \mathbf{n}(x',t')\mathbf{n}_F\ \mathbf{n}(x,t)\ + \\ &+\ i\mathrm{Tr}\ \mathbf{n}(x,t)\mathbf{n}_F\ \mathbf{n}(x',t')\ =\ 2\mathfrak{Im}\left\{\mathrm{Tr}\ \mathbf{n}(x',t')\mathbf{n}_F\ \mathbf{n}(x,t)\right\}. \end{aligned}$$

Now we set $t' = 0$ without any loss of generality, as the response function devolves upon equilibrium quantities only so that the dependence on time arguments has the form $t - t'$. The trace will be written explicitly, the projector implies another summation which will be denoted by an exclamation sign $\sum_{k!}$ to indicate that we add terms with energy less than E_F.

$$\begin{aligned} 2\mathfrak{Im}\left\{ \sum_{j,k!} \left\langle \phi_j | x' \right\rangle \left\langle x' | \phi_k \right\rangle \left\langle \phi_k | x \right\rangle \left\langle x | \phi_j \right\rangle e^{-i(E_j - E_k)t} \right\} = \\ = 2\mathfrak{Im}\left\{ \sum_j \phi_j(x)\phi_j^*(x')e^{-iE_j t}\ \sum_{k!} \phi_k(x')\phi_k^*(x)e^{iE_k t} \right\} \end{aligned}$$

We can employ the general form of a Green's function contained in the Eq. 2.14 since we contemplate only $t > 0$.

The other sum can be proven to be the integral

$$-\frac{1}{\pi}\int_0^{E_F} e^{i\omega t}\mathfrak{Im}\left\{G(x',x,\omega)\right\}\mathrm{d}\omega \equiv -iC(x',x,-t) \tag{3.7}$$

in the same fashion as the Eq. 3.2. We accomplish our effort with the main result of this section

$$\chi(x,t|x',t') = 2\mathfrak{Im}\left\{G^r(x,t|x',t')C(x',x,t'-t)\right\}. \tag{3.8}$$

As an example the response function of a homogeneous electron gas is derived in the Appendix B.

3.4.1 Electron gas with a delta-barrier

The latter equation will be used to study the electron gas with a potential $c\delta(x)$. This barrier is treated as a part of the unperturbed Hamiltonian $\mathcal{H}_0$. The potential $V(x,t)$ will represent an external field that drives the system out of equilibrium. Thus the Green's functions that form the Eq. 3.8 are one-particle Green's functions of an electron with a delta-barrier potential. We need two ingredients for the response function. The Green's function in a direct space and time $G^r(x,t|x',t')$ calculated in the Appendix A reads

$$G^r(x,t|x',0) = \frac{-i}{\sqrt{2\pi i t}}e^{i\frac{r^2}{2t}}\,\theta(t) + \\ + \frac{ic}{2}\exp\left\{i\frac{c^2}{2}t + c\xi + \ln\,\mathrm{erfc}\sqrt{\frac{i}{2t}}(ct - i\xi)\right\}\theta(t).$$

in the notation $\xi = |x| + |x'|$ and $r = |x - x'|$. Well, that's not a "nice-looking" function. The other necessary term C is an integral which has to be evaluated numerically. With the aid of Eq. 2.22 we have

$$C(x',x,t) = \frac{1}{i\pi}\int_0^{E_F}\mathrm{d}\omega\mathfrak{Im}\left\{\frac{e^{ikr}}{ik} + \frac{c}{ik-c}\frac{e^{ik\xi}}{ik}\right\}\,e^{i\frac{k^2}{2}t}.$$

The singularity is removed by replacing $k^{-1}\mathrm{d}\omega = \mathrm{d}k$ so that we finish with

$$C(x',x,t) = \frac{1}{i\pi}\int_0^{k_F}\mathrm{d}k\mathfrak{Im}\left\{-ie^{ikr} - \frac{ic}{ik-c}e^{ik\xi}\right\}\,e^{i\frac{k^2}{2}t}. \tag{3.9}$$

This is a job for a computer.

3.5 Current density. Induced potential

For the sake of reference we review shortly some auxiliary relations concerning a charged line. In a closed one-dimensional system current density

$j(x,t)$ and particle density satisfy the continuity equation

$$\frac{\partial}{\partial t}n(x,t) \;=\; \frac{\partial}{\partial x}j(x,t)$$

which in turn can be integrated

$$j(x,t) = \frac{\partial}{\partial t}Q(x,t), \quad Q(x,t) \equiv \int_{-\infty}^{x} n(x',t)\mathrm{d}x'.$$

The current in a steady state obtained from the linear response theory can be compared to the Landauer formula (see Eq. 1.2).
The density $n(x,t_0)$ at a certain time induces additional electric field described by the potential $\phi_i(x,t_0)$ subject to the Poisson's equation

$$\frac{\partial^2}{\partial x^2}\phi_i(x,t_0) = 4\pi n(x,t_0).$$

Note that in the latter equation we have put the electron density instead of the usual charge density. On inverting we arrive at the expression

$$\phi_i(x,t_0) = \int_{-\infty}^{x} (x'-x)\; n(x',t_0)\; \mathrm{d}x' \;= \\ = \int_{-\infty}^{x} x' n(x',t_0)\; \mathrm{d}x' \;-\; xQ(x,t_0). \quad (3.10)$$

Chapter 4

Numerical methods

As stated in the Introduction, the main task is the calculation of the density response (Eq. 3.5) of an inhomogeneous gas to the potential (Fig. 1). The inhomogeneity is simulated by placing the delta-function barrier. The specification of the task for the numerics is:

1. Complex error function necessary for the calculation of Green's function
2. The function C of Eq. 3.9. Having obtained the response function we need to
3. integrate in space and time (Eq. 3.5) to get the density response to the potential.

Ad 1 The complementary error function[1]

$$\mathrm{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-\tau^2} \mathrm{d}\tau \tag{4.1}$$

has been evaluated in the first quadrant by a series approximation

$$\mathrm{erfc}(z) = 1 - \frac{2}{\sqrt{\pi}} e^{-z^2} \sum_{n=0}^{\infty} \frac{2^n}{1 \cdot 3 \cdot 5 \ldots (2n+1)} z^{2n+1} \tag{4.2}$$

for the argument values $|z| < 1,5$. For arguments with greater $|z|$ we have employed the continued fraction approach

$$\mathrm{erfc}(z) = e^{-z^2} \frac{2z}{\sqrt{\pi}} \left\{ \frac{1}{2z^2 + 1 -} \frac{1 \cdot 2}{2z^2 + 5 -} \frac{3 \cdot 4}{2z^2 + 9 -} \ldots \right\}, \quad |z| > 1.5 \tag{4.3}$$

[1] For the definition and properties we refer to [5]

The function values in other quadrants can be obtained by the reflection properties $\mathrm{erfc}(\bar{z}) = \overline{\mathrm{erfc}(z)}$ and $\mathrm{erfc}(-z) = 2 - \mathrm{erfc}(z)$.
With this device we are ready to calculate the Green's function (Eq. A.1). We have tested this function in the case of a one-electron wave-packet propagating towards a delta-function barrier.

Ad 2 The integrand of Eq. 3.9 is an oscillating function. We manage this task by employing the Gauss-Kronrod rule for the numerical approximation of this definite integral.

Ad 3 Fig. 4.1 displays the time-dependence of a response function in the case $c = 0$ for various values of the spatial stride (to be discussed later). It's clear that due to the singular oscillating behavior at $t = 0$ (also apparent in the Eq. B.1 and similarly when $c \neq 0$) linear discretization of the time axis is not helpful at all. In the Eq. 3.5 we must substitute $t' = e^s$ and discretize the variable s. The integral becomes

$$\delta n(x,t) = \int \mathrm{d}x' \int_{-\infty}^{\ln t} \tilde{\chi}(x,x',\ln t - s)\mathrm{d}s \tag{4.4}$$

where $\tilde{\chi}(x,x',s) = \chi(x,x',e^s) \times e^s$. The integrand is plotted in the Fig. 4.2. A suitable low range for the integral can be introduced (typically -6.0 is fine). Then, the approximation to the latter time integration can be obtained by the means of a Simpson's rule. Number of instants in the sum is usually more than 200 (concerning the results presented in the next section).
The spatial dependence of the response function is oscillatory as well. However, we expect the oscillations have a typical quasi-period of the order of λ_F, the Fermi wave-length. The spatial integration was performed in a restricted area only, ie $\int_{-\infty}^{\infty} \to \int_{-\mathrm{ext}/2}^{\mathrm{ext}/2}$, ext being about ≈ 150. The integral was approximated by a trapez rule with stride less than $\frac{1}{20}$ in the units of λ_F, ie we included more than 20 points per Fermi wave-length to the integral of Eq. 4.4.

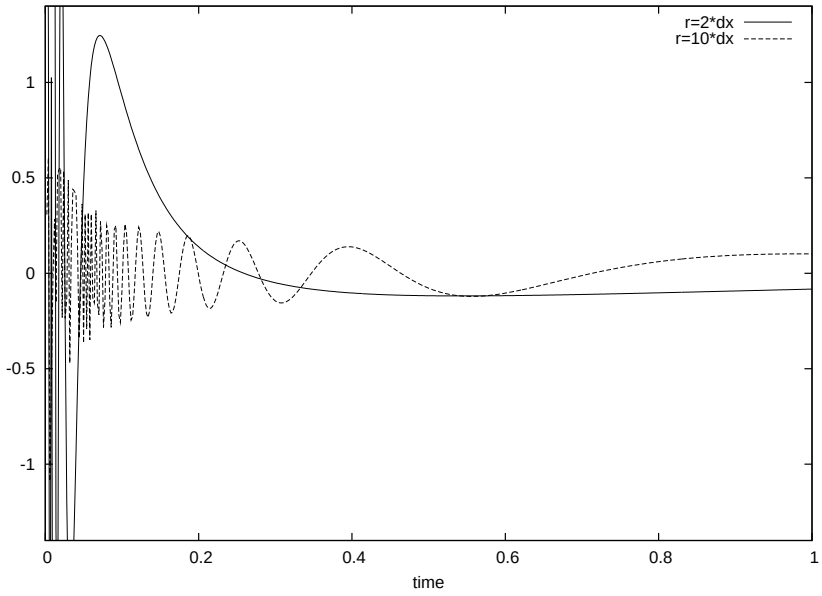

Figure 4.1: *Time dependence of a response function for two values of* $r = |x - x'|$. *Here* $\mathrm{d}x$ *is a stride of the spatial discretization.*

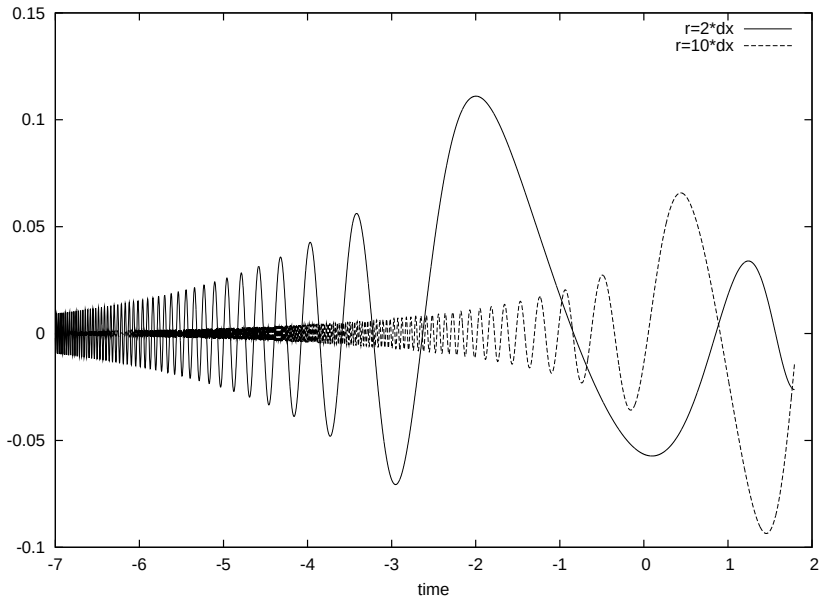

Figure 4.2: *The function* $\tilde{\chi}(x, x', s)$ *of the Eq. 4.4. Here dx is a stride of the spatial discretization.*

Chapter 5

Results

Figs. 5.1-5.4 show the first order density change $\delta n(x,t)$ as a result of turning on the perturbing potential at $t = 0$. The potentials employed have the form of Fig. 1. The calculations have been performed with various values of the slope width a, ie the region of a constant field strength. The voltage bias ΔV has had a fixed value 20. We stress that the actual units of δn are a_B^{-1}, though this is not relevant due to the linear dependence on the bias. The range of a has been $\langle 0.5; 20\rangle$, what can be compared to the Fermi wave length $\lambda_F = 4.0558$ of the electron gas. The change of the electron density $\delta n(x,t)$ has been calculated always at the point $x = 10$. We note that the method of time integration has been the equally-spaced trapez rule, what could be a source of possible errors. Another parameter that has been varied is the magnitude of the delta-function barrier c (see Sec. 3.4.1).

All the plots show the onset of a steady state. We define the relaxation time τ as the instant when the density change $\delta n(x,t)$ varies no more than 10% from it's steady-state value. The relaxation time for electron gasses with a variety of barriers is presented in the Fig. 5.5.
Additionally we present the spatial dependence of $\delta n(x,t)$ in the Fig. 5.6. The density for $x < 0$ reaches a maximum and then we observe broadening of the front. For $x > 0$ the process is the same up to a sign. Fig. 5.7 plots the induced potential to the density distribution of Fig. 5.6. These last two plots were obtained by employing the logarithmic discretization of the time axis, as described in the Chap. 4.
The behavior of the homogeneous gas can be interpreted easily. For values of a much smaller than the actual λ_F the electron gas is insensible to any change of a. This saturation holds true even if $c \neq 0$ and the disorder becomes invisible. Dimensional analysis yields for the relaxation time τ when $a \ll \lambda_F$ the law $\tau = \frac{10}{v_F} + \tau_0$ where $\tau_0 \propto E_F^{-1}$. Exact calculation [8] for the homogeneous gas of electrons comes with $\tau_0 = \frac{2\pi}{E_F}$, what is different from the numerical value. The source of this discrepancy could be seen in

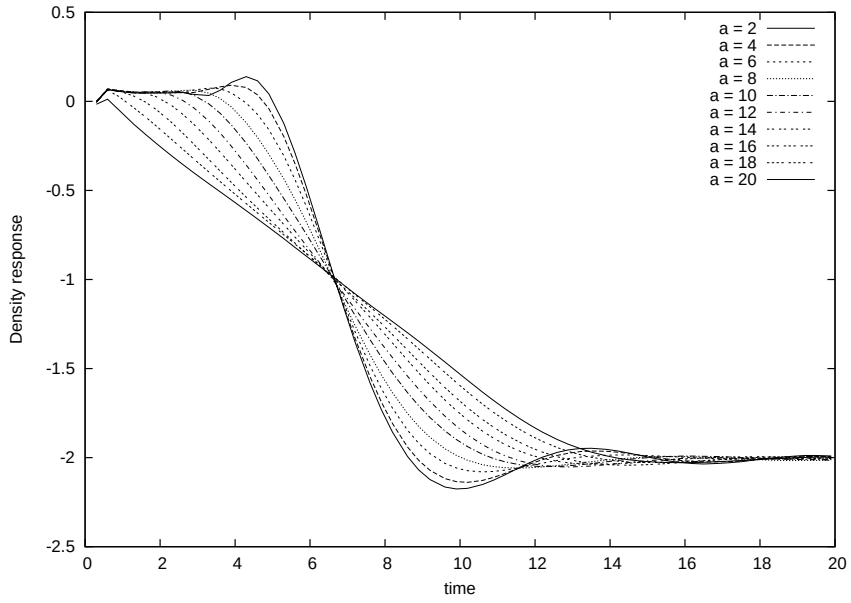

Figure 5.1: Density response at $x = 10$ of a homogeneous electron gas ($c = 0$) against time parameterized by the width of the potential drop.

Fig. 5.1. Notice that the blob of positive change in density is unphysical (as well as the positive background for $t < 4$). We have found that the source of this error dwells in the numerical integrator in time. Linear mesh fails to do the job, as described in Chap. 4.
For a homogeneous electron gas at $a \gg \lambda_F$ there's a domain of proportionality. The onset of a steady state is determined by the "impulse" that arrives from the furthest corner of the constant field, ie $-\frac{a}{2}$. The relaxation time becomes $(10 + a/2)/v_F$. In the Fig. 5.5 τ raises with a with the factor of ≈ 0.226. The trend in the a-dependence of τ for growing value of c must be decreasing for there is an obstacle in the coordinate origin. This is exhibited in the Fig. 5.5 as well.
There is a hope that the logarithmic discretization will patch the numerical error that is present in the calculation of the relaxation time.
In the Fig. 5.6 we see a non-zero electric dipole

$$p(t) = -\int_{-\infty}^{\infty} \delta n(x,t)\ x\mathrm{d}x \tag{5.1}$$

that keeps on broadening with the Fermi velocity. This is a clear indication of the fact that non-interacting approximation becomes completely inadequate for the modelling of time-dependent electron transport. What must happen physically is the attraction between the valley ($x > 0$) and the peak ($x < 0$).

This is further elaborated in the Fig. 5.7. We have calculated the induced potential (cf. Eq. 3.10). The induced electric field has opposite effect as the external driving field, hence we have found a serious objection against this model of a nanoscopic junction.

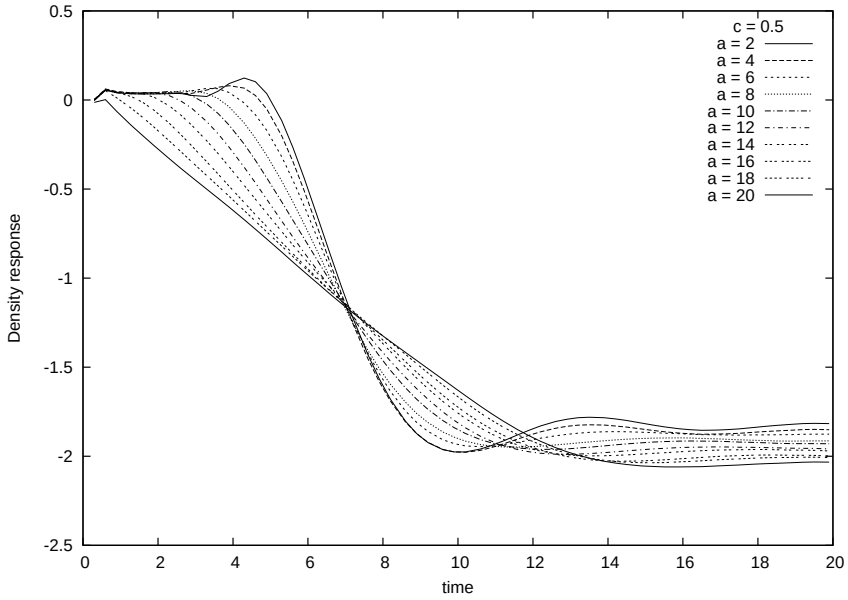

Figure 5.2: Density response at $x = 10$ of the inhomogeneous electron gas ($c = 0.5$) against time parameterized by the width of the potential drop.

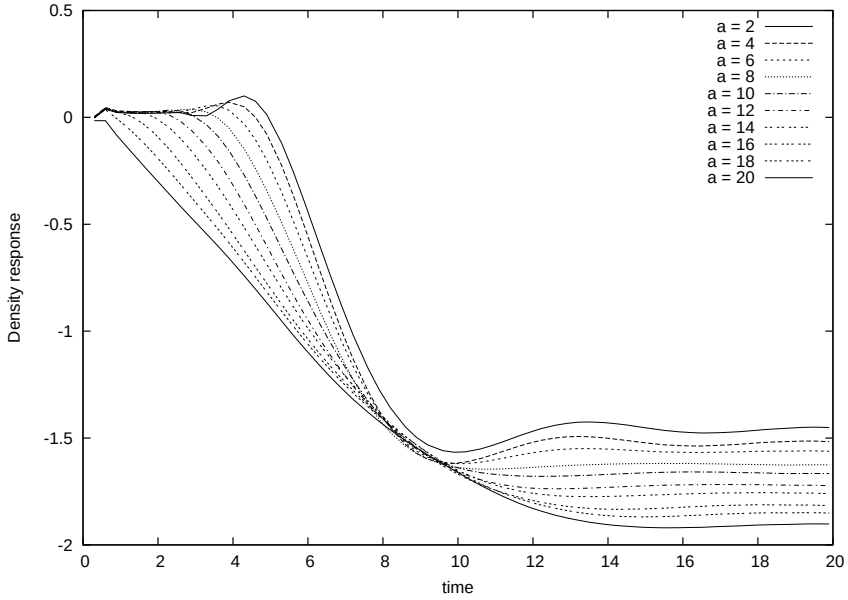

Figure 5.3: Density response at $x = 10$ of the inhomogeneous electron gas ($c = 1$) against time parameterized by the width of the potential drop.

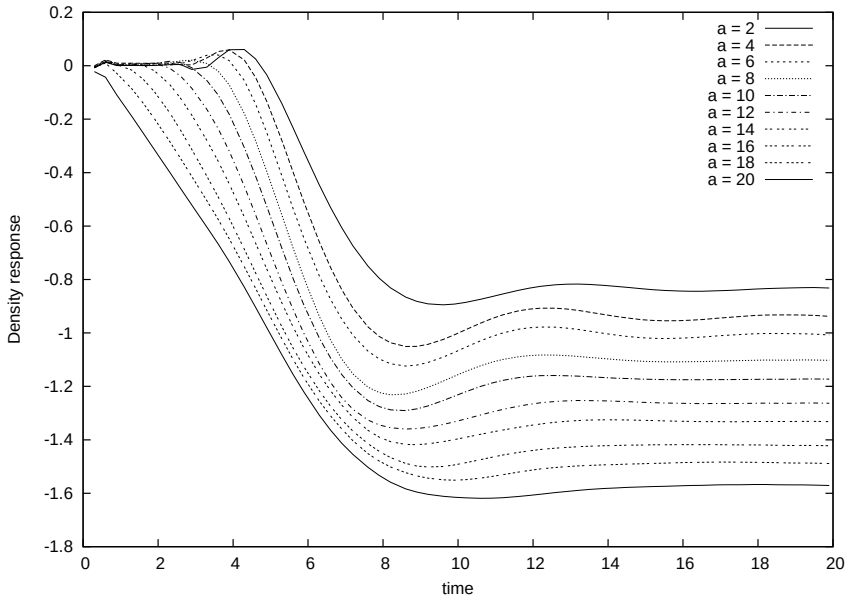

Figure 5.4: Density response at $x = 10$ of the inhomogeneous electron gas ($c = 2$) against time parameterized by the width of the potential drop.

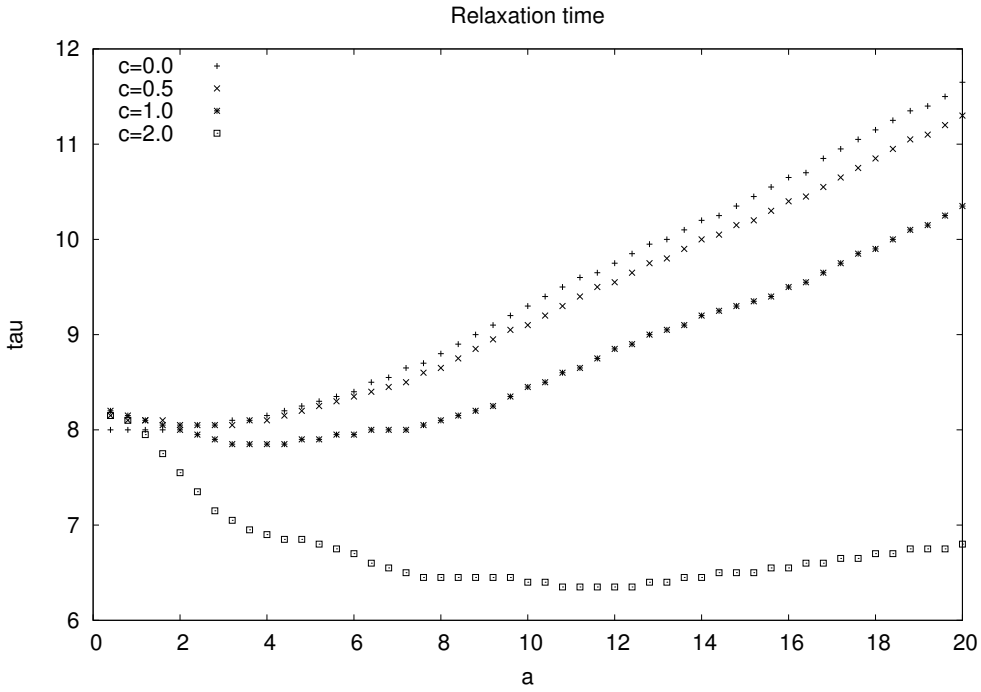

Figure 5.5: Relaxation time of the electron density at $x = 10$ as a function of the potential drop width for the electron gasses with various barriers $c = 0, 0.5, 1, 2$.

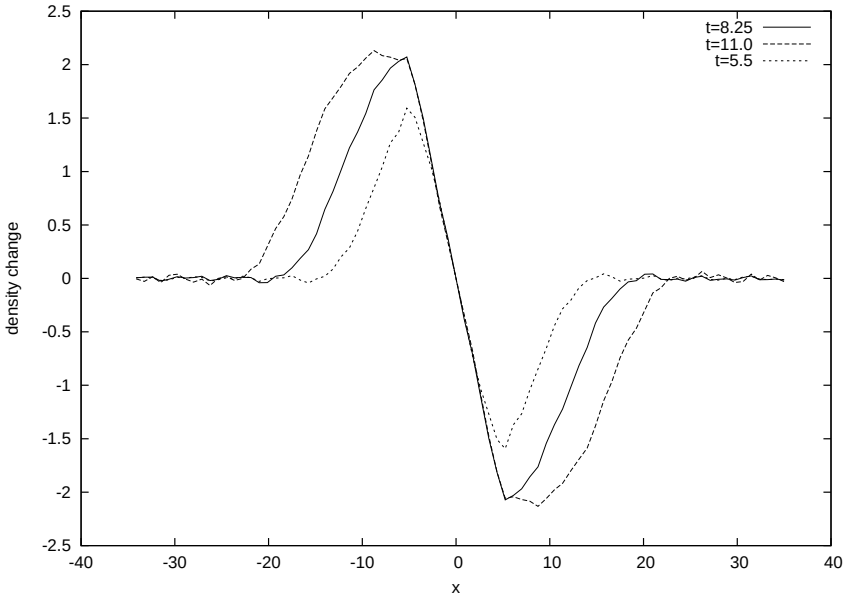

Figure 5.6: Density change as a function of a coordinate at three instants of time for a homogeneous electron gas.

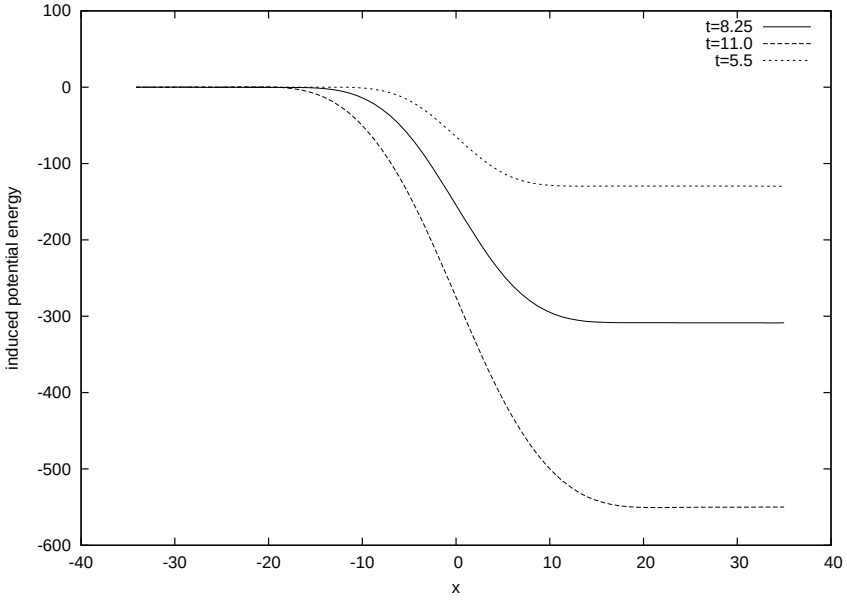

Figure 5.7: Induced potential energy to the density of Fig. 5.6

Chapter 6

Conclusion and Outline

In this work the onset of a steady state in the inhomogeneous electron gas has been investigated. For this goal the quantum mechanics of a many-electron system had to be studied. The first order perturbation theory (linear regime) has been employed in order to formulate the response equation. The time evolution of a many-electron system has been studied by the means of one particle Green's functions.
The main quantity of our interest has been the electron density. We have calculated the change in density in a transient state as a consequence of the application of external field. The particular shape of the electric potential has served us to investigate the transient state in a nanoscopic junction with a disorder.
Numerical results have shown relaxation in the non-interacting approach. It's dependence on the magnitude of the disorder and the external potential has been discussed. The results of numerical simulations lead to a qualitative understanding of the essential features of the relaxation dynamics - dictated by the fronts of the density change moving at the Fermi velocity.
To end up we summarize some of our own contributions and achievements and point out the direction of further investigation in this field.

- Eq. 3.8 which expresses the density response function through one-particle Green's functions.
- The detailed derivation of the constituents that enter the Eq. 3.8, especially the Green's function in a direct space and time of an electron with delta-potential.
- The implementation of Eq. 3.5 in a computer program for an arbitrary potential.
- Analysis of the relaxation time dependence on the parameters a, c.
- Study of space-time dependence of χ

Numerical problems with the time integration have been mentioned. They could be overcome if we used the logarithmic discretization of the time axis. We have argued that the possible inclusion of electron-electron interaction can render the onset of a steady state doubtful. This could be shown in the RPA approximation (self-consistent time dependent Hartree approximation) using the same model system, modifying the potential energy every time by the induced potential.

Are there any physical reasons for this breakdown? We suppose that the picture of screening in the leads is incorrect, that we must consider a finite relaxation time in the bulk as well. Taking this into account we will employ an external potential for which the field strength is nonzero in the whole space, but for an arbitrarily short time. We assume that in this model the charge neutrality is not violated.

Appendix A

Green's function for a delta-barrier in a closed form

On evaluating the Green's function for the δ-barrier (Eq.2.23) we arrive at the integral

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{c}{i\sqrt{2\omega+i\delta}-c}\,\frac{e^{-i(\omega+i\delta)t+i\sqrt{2\omega+i\delta}\xi}}{i\sqrt{2\omega+i\delta}}\mathrm{d}\omega\equiv I,$$

or

$$\frac{1}{2\pi}\int_{-\infty+i\delta}^{+\infty+i\delta}\frac{c}{i\sqrt{2\omega}-c}\frac{e^{-i(\omega+i\delta)t+i\sqrt{2\omega}\xi}}{i\sqrt{2\omega}}\mathrm{d}\omega,$$

where $\xi=|x|+|x'|$. From now on we contemplate only $t>0$, due to the retarded behavior. We split the ω integration into two parts.
Now the first part

$$\frac{1}{2\pi}\int_{0}^{\infty}\frac{c}{i\sqrt{2\omega}-c}\frac{e^{-i(\omega+i\delta)t+i\sqrt{2\omega}\xi}}{i\sqrt{2\omega}}\mathrm{d}\omega=\frac{1}{2\pi}\int_{0}^{\infty}\frac{c}{ik-c}\frac{e^{-i\frac{k^2}{2}t+ik\xi}}{ik}k\mathrm{d}k,$$

where the substitution $\omega=\frac{k^2}{2}$ has been employed. Similarly we perform the $\omega=-\frac{k^2}{2}$ substitution in the domain of integration $\mathfrak{Re}\{\omega\}<0$, so that

$$\begin{aligned}&\frac{1}{2\pi}\int_{\infty}^{0}\frac{c}{i^2k-c}\frac{e^{i\frac{k^2}{2}t+i^2k\xi}}{i^2k}(-k\mathrm{d}k)\;=\\&=\;\frac{1}{2\pi}\int_{i\infty}^{0}\frac{c}{-k-c}e^{i\frac{k^2}{2}t-k\xi}\mathrm{d}k\;=\\&=\;\frac{1}{2\pi i}\int_{-\infty}^{0}\frac{c}{ik'-c}e^{-i\frac{k'^2}{2}t+ik'\xi}\mathrm{d}k'.\end{aligned}$$

We have rotated the integration path, since the integrand is analytic for $\mathfrak{Re}\{k\} > 0$ and falls off at least exponentially as $\mathfrak{Re}\{k\}$ tends to infinity. Now we have

$$\begin{aligned} I = & \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{c}{ik'-c}e^{-i\frac{k'^2}{2}t+ik'\xi}\mathrm{d}k' = \\ = & \frac{1}{2\pi i}e^{i\frac{\xi^2}{2t}}\int_{-\infty}^{\infty}\frac{c}{ik'-c}e^{-i(k'-\frac{\xi}{t})^2\frac{t}{2}}\mathrm{d}k' = \\ = & \frac{1}{2\pi}e^{i\frac{\xi^2}{2t}}\int_{-\infty}^{\infty}\frac{c}{\gamma-k}e^{-ik^2\frac{t}{2}}\mathrm{d}k, \end{aligned}$$

where $\gamma \equiv -\xi/t - ic$. Since c is always positive, we are allowed to employ the integral representation

$$\frac{1}{\gamma-k} = i\int_0^{\infty} e^{-i(\gamma-k)\tau}\mathrm{d}\tau.$$

Hence

$$\begin{aligned} I = & \frac{ic}{2\pi}e^{i\frac{\xi^2}{2t}}\int_{-\infty}^{\infty}dk\int_0^{\infty}\mathrm{d}\tau e^{-ik^2\frac{t}{2}-i(\gamma-k)\tau} = \\ = & \frac{ic}{2\pi}e^{i\frac{\xi^2}{2t}}\int_{-\infty}^{\infty}dk'\int_0^{\infty}\mathrm{d}\tau e^{i\frac{\tau^2}{2t}-i\gamma\tau}e^{-i\frac{t}{2}k'^2} = \\ = & \frac{ic}{2\pi}e^{i\frac{\xi^2}{2t}}\sqrt{\frac{2\pi}{it}}\int_0^{\infty}e^{i\frac{\tau^2}{2t}-i\gamma\tau}\mathrm{d}\tau, \end{aligned}$$

in virtue of the Gaussian integration

$$\int_{-\infty}^{\infty}e^{-i\frac{t}{2}k^2}\mathrm{d}k = \sqrt{\frac{2}{it}}\int_0^{i\infty}e^{-u}\frac{\mathrm{d}u}{\sqrt{u}} = \sqrt{\frac{2\pi}{it}}.$$

We now shift the integration variable and split the integral:

$$\begin{aligned} I = & \frac{ic}{2\pi}\sqrt{\frac{2\pi}{it}}e^{i\frac{\xi^2}{2t}}e^{-it\gamma^2/2}\int_{-\gamma t}^{\infty}e^{i\frac{\tau^2}{2t}}\mathrm{d}\tau = \\ = & \sqrt{\frac{ic^2}{2\pi t}}e^{i\frac{\xi^2}{2t}-i\frac{t}{2}\gamma^2}\Big(\int_0^{\infty}+\int_{-t\gamma}^{0}\Big)e^{i\frac{\tau^2}{2t}}\mathrm{d}\tau = \\ = & \frac{ic}{2}e^{i\frac{\xi^2}{2t}-i\frac{t}{2}\gamma^2} - \sqrt{\frac{ic^2}{2\pi t}}e^{i\frac{\xi^2}{2t}-i\frac{t}{2}\gamma^2}\int_0^{-t\gamma}e^{i\frac{\tau^2}{2t}}\mathrm{d}\tau. \end{aligned}$$

This reduces to

$$\begin{aligned} I = & \frac{ic}{2}e^{i\frac{c^2t}{2}+c\xi}\Big(1-\sqrt{\frac{2}{\pi ti}}\int_0^{-t\gamma}e^{i\frac{\tau^2}{2t}}\mathrm{d}\tau\Big) = \\ & = \frac{ic}{2}e^{i\frac{c^2}{2}t+c\xi}\ \Big\{1-\mathrm{erf}\Big[\sqrt{\frac{i}{2t}}(ct-i\xi)\Big]\Big\}, \end{aligned}$$

with obvious definition of complex *error-function*

$$\mathrm{erf}(z) \equiv 1 - \mathrm{erfc}(z) \equiv \frac{2}{\sqrt{\pi}} \int_0^z e^{-s^2} \mathrm{d}s.$$

The Green's function of an electron in a delta-function potential then reads

$$G^r(x', t'|x, t) = \frac{-i}{\sqrt{2\pi i(t'-t)}} e^{i\frac{(x'-x)^2}{2(t'-t)}}\ \theta(t'-t) + \\ + \ \frac{ic}{2} e^{i\frac{c^2}{2}(t'-t)+c\xi}\ \mathrm{erfc}\sqrt{\frac{i}{2t'-2t}}(ct'-ct-i\xi) \times \theta(t'-t) \quad \text{(A.1)}$$

where the first term is the Green's function of a free electron.

Appendix B

Response function of a homogeneous electron gas

We denote the density response function of a homogeneous gas by

$$\chi_0(x,t|x',0) = \chi_0(x-x',t)$$

in view of the space-time symmetry.
The Hamiltonian $\mathcal{H}_0$ must not contain any potentials for we deal with a homogeneous electron system. Thus we can use the Green's functions Eqs.2.11 and 2.12 derived in Chapter2 in the recipe for calculating the response function Eq.3.8.
Firstly we struggle with the integral

$$C(x',x,-t) = \frac{1}{i\pi}\int_0^{k_F} \mathfrak{Im}\left\{-ie^{ik|x-x'|}\right\} e^{i\frac{1}{2}k^2t}\ \mathrm{d}k$$

where $k_F = \sqrt{2E_F}$ after substituting $\omega = k^2/2$. Further

$$\begin{aligned}
C(x',x,-t) &= \frac{i}{\pi}\int_0^{k_F} \mathfrak{Re}\left\{e^{ik|x-x'|}\right\} e^{i\frac{1}{2}k^2t}\ \mathrm{d}k = \\
&= \frac{i}{2\pi}\int_{-k_F}^{k_F} e^{i(\frac{1}{2}k^2t+k|x-x'|)}\ \mathrm{d}k = \\
&= \frac{i}{2\pi}e^{-i\frac{r^2}{2t}}\int_{-k_F+r/t}^{k_F+r/t} e^{i\frac{1}{2}k'^2t}\ \mathrm{d}k' = \\
&= \frac{i}{2\pi}\sqrt{\frac{2i}{t}}\ e^{-i\frac{r^2}{2t}}\int_{(-k_F+r/t)\sqrt{-it/2}}^{(k_F+r/t)\sqrt{-it/2}} e^{-\tau^2}\mathrm{d}\tau = \\
&= \frac{i}{2}\sqrt{\frac{i}{2\pi t}}\ e^{-i\frac{r^2}{2t}}[\mathrm{erf}\sqrt{\frac{t}{2i}}(\frac{r}{t}-k_F) - \mathrm{erf}\sqrt{\frac{t}{2i}}(\frac{r}{t}+k_F)]
\end{aligned}$$

and $\quad r \equiv |x-x'|$.

On inserting the Green's function

$$G_0^r(r,t) = \frac{-i}{\sqrt{2\pi i t}} e^{i\frac{r^2}{2t}}\ \theta(t)$$

we encounter the result

$$\chi_0(r,t) = \frac{1}{2\pi t}\mathfrak{Im}\left\{\mathrm{erf}\sqrt{\frac{t}{2i}}(\frac{r}{t} - k_F) - \mathrm{erf}\sqrt{\frac{t}{2i}}(\frac{r}{t} + k_F)\right\}. \tag{B.1}$$

in terms of complex error-functions.

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