Bias and temperature dependence analysis of the tunneling current of normal metal-insulator-normal metal tunnel junctions

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Tunnel junctions are very important in the application of nanoelectronics. In spite of this, there does not exist a well established theory to explain several important facts of physics of tunnel junctions and the production of components involving them is mainly based on empirical rules.

In this thesis I will present a semiclassical model to explain the bias and temperature dependence of the tunneling current and conductance in normal metal–insulator–normal metal (NIN) tunnel junctions. The model explains quantitatively the observed temperature dependence of the tunneling conductance in the region between liquid helium temperature 4.2K and room temperature 295K.

The model was developed in parallel with experiments. We made measurements on a number of Al–AlO₉—Al tunnel junctions. The measured quantities were the Coulomb blockade at 4.2K, the zero bias conductance and conductance vs. bias at temperatures from 4.2K to 295K.

From our new model, a set of equations is derived and we obtain all required information to determine the fundamental junction parameters: the thickness and the height of the tunneling barrier and the dielectric constant of the insulating AlO₉ layer.
## Contents

1 Introduction  

2 Tunneling in normal metal – insulator – normal metal tunnel junctions  

2.1 Tunneling through a finite square barrier  

2.2 Wentzel–Kramers–Brillouin (WKB) approximation  

2.3 Tunneling in the formalism of the occupation number representation  

2.3.1 Formalism of the second quantization for fermions  

2.3.2 Time dependent perturbation theory and Fermi’s golden rule  

2.3.3 Transmission rates and the tunneling current  

2.4 Charging effects in NIN tunnel junctions  

2.5 The shape of the potential barrier on metal – insulator – metal tunnel junction  

2.6 Examples of the operational principles of recent applications  

2.6.1 Coulomb Blockade Thermometer (CBT)  

2.6.2 Normal state Single Electron Transistor (SET)  

3 Simmons’ model of tunneling current in NIN structures  

4 Bias and temperature dependence of the tunneling current  

4.1 Approximative image potential  

4.1.1 Barrier height  

4.2 Parabolic shape of the total barrier and the tunneling matrix element  

4.3 Tunneling current — the three dimensional model
4.4 Predictions from the model ........................................ 43

5 Experiments ......................................................... 45
  5.1 Fabrication of planar tunnel junctions ......................... 45
  5.2 Measurement setup ............................................. 47
  5.3 Experiments on Al–AlO_x–Al tunnel junctions ............... 50

6 Results and Conclusions .......................................... 51
  6.1 Temperature dependence of the tunneling conductance ...... 52
  6.2 Voltage dependence of the tunneling conductance .......... 53
  6.3 Absolute measurements of junction parameters ............. 57
  6.4 Conclusion .................................................... 61

Bibliography ......................................................... 63

Appendix .............................................................. 67
  A Next to the leading order calculation of $\delta x$ and barrier height 67
    A.1 Calculation of $\delta x$ ...................................... 67
    A.2 Barrier height $V_h$ ......................................... 68
  B Tunneling matrix element calculation for a parabolic barrier 70
  C Three dimensional tunneling current integral ............... 73
  D Tunneling conductance ....................................... 75
Chapter 1

Introduction

Miniaturization of electronics has reached such a level, that quantum mechanics begins to play an important role in these systems and the classical physics is not enough to explain new, interesting, effects in these systems nor to give a good description of the physics itself. For future applications it is very important to understand the underlying physics of metal nanostructures. In this master’s thesis we will concentrate to metal-insulator-metal tunneling nanostructures, which are widely used and studied for applications of nanoelectronics. In the future the role of these structures will be even more important. Metal-insulator-metal tunnel junctions can be used for the solid state realization of the quantum bit (SQUBIT, Superconducting Quantum BIT) [1, 2], Single electron transistors (SET) [3], SINIS coolers [4], Coulomb Blockade Thermometers (CBT) [5] and an emerging application as wide temperature range sensors [6], just to name few of these applications.

In this thesis we have studied the physics of the tunneling phenomena, i.e. electron transportation, in normal metal – insulator – normal metal (NIN) junctions theoretically and experimentally. Specially the temperature and bias voltage dependence of the tunneling current has been our main point of interest, because of their importance for applications.

In chapter 2 we will introduce the tunneling phenomena in NIN tunnel junctions. Here we use the formalism of the second quantization, i.e. the occupation number representation to derive the tunneling current. In this chapter we will also introduce
the operation principles of few applications based on NIN tunnel junctions.

In 1963 John G. Simmons presented a simple model for tunneling current in NIN junctions [7, 8]. This model is called Simmons’ model and it is introduced in chapter 3. Simmons’ model has been used as a standard reference for decades. We show criticism towards this model, because it seems to be unphysical at some points. We have done the corrections to the Simmons’ model and derived the three dimensional tunneling current equation for NIN junctions. This model is applicable for junctions, which contain similar metals at the both sides of the insulating barrier. This new model predicts the temperature and the bias voltage dependence of the tunneling current through the junction. Our model is described in the chapter 4. This chapter also contains the comparison in between the different models, we have calculated the current voltage characteristics in three different models.

Chapter 5 contains the experimental part of this thesis. Here we will describe the experimental setup to measure the tunneling current and the differential conductance as a function of the bias voltage. Also the fabrication methods of the tunnel junctions are introduced in chapter 5. We have done the experiments with tunnel junctions, that contain aluminum or niobium as an electrode and barrier is made of aluminum oxide AlO$_x$. Experiments are done in the temperature interval from room temperature, i.e. $\sim$ 300 K, down to liquid helium temperature, which is 4.2 K. These experiments show us the temperature and bias voltage dependence of the tunneling conductance.

In the last chapter we will conclude the results within the experiments and theoretical model. Here we also discuss ideas for the future research of the NIN nanostructures.
Chapter 2

Tunneling in normal metal – insulator – normal metal tunnel junctions

Tunneling is the one of the basic concepts in the quantum mechanics: by tunneling phenomena we can understand the alpha decay in heavy nuclei [9] as well as the current voltage characteristics in artificially made tunneling nanostructures. In this chapter we will first introduce the theoretical basis of electron tunneling and then describe the tunneling phenomena in normal metal – insulator – normal metal tunnel junctions.

Metal – insulator – metal tunnel junction contains two electrodes separated by a thin insulating layer. Insulator in between two metals forms a potential barrier. Classically electrons with energies less than the barrier height can not move from one electrode into another, but if the width of the barrier is small enough, i.e. if system we consider is microscopic, electrons can transport through the barrier due to the quantum mechanical tunneling phenomena. Here electrons have a certain probability to transport through the barrier, this probability can be calculated by solving the time independent Schrödinger equation for the system

\[ \hat{H}\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) , \]  

(2.1)
where $\hat{H}$ is the Hamiltonian of the system, $\Psi(r)$ is the wavefunction of the penetrating particle and $E$ is the energy eigenvalue. Schrödinger equation can be analytically solved for some rather simple barriers, the tunneling probabilities can be calculated from the wave functions. The tunneling or transmission probability is the ratio of the absolute square of the transmitted and incident waves, i.e. it is the ratio of the penetrated and incident flux.

Usually the transmission probability can be calculated within some approximation, for example by WKB\(^1\) approximation or by solving the Schrödinger equation (2.1) numerically. As an example we will solve the Schrödinger equation analytically for rectangular barrier in the next section and then concentrate on approximative methods.

### 2.1 Tunneling through a finite square barrier

For a rectangular barrier with a finite height $\phi_0$ and width $x_0$, see figure 2.1, the tunneling probability can be easily calculated by solving Schrödinger equation (2.1). In the case of square barrier the Hamiltonian of the system has the form

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \phi_0 .$$ (2.2)

In the figure 2.1 the system is divided into three regions. In the region $I$ the wave function is the superposition of the propagating wave and the reflected wave, therefore in region $I$

$$\psi_I = A e^{ikx} + B e^{-ikx}, x < -x_0/2 ,$$ (2.3)

where $A$ and $B$ are complex numbers and $k^2 = 2mE/\hbar^2$. This is a general solution of (2.1) for a free particle.

Region $II$ is classically forbidden region in the energies below the height of the barrier, i.e. when $E < \phi_0$. Here the solution of (2.1) is that wave function decays exponentially

$$\psi_{II} = C e^{\kappa x} + D e^{-\kappa x}, |x| < x_0/2 ,$$ (2.4)

\(^1\)See section 2.2
where $C$ and $D$ are complex numbers and $\kappa^2 = 2m(\phi_0 - E)/\hbar^2$.

In region $III$ the wave function is again free particle solution, i.e. plane wave propagating to $x$ direction\(^2\)

$$\psi_{III} = Fe^{ikx}, x > x_0/2,$$  \hspace{1cm} (2.5)

where $F$ is a complex number. The boundary conditions for Schrödinger equation (2.1) requires the continuity of both the wave function $\psi(x)$ and its derivative $\psi'$. From this condition the coefficients can be determined.

The tunneling (transmission) probability $|T|^2$ is obtained by a definition

$$|T|^2 = \frac{\text{penetrated flux}}{\text{incident flux}} = \frac{|F|^2}{|A|^2}. \hspace{1cm} (2.6)$$

The transmission probability for the rectangular barrier is [10]

$$|T|^2 = \left[1 + \left(\frac{\kappa^2 + \kappa^2}{2k\kappa}\right)^2 \sinh^2(\kappa x_0)\right]^{-1}. \hspace{1cm} (2.7)$$

If the height of the potential is large compared to the energy of penetrating particle, i.e. $\kappa x_0 \ll 1^3$, the tunneling probability in the previous equation can be written\(^2\)\(^3\)
approximately

\[ |T|^2 = \left( \frac{2k\kappa}{k^2 + \kappa^2} \right) e^{-2\kappa x_0}. \] (2.8)

Hence the transmission probability is exponentially depending on barrier thickness, i.e. small changes in the barrier thickness have large effect on the transmission probability.

### 2.2 Wentzel–Kramers–Brillouin (WKB) approximation

Wentzel–Kramers–Brillouin (WKB) approximation is commonly used for calculating the tunneling matrix elements or tunneling probabilities through a barrier, it can be easily applied only in one dimensional problems [11]. In the barrier penetration problems this means that, the tunneling phenomena happens strictly in one dimension.

The WKB approximation in general form is introduced in detailed way in references [11, 12, 10]. The WKB approximation is valid for a slowly varying potential, which means that the potential \( V(x) \) changes only slightly over the de Broglie wavelength of the penetrating particles [10]. The WKB criterion is [11]

\[ \frac{|m\hbar V'(x)|}{2m(E - V(x))^{3/2}} \ll 1, \] (2.9)

where \( V'(x) \) is the derivative of the potential in respect to \( x \), \( m \) is the mass of the particle and \( E \) its energy.\(^4\)

The WKB criterion can be also written in the terms of de Broglie wave length of the particle [10]

\[ \left| \frac{\lambda(x)}{2\pi p(x)} p'(x) \right| \ll 1, \] (2.10)

where \( \lambda(x) = \hbar/p(x) \) is the de Broglie wave length of the particle, \( p(x) \) its momentum and \( p'(x) = dp(x)/dx \) is the derivative of the momentum in respect to \( x \). This

\(^4\)In the classical turning points, where \( E = V(x) \), i.e. the velocity of the particle vanishes and changes the sign, the WKB criterion (2.9) breaks down. Therefore the WKB approximation is valid only far away from these points.
expression of course means that the relative change in the momentum of the particle has to be small compared to its de Broglie wavelength. In the other words, the potential has to change so slowly, that momentum is almost constant within many de Broglie wave lengths.

In the WKB approximation the tunneling probability can be written in the form [12]

\[ |T|^2 = \exp \left( -\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{8m(V(x) - E)} \right), \]  

(2.11)

where \( x_1 \) and \( x_2 \) are left and right boundaries of the barrier. The derivation of the tunneling probability within WKB approximation is rather long, but the result in the equation (2.11) can be also explained in more heuristic way: If we consider a smooth, slowly varying, barrier, which is divided into rectangular pieces, see figure 2.2. The transmission coefficients are independent for each piece. Therefore the transmission probability through the whole barrier can be written in an approximative form

\[ |T|^2 = \prod_i \exp \left( -\frac{1}{\hbar} \sqrt{8m(V(x) - E)} \Delta x_i \right) = \exp \left( -\frac{1}{\hbar} \sum_i \sqrt{8m(V(x) - E)} \Delta x_i \right). \]  

(2.12)

This results in the limit \( \Delta x_i \to 0 \) to

\[ |T|^2 = \exp \left( -\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{8m(V(x) - E)} \right), \]  

(2.13)

which is the WKB result.

The tunneling probability in the WKB approximation can be calculated analytically in some limited cases, i.e. when the integral can be calculated in equation (2.11). Probabilities can be calculated in the closed form quite easily for rather simple barriers: for example barriers with trapezoidal or parabolic shape.
Figure 2.2: The potential barrier, which is divided into rectangular pieces.

### 2.3 Tunneling in the formalism of the occupation number representation

#### 2.3.1 Formalism of the second quantization for fermions

In the formalism of the second quantization, i.e. occupational number representation, the many particle state of the \( N \) particle system is described by the state vector

\[
|n_1, n_2, \ldots, n_N\rangle \equiv |\{n_i\}\rangle , \tag{2.14}
\]

where \( n_i \) is the number of particles at the state \( i \), \( n_i \) is called occupation number of the state \( i \). Electrons, like other fermions, obey Pauli exclusion principle, therefore each of the states can contain only zero or one particle. Hence for electrons \( n_i \in \{0, 1\} \) for all \( i \in \{1, 2, \ldots, N\} \). State (2.14) is called as vacuum state if \( n_i = 0 \), \( \forall i \).

All possible states \( |\{n_i\}\rangle \) forms the Fock’s space, which is complete and orthonormal in respect to the occupation numbers.

Next we will introduce the fermionic creation and annihilation operators \( c_i^\dagger \) and

---

5Note that sometimes the vacuum state can also be determined as the ground state of the system and therefore it can be completely nontrivial state.
The fermionic anticommutation relations for creation and annihilation operators can be derived easily derived \[13\]. It appears, that these operators satisfy anticommutation relations

\[
\{c_i, c_j^\dagger\} = \delta_{ij} \\
\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0.
\]

Particle number of the given state is obtained by defining the particle number operator

\[
\hat{n}_i = c_i^\dagger c_i.
\]

This is a good definition, because the arbitrary state \(|\{n_i\}\rangle\) is the eigenstate of this operator with eigenvalue \(n_i\).

Within the definitions (2.15)–(2.18) of the creation and annihilation operator the general \(N\) particle state can be created from the vacuum state by relation

\[
|n_1, n_2, \ldots, n_N\rangle = (c_N^\dagger)^{n_N} \ldots (c_2^\dagger)^{n_2} (c_1^\dagger)^{n_1} |0\rangle,
\]

where \(n_i \in \{0, 1\}, \forall \ i \in \{1, 2, \ldots, N\}\).

### 2.3.2 Time dependent perturbation theory and Fermi’s golden rule

Usually quantum mechanics is presented in Schrödinger’s representation, where time dependence of the system is included into states. For considering the transitions in between states it is more natural to use interaction representation\(^6\). In this

\(^6\)This is also called Dirac’s representation.
representation operators have the form

\[ H = H_0 + V , \]  

(2.22)

where \( H_0 \) is time–independent and \( V \) can depend on time. Time evolution operator in this representation can be written in the form

\[ U_I(t, t_0) = e^{iH_0 t / \hbar} U(t, t_0) e^{-iH_0 t_0 / \hbar} , \]  

(2.23)

where subscript \( I \) refers to 'interaction', \( H_0 \) is the time–independent Hamiltonian and \( U(t, t_0) \) is the time evolution operator in Schrödinger’s representation.

In Schrödinger’s representation the equation of motion is the time dependent Schrödinger’s equation. In the interaction representation the equation of motion has the form

\[ i \hbar \frac{dU_I(t, t_0)}{dt} = V_I(t) U_I(t, t_0) , \]  

(2.24)

The time evolution operator \( U_I(t, t_0) \) can be written in expanded form by solving the previous equation as an integral equation. This expansion is [12]

\[ U_I(t, t_0) = 1 + \sum_{n=1}^{\infty} \left( \frac{-i}{\hbar} \right)^n \int_{t_0}^{t} dt_1 V_I(t_1) \int_{t_0}^{t_1} dt_2 V_I(t_2) \ldots \int_{t_0}^{t_{n-1}} dt_n V_I(t_n) . \]  

(2.25)

In the time–dependent perturbation theory the Hamiltonian of the system is divided into two parts: time–dependent and time–independent. The transmission probability from an initial state \( |\phi_i\rangle \) into a final state \( |\phi_f\rangle \) is

\[ P_{fi} = |\langle \phi_f | \phi_i(t) \rangle|^2 = |\langle \phi_f | U_I(t, t_0) |\phi_i\rangle|^2 , \]  

(2.26)

by substituting the expansion of the time evolution operator from equation (2.25) into this, the transition probability in the lowest order is

\[ P_{fi} = \frac{1}{\hbar^2} \left| \int_{t_0}^{t} dt e^{i(E_f - E_i)(t-t_0)} \langle \phi_i | V(t) |\phi_f\rangle \right|^2 , \]  

(2.27)

where \( E_f \) and \( E_i \) are the energies of the final and the initial states. Now, in the case where perturbed Hamiltonian \( V \) is time independent, the transition rate, i.e. the time derivative of the transition probability, is

\[ w_{fi} \equiv \frac{dP_{fi}}{dt} = \frac{2\pi}{\hbar} |\langle \phi_f | V |\phi_i\rangle|^2 \delta(E_f - E_i) , \]  

(2.28)

\[ ^7 \text{This can be easily derived from the matrix element invariance in between the representations.} \]
which is also called Fermi’s golden rule.

### 2.3.3 Transmission rates and the tunneling current

Usually quantum mechanical transitions from one state into another can be calculated by using time dependent perturbation theory as a good approximation. In this subsection we introduce the transmission, i.e., tunneling, rates through the tunneling barrier by applying the formalism of the second quantization and the time-dependent perturbation theory.

The tunneling is the transmission of electrons from one electrode into another, therefore we have to construct a Master equation for tunneling, which contains the transmission probabilities from state \( k \) on electrode 1 to state \( q \) on electrode 2 and the occupation probabilities of these states.

For the system, which contains two electrodes and the potential barrier in between, the total Hamiltonian has the form [14]

\[
H = H_{\text{int}} + H_T ,
\]  

where \( H_{\text{int}} \) describes the internal energy of the electrodes and \( H_T \) is the tunneling Hamiltonian. Tunneling Hamiltonian can be written in terms of creation and annihilation operators in Fock space: In tunneling process one electron\(^8\) is annihilated from one electrode in state \( k \) and created into another electrode to state \( q \), and this happens with certain probability, which is obtained from the tunneling matrix elements \( T_{kq} \). Hence the tunneling part of the Hamiltonian has the form [14]

\[
H_T = \sum_{kq\sigma} [T_{kq} c_{\sigma}^\dagger c_{k\sigma} + T_{kq}^* c_{k\sigma}^\dagger c_{q\sigma}] .
\]  

\(^8\)Actually particles in the electrodes are quasiparticles: negative charge surrounded by positively charged cloud.

Next we will use the Fermi’s golden rule (2.28) to calculate the transmission rates. Here we consider the tunneling Hamiltonian (2.30) as a perturbed Hamiltonian, therefore we obtain for the transmission rate from the state \( q \) to the state \( k \) for the
voltage biased junction, see figure 2.3

\[ \Gamma_{qk} = \frac{2\pi}{\hbar} |\langle f | H_T | i \rangle|^2 \delta(\epsilon_f - \epsilon_i), \]  
\hspace{1cm} (2.31)

where \( i \) refers to initial state of the system and \( f \) final. The initial and final states are of the form

\[ |i\rangle = |n_{1}^{i}, n_{2}^{i}, \ldots, n_{k}^{i}, \ldots, n_{q}^{i}, \ldots\rangle \]
\[ |f\rangle = |n_{1}^{f}, n_{2}^{f}, \ldots, n_{k}^{f}, \ldots, n_{q}^{f}, \ldots\rangle, \]  
\hspace{1cm} (2.32)

where \( n_{j}^{i,f} \in \{0, 1\} \) for all \( j \). By using the properties of the fermion creation and annihilation operators, introduced in the previous section, and the orthonormality of the states \( f \) and \( i \), we obtain\(^9\) for the transmission rate from electrode 1 to 2, with positive bias voltage \( eV \),

\[ \Gamma_{1\rightarrow 2}(V) = \sum_{f,i} \frac{2\pi}{\hbar} |T_{kq}|^2 f(\epsilon_q)[1 - f(\epsilon_k)] \delta(\epsilon_q + eV - \epsilon_k) \]
\[ = \int \int \frac{2\pi}{\hbar} |T_{kq}|^2 \rho_1(\epsilon_q) \rho_2(\epsilon_k)f(\epsilon_q)[1 - f(\epsilon_k)] \delta(\epsilon_q + eV - \epsilon_k)d\epsilon_q d\epsilon_k \]  
\hspace{1cm} (2.33)

where \( \rho_{1,2} \) is the density of states on electrodes 1 and 2, \( f \) is the Fermi–Dirac distribution. In the last equation we have used the notation \( \epsilon \equiv \epsilon_q \). The transmission rate from electrode 2 to electrode 1 is calculated in the similar way and it results

\[ \Gamma_{2\rightarrow 1}(V) = \Gamma_{1\rightarrow 2}(-V) = \frac{2\pi}{\hbar} \int |T_{kq}|^2 \rho_1(\epsilon - eV) \rho_2(\epsilon)f(\epsilon - eV)[1 - f(\epsilon)]d\epsilon. \]  
\hspace{1cm} (2.34)

\(^9\)This is done explicitly for example in [13] or [14].
Therefore the total flux through the barrier is obtained from relation

\[ \Gamma = \Gamma_{1\rightarrow 2}(V) - \Gamma_{2\rightarrow 1}(V) \] (2.35)

and the total current is the total transmission rate multiplied by electron charge, i.e. \( I = e\Gamma \). Total tunneling current can be expressed in terms of the tunneling resistance \( R_T \) [14]

\[ I = \int \frac{1}{eR_T} [f(\epsilon) - f(\epsilon + eV)] d\epsilon , \] (2.36)

where tunneling resistance is defined by relation

\[ R_T^{-1} = \frac{2\pi e^2}{\hbar}\rho_1\rho_2|T(\epsilon)|^2 . \] (2.37)

Here the density of states on each electrode is assumed to be constant, i.e. \( \rho_{1,2} = \rho_{1,2}(E_F) \). This is a justified approximation, when considered energies are small compared to the Fermi energy of the metal\(^{10} \). From equations (2.36) and (2.37) we can see, that the properties of the oxide barrier are included in the tunneling resistance only, because this term contains the tunneling matrix element. Hence \( R_T \) contains a lot of information about the physics of the system itself.

In the chapter 4 we will concentrate on this term and study the properties of the barrier in more detailed way. Usually the tunneling resistance in (2.36) is assumed to be energy independent and therefore it is treated as a constant in respect to the integration over energy. This is valid assumption at low temperatures and with low bias voltages. But in chapter 4 we discuss about the temperature dependence of the tunneling current in the wide temperature range\(^{11} \) and therefore this simplification is not valid anymore.

If the approximation about the energy independence of the tunneling resistance \( R_T \) is made, the transmission rate from one electrode into another has the form at low bias voltage and at low temperature\(^{12} \)

\[ \Gamma_{1\rightarrow 2}(V) = \frac{1}{R_T e^2} \frac{eV}{1 - \exp \left( -eV/k_B T \right)} \] (2.38)

\(^{10}\)This criterion is usually fulfilled, because for example for aluminum \( E_F \approx 10 \text{ eV} \) [15], which corresponds temperature \( T \approx 10^5 \text{ K} \).

\(^{11}\)Wide temperature range here means from 4.2 K up to \( \sim 300 \text{ K} \).

\(^{12}\)This result is easily obtained by changing variables \( x = \exp[(\epsilon - E_F)/k_B T] \) in the integration over Fermi–Dirac distribution.
and therefore the current has an ohmic behaviour

\[ I(V) = e[\Gamma_{1\rightarrow 2}(V) - \Gamma_{1\rightarrow 2}(-V)] = \frac{V}{R_T} \]  

(2.39)

Ohmic behaviour of the tunneling current in the previous equation is the reason and justification for calling \( R_T \) a tunneling resistance.

### 2.4 Charging effects in NIN tunnel junctions

Because the tunnel junction contains two electrodes separated by an insulating film it has certain capacitance \( C \). The capacitance depends on the properties of the insulating layer, like thickness, dielectric constant and the area of the junction. If the parallel plate geometry of the tunnel junction, i.e. tunnel junction is planar, is assumed, then the capacitance of the junction has the form

\[ C = \frac{\varepsilon \varepsilon_0 A}{x_0}, \]  

(2.40)

where \( \varepsilon \) is the dielectric constant of insulator, \( \varepsilon_0 \) vacuum permittivity, \( A \) is the area of the junction and \( x_0 \) is the thickness of the insulating layer.

Let us next consider a system, which consists two normal metal tunnel junctions. In between the junctions is a normal metal island, which is isolated from the rest of the circuit. Therefore the island has a certain charging energy \( E_C \), which has the form

\[ E_C = \frac{e^2}{2C^*}, \]  

(2.41)

where \( C^* \) is the total capacitance of the junctions, for identical junctions \( C^* = 2C \) if the ground capacitance of the island is assumed to be zero.

Electrons tunneling through the junction to the island have to exceed this energy, because of the Coulomb repulsion in between the electrons. Electrons with smaller energy than the charging energy \( E_C \) are blocked from the island, this phenomenon is called Coulomb blockade, it was first studied by Averin and Likharev [16]. This means, that for a typical tunnel junction at low temperatures or at low bias voltage regime there is no current flowing through the barrier, see figure 2.4. The Coulomb
blockade phenomena can be understood easily by the energy level diagram presented in the figure 2.5.

![Energy Level Diagram](image)

Figure 2.4: Sketch of a current voltage characteristics through the double junction system at zero temperature. Here if electron energy $e|V| < E_c$ electrons are blocked by the charging energy of the island.

In the figure 2.4 is shown the ideal Coulomb blockade at zero temperature, at nonzero temperatures the edges of this gap are rounded due to thermal excitation of electrons on electrodes. The Coulomb gap can be seen as a dip in the voltage dependence of the tunneling conductance$^{13}$, measured Coulomb blockade at 4.2 K is shown in the figure 2.6.

At finite temperature, where $k_B T \approx E_C$, the full width at half minimum (FWHM) of the conductance dip is $[17, 18]$

$$V_{1/2} = \frac{5.44 N k_B T}{e},$$

and the height of the dip is

$$\frac{\Delta G}{G_T} = \frac{1}{6} \frac{2(N-1)}{N} \frac{E_C}{k_B T}.$$  \hspace{1cm} (2.43)

where $N$ is the number of junction in series, $G_T$ is the asymptotic value of the tunneling conductance at low bias voltages.

$^{13}$Tunneling conductance is the differential conductance $dI/dV$. 

15
Figure 2.5: In both figures $E_F$ is the fermi energy of the metal and temperature is zero. In the island free energy levels are marked with dotted lines and occupied ones with solid line. In figure (A) junctions are biased by a voltage $V > E_C/e$ and current is flowing through the island by tunneling through the barrier. In figure (B) bias voltage is zero and because of the zero temperature there is not enough energy to excite electrons from the electrodes to free states in the island, hence there is no current flowing through the system.

2.5 The shape of the potential barrier on metal – insulator – metal tunnel junction

The insulating layer in tunnel junction forms a potential barrier in between the electrodes. The basic shape of this barrier is assumed to be rectangular with height $\phi_0$ and thickness $x_0$.

The height of the barrier is the difference in between the Fermi level of the metal electrode and the conduction band of the insulator. Barrier height can be also called effective work function of the metal. Effective work function is lower than the work function of the metal in respect to the vacuum level, hence it requires less energy to excite electron from metal to the conduction band of an insulator than emit electron from metal to the vacuum. Thickness of the insulator determines the thickness of the barrier.

When bias voltage is applied across the junction, the Fermi levels of the metals are displaced by the amount of $eV$, see figure 2.3. For an initially rectangular barrier, the shape of the barrier is changed from rectangular to trapezoidal. Hence the total
Figure 2.6: Measured Coulomb blockade at 4.2 K, $G_T$ is a asymptotic value of the tunneling conductance at low bias voltages.

There is also a third contribution to the total potential, which comes from the tunneling electron. An electron which is approaching the metal surface polarizes the charge distribution in metal. Hence electron feels an attractive force. In tunnel junctions the tunneling electron in between electrodes polarizes the charge distribution in the both metal surfaces. As a result both of the electrodes has an influence to the potential barrier: the barrier thickness and height is reduced due to attractive interaction caused by image forces. Image forces, and therefore the image potential, can be calculated classically by applying image charge methods [19].

Calculating the image potential by image force methods we take the tunneling electron, with charge $-e$, to be positioned in between the electrodes, which are separated by the thickness of an insulating barrier $x_0$. Therefore the distance of the tunneling electron from one electrode is $x$ and from another is $x_0 - x$. Then we

$$V_{tot} = \phi_0 - \frac{eV}{x_0}x.$$  \hspace{1cm} (2.44)
calculate the Coulomb interaction with two image charges placed to distances $x$ and $x_0 - x$ in the metal, see figure 2.7. Then we calculate forces in between the image charges and the counter images, and so on. This method results to the infinite sum of the image charges, and therefore the total image potential is \[ V_i(x) = -K \left\{ \frac{1}{2x} + \sum_{n=1}^{\infty} \left[ \frac{n x_0}{(n x_0)^2 - x^2} - \frac{1}{n x_0} \right] \right\}, \] (2.45)

where $K := e^2/(8\pi\varepsilon\varepsilon_0)$, $\varepsilon$ is dielectric constant of an insulator, $\varepsilon_0$ permittivity of vacuum and $x_0$ the barrier thickness.

Figure 2.7: Image forces acting to the tunneling electron in between two metal electrodes.

Here one should note, that in the prefactor $K$ there is the factor $8\pi$ instead of $4\pi$, which is usual prefactor in Coulomb interaction potential. The reason for the difference of factor two comes from the image force itself: The magnitude of the Coulomb force in between two point charges has to be \[ F = \frac{e^2}{4\pi\varepsilon\varepsilon_0} \frac{1}{r^2}, \] (2.46)

where $r$ is the distance in between the charges, here $r^2 = (2x)^2$ for distance in between the electron and the image charge in the left hand side on the figure 2.7. Now if we use the factor $4\pi$ instead of $8\pi$ in the potential, this results to force \[ F = -\frac{dV_i}{dx} = \frac{e^2}{2\pi\varepsilon\varepsilon_0} \frac{1}{(2x)^2}, \] (2.47)
which is a wrong result. Now by using factor $8\pi$ the image force comes out in a right way: the image potential is

$$V_i = \frac{e^2}{8\pi \varepsilon \varepsilon_0} \frac{1}{2x}$$

(2.48)

and the corresponding image force is therefore

$$F = -\frac{dV_i}{dx} = \frac{e^2}{4\pi \varepsilon \varepsilon_0} \frac{1}{(2x)^2}.$$  

(2.49)

The shape of the total potential barrier is sum of three components: the rectangular part, the bias part and the image charge contribution. Therefore the total potential barrier in between the electrodes is

$$V_{tot} = \phi_0 - \frac{eV}{x_0} x - K \left\{ \frac{1}{2x} + \sum_{n=1}^{\infty} \left[ \frac{n x_0}{(n x_0)^2 - x^2} - \frac{1}{n x_0} \right] \right\}.$$  

(2.50)

Sketch of the total potential with image forces is represented in the figure 2.8

![Figure 2.8: Total potential with image forces.](image)

Here we have calculated the image potential classically. The more precise way to determine the shape of the barrier is to do quantum mechanical calculations to solve the contribution of the image charge effects. These calculations can be done by applying the density function theory (DFT), which was developed by Kohn and Sham [21]. The problem here is reduced to solve the electron density and the
potential at the metal surface. The starting point in these calculations is to take the semi–infinite metal slab and calculate the electron density at the surface. The energy of the system, which contains the potential, is the functional of the electron density. Within the DFT the problem is to solve the set of second order differential equations, so called Kohn–Sham equations \[22, 23\]

\[-\frac{1}{2} \nabla^2 \psi_i(r) + v_{\text{eff}}(r) \psi_i(r) = \epsilon_i \psi_i(r), \quad (2.51)\]

where \(\psi_i\) is the single particle wave function and \(v_{\text{eff}}\) is the effective potential, which contains the external potential and the exchange and correlation energies, i.e. all effects due to many–particle quantum mechanics are taken into account. The electron density is obtained from wave function by relation

\[n(r) = \sum_i |\psi_i|^2, \quad (2.52)\]

and the electrostatic potential can be calculated from the density by solving Poisson’s equation \[19\]

\[\nabla^2 \phi(r) = -\frac{en(r)}{\epsilon \epsilon_0}. \quad (2.53)\]

The equations (2.51) can be solved self–consistently.

The total potential is calculated for the interface in between vacuum and metal in references \[24, 25\]. In these calculations it is convenient to use the jellium model. In this model the exact crystal structure of the metal is neglected and atoms in the lattice are considered as uniform positive background charge — background ions form a rigid positively charged jelly, where electrons are moving.

Electron density at the metal surface is not a sharp step function, but electrons spill out from the surface creating an electrostatic dipole layer \[22\]. Therefore there is no sharp edge on the electron density nor the potential at surface. We have calculated the electron density and potential within DFT for aluminum–vacuum interface, results are shown in figures 2.9 and 2.10. Here one can see, that potential at the surface is a smooth function of a distance.

It is rather simple to calculate the total potential quantum mechanically at metal–vacuum interface, but it is more complicated at metal–insulator interface.
Figure 2.9: Electron density at aluminum surface. Oscillations at surface here are so called Friedel oscillations [15].

Because there one has to take into account the properties of an insulator, therefore this is not done in this thesis and all calculations for example in chapter 4 are done within the classical image potential.

2.6 Examples of the operational principles of recent applications

2.6.1 Coulomb Blockade Thermometer (CBT)

The Coulomb blockade phenomena can be used for a primary thermometry because of the universal relation (2.42) is not dependent on any other quantities than temperature. This kind of thermometer is called Coulomb blockade thermometer (CBT). The CBT is a commercial application of the nanoelectronics [26], SEM image of
a CBT is shown in figures 2.11 and 2.12. The CBT sensor contains a matrix of tunnel junctions, typically 20 junctions in series and 5 chains in parallel, sketch of a CBT is shown in the figure 2.13. The Coulomb blockade thermometer operates at temperatures $E_C \sim k_B T$, hence by adjusting the charging energy of a junctions temperature range can be selected.

The measured Coulomb blockade in the figure 2.6 is a conductance spectrum of a typical CBT matrix at low bias voltages\textsuperscript{14}. The Coulomb blockade thermometers have great advantages in comparison to other low temperature thermometers. In addition to the primary thermometry, the measured dip is independent of the magnetic field, CBT sensor has a small size and therefore quick response time, CBT sensor is also very accurate.

The measuring range of a CBT is from 0.02 K to 30 K. At higher temperatures

\textsuperscript{14}In the fig. 2.6 the coulomb blockade is plotted in the scale, where bias voltage is per junction. The FWHM is about 2mV per junction at 4.2K.
CHAPTER 2. TUNNELING IN NORMAL METAL – INSULATOR – NORMAL METAL TUNNEL JUNCTIONS

Figure 2.11: SEM image of a commercially available CBT tunnel junction matrix [27].

Figure 2.12: Zoomed image of single tunnel junction chain in the CBT matrix. Bright spots are individual tunnel junctions [27].

charging effects are reduced due to high temperature. For example the planar tunnel junction with barrier thickness 10 Å and dielectric constant of a barrier 4, the junction area should be $\sim (10 \times 10)\text{nm}^2$ to obtain a charging energy $E_C \approx k_B T$ at 300 K. Even if the size of the tunnel junctions would be small enough, i.e. charging energy is high, CBT cannot be directly used at room temperatures because the full width of a half minimum is wide and therefore the effects of a high bias voltage start to mix up with the Coulomb blockade: At high bias voltage there is no 'asymptotic' conductance $G_T$ anymore, but the conductance increases rapidly with voltage, see for example figure 2.14. At low temperatures there are two problems: Electrodes
have to be kept in normal state, because in superconducting state the superconducting gap [28, 29] mixes up with a Coulomb blockade. This is a technical problem, which is under development [30, 31, 32, 33]. At very low temperatures the CBT does not measure anymore the lattice temperature of a substrate, but measures the electron temperature instead.

Coulomb blockade thermometers can be also used as a wide range thermometers. For this purpose one measures the temperature dependence of the tunneling conductance instead of a Coulomb blockade [6, 34]. Temperature dependence of a tunneling conductance is discussed in chapter 4.

Figure 2.13: Sketch of the structure of the CBT sensor.
CHAPTER 2. TUNNELING IN NORMAL METAL – INSULATOR – NORMAL METAL TUNNEL JUNCTIONS

Figure 2.14: Measured spectrum of a CBT sensor at 4.2 K. At higher bias voltages there is no signal of an asymptotic value of a tunneling conductance, therefore at high temperatures even, if the charging energy would be high enough: Coulomb Blockade mixes up with high bias part because of its full width of a half minimum $V_{1/2} = 2.8 V$ at 300 K.

2.6.2 Normal state Single Electron Transistor (SET)

Normal state single electron transistor (SET) contains two normal state tunnel junctions in series, separated by an island in between. In addition to the normal system with two junctions in series, there is capacitive connection to the island, so called gate capacitor $C_g$, sketch of the SET is shown in the figure 2.15.

The charging energy of the island is now [13, 29, 35]

$$E_C = \frac{(ne + Q_G)^2}{2C_\Sigma} ,$$

(2.54)
where $C_{\Sigma} = 2C + C_G$, when additional ground capacitance is neglected and $Q_G$ is the charge of the gate capacitor and $ne$ is the number of excess electrons in the island.

The charging energy of the island can be varied by changing the gate voltage $V_g$, i.e. the electric field through the capacitive finger, because the charge of the capacitor is related to the gate voltage. Hence by gate modulation the conductivity of the tunnel junction at low bias voltages can be adjusted. The Coulomb blockade dip can be completely suppressed away with the additional gate voltage, hence by the gate voltage the tunneling of single electrons through the system can be adjusted. The more detailed operating principles of the SET are presented for example in references [3, 13, 14, 36, 35].

![Figure 2.15: Sketch of the SET. Here $C$ is the capacitance of the tunnel junction, $V_g$ the gate voltage and $C_g$ the gate capacitance.](image)

Figure 2.15: Sketch of the SET. Here $C$ is the capacitance of the tunnel junction, $V_g$ the gate voltage and $C_g$ the gate capacitance.
Chapter 3

Simmons’ model of tunneling current in NIN structures

In 1963 John G. Simmons introduced a model for tunneling in NIN structures, where the image charge effects were taken into account [7, 8]. Simmons’ model has been used as a standard in the analysis of the tunneling spectra — i.e. investigation of the current voltage characteristics of the tunneling current or conductance — for last four decades [37, 38, 39]. Simmons’ model is semi-classical, which means that the shape of the potential barrier, i.e. image forces, has been calculated classically and after that quantum mechanics is applied into this barrier.

In this model the image potential (2.45) has been approximated with expression [7]

\[ V_i(x) = -1.15\lambda \frac{x_0^2}{x(x_0 - x)}, \]  

(3.1)

where parameter \( \lambda \) is

\[ \lambda = \frac{e^2 \ln(2)}{8\pi\varepsilon_0 x_0}. \]  

(3.2)

Therefore the total potential in the Simmons’ approximation is

\[ V_{tot}(x) = \phi_0 - eV \frac{x}{x_0} - 1.15\lambda \frac{x_0^2}{x(x_0 - x)}. \]  

(3.3)

In this model the tunneling current for the voltage biased junction is [7]

\[ I(V, T) = \frac{meA}{2\pi^2\hbar^3} \int_0^{E_m} D(E_x, eV) \int_0^\infty [f(E) - f(E + eV)] dE_x dE_x, \]  

(3.4)
where $A$ is the area of the junction, $D(E_x, eV)$ tunneling probability and $f(E)$ is the Fermi–Dirac distribution. Here the energy of the electrons is divided into two parts $E = E_x + E_r$ due to the velocity components $E_x$ pointing towards and $E_r$ parallel to the barrier. Equation (3.4) shows, that in this model electrons in electrodes are treated as three dimensional electron gas, but the tunneling takes place only in one direction: perpendicular in respect to the barrier. Hence the tunneling probability $D$ is only $E_x$ dependent and is calculated by WKB approximation

$$D(E_x, eV) = \exp \left( -\frac{\sqrt{8m}}{\hbar} \int_0^{x_0} \sqrt{V_{\text{tot}}(x) - E_x} \, dx \right).$$  (3.5)

At relatively low voltages the tunneling conductance can be written in the quadratic form [7]

$$G = \frac{dI}{dV} = G_0 \left( 1 + \frac{V^2}{V_0^2} \right).$$  (3.6)

where $G_0$ is the zero–bias conductance and $V_0 = [4\hbar^2/(e^2m)]\phi_0/s^2$.

Simmons’ model is widely used, because image charge effects to the tunneling are taken into account. There are several aspects in this model, which seems to have somewhat unphysical nature. The image forces approximation (3.1) leads to the divergence of the potential at both of the metal–insulator surfaces in the junction. As seen in the equation (3.1) potential diverges to the minus infinity at points $x = 0$ and $x = x_0$. The barrier at the surface should be continuous, as shown in the figure 2.10. Simmons has also used the WKB approximation for the approximative, divergent, barrier. It is sure, that the WKB criterion (2.9) is not satisfied in this case. Therefore WKB approximation should not be used for such a barrier. We have constructed a semi–classical model in the next chapter, which avoids the unphysical divergence of the barrier.
Chapter 4

Bias and temperature dependence of the tunneling current

In this chapter we will construct a model for the bias voltage and temperature dependence of the tunneling current. In this model we have made higher order corrections to the approximative potential in Simmons’ model, which was presented in chapter 3. Our construction also avoids the unphysical divergence of the barrier on the metal surface. First we introduce the potential with image forces included and calculate the properties of the tunneling barrier. Then we derive the tunneling current from tunneling matrix elements and Fermi-Dirac statistics.

4.1 Approximative image potential

The classical image potential of two planar conductors with insulator in between has the explicit form (see section 2.5 in chapter 2)

\[ V_i = -K \left\{ \frac{1}{2x} + \sum_{n=1}^{\infty} \left[ \frac{n x_0}{(n x_0)^2 - x^2} - \frac{1}{n x_0} \right] \right\} \]

(4.1)

\[ = -K \frac{x_0}{x(x_0 - x)} \left\{ \frac{x_0 - x}{2} + x(x_0 - x) \sum_{n=1}^{\infty} \left[ \frac{n x_0}{(n x_0)^2 - x^2} - \frac{1}{n x_0} \right] \right\} \]

(4.2)

where \( K := e^2/(8\pi\epsilon\epsilon_0) \), \( \epsilon \) is the dielectric constant of insulator, \( \epsilon_0 \) is the permittivity of the vacuum and \( x_0 \) is the barrier thickness.
We can approximate this potential with power series

\[ V_i = -K \frac{x_0}{x(x_0 - x)} f(x) , \quad (4.3) \]

where \( f(x) \) is a slowly varying (polynomial) function of \( x \) near by point \( x = x_0/2 \), i.e. peak value of the potential without bias voltage. This is a correction to the image potential in Simmons’ model (3.1). From numerical calculation of the analytic form (4.2) we obtain, that \( f(x) \) has the parabolic form

\[ f(x) = \alpha_0 + \alpha_1 \left( \frac{1}{2} - \frac{x}{x_0} \right)^2 + \alpha_2 \left( \frac{1}{2} - \frac{x}{x_0} \right)^4 + \ldots , \quad (4.4) \]

where \( \alpha_0, \alpha_1 \) and \( \alpha_2 \) are constants, that define the curvature of the function \( f(x) \). These constants can be extracted from the polynomial fit to the numerical calculation of equation (4.2). Results of numerical calculation and fit are shown in figure 4.1. Here fourth order polynomial seems to fit perfectly to numerical data with coefficients \( \alpha_0 \approx 0.3465, \alpha_1 \approx 0.7215 \) and \( \alpha_2 \approx -0.4274 \). From the figure we see, that Simmons’ approximation — constant value for \( f(x) \) — is off from the real value at the peak position \( x = x_0/2 \).

The total potential of the tunneling barrier is the superposition of the effective work function \( \phi_0 \), the bias voltage part and the image potential \( V_i \). Hence the total potential is

\[ V_{tot} = \phi_0 - \frac{eV}{x_0} x - K \frac{x_0}{x(x_0 - x)} f(x) , \quad (4.5) \]

where \( \phi_0 \) is the effective work function and \( V \) is the bias voltage.

Let us next find the peak value of the potential, for this we need to find the roots of the first derivative of the potential. The derivative of the potential (4.5) is

\[ \frac{dV_{tot}}{dx} = -\frac{eV}{x_0} - Kx_0 \left[ \frac{f'(x)}{x(x_0 - x)} - \frac{f(x)}{x^2(x_0 - x)} + \frac{f(x)}{x(x_0 - x)^2} \right] . \quad (4.6) \]

Substituting \( f(x) \) as fourth order polynomial into this equation and solving the roots is very difficult, therefore we are going to do the next to the leading order calculation, i.e. in this case we take \( f(x) \) as second order polynomial — this is the parabolic approximation to the image potential: \( f(x) = \alpha_0 + \alpha_1 (1/2 - x/x_0)^2 \). We
Figure 4.1: The function $f(x)$ in equation (4.3) calculated numerically. (○) represents the explicit the numerical calculation of sum in equation (4.2), solid line is fourth order polynomial fit with parameters $\alpha_0 = 0.3465$, $\alpha_1 = 0.7215$ and $\alpha_2 = -0.4274$. Dotted line is a second order approximation of fourth order fit, i.e. $f(x)$ only with terms including $\alpha_0$ and $\alpha_1$. Dashed line is Simmons’ approximation (3.1).

will consider only small bias voltage\(^1\) — i.e. small perturbations to the peak value at zero bias — therefore we will set up the condition

$$\frac{dV_{tot}}{dx} \bigg|_{x=x_0+\delta x} = 0 \quad (4.7)$$

Here $\delta x$ is a small perturbation to the peak position at zero bias $x = x_0/2$. Substi-

\(^1\)Here small means that bias voltage is lot smaller than work function, i.e. $eV \ll \phi_0$. 

31
tuting the \( f(x) \) in second order into equation (4.6) we get\(^2\)
\[
\frac{dV_{\text{tot}}}{dx} \bigg|_{x=x_0/2+\delta x} = -eV \frac{x_0}{x_0} - \frac{4K(\alpha_1 + 4\alpha_0)}{x_0^2} \left( \frac{\delta x}{x_0/2} \right) = 0, \quad (4.8)
\]
resulting \( \delta x \) into form
\[
\delta x = -\frac{eV^2}{8K(\alpha_1 + 4\alpha_0)} - \frac{eV}{16.86K} \quad (4.9)
\]
\( \delta x \) represents the change of the peak position at low bias voltages. The maximum bias used in experiments is typically about 200 mV per junction, this changes peak position about 6.6% in the previous equation\(^3\).

The result (4.9) is applicable for calculating the barrier height \( V_h \) at point \( x = x_0/2 + \delta x \), i.e. \( V_h = V(x_0/2 + \delta x) \).

### 4.1.1 Barrier height

In the second order approximation in respect \( x \) of function \( f(x) \), the total potential barrier (4.5) takes the form
\[
V(x) = \phi_0 - \frac{eV}{x_0} \left( \frac{x_0}{2} + \frac{x}{x_0} - \frac{Kx_0}{x_0} \left[ \alpha_0 + \alpha_1 \left( \frac{1}{2} - \frac{x}{x_0} \right)^2 \right] \right). \quad (4.10)
\]
Let us next calculate the barrier height, i.e. \( V(x) \) at point \( x = x_0/2 + \delta x \), within the second order in \( \delta x \). Hence the barrier height is
\[
V_h = \phi_0 - \frac{eV}{x_0} \left( x_0/2 + \delta x \right) - \frac{Kx_0}{(x_0/2 + \delta x) - \frac{Kx_0}{x_0} \left[ \alpha_0 + \alpha_1 \left( \frac{\delta x}{x_0} \right)^2 \right]} \quad (4.11)
\]
Next we apply the Taylor expansion into term \( [(x/2)^2 + (\delta x)^2]^{-1} \) and take the expansion within the second order in respect to \( \delta x \). Then by substituting the \( \delta x \) from equation (4.9) into this form gives us finally the total barrier height\(^4\)
\[
V_h = \phi_0 - \frac{eV}{2} - \frac{\delta x}{x_0} eV - \frac{Kx_0}{(x_0/2)^2 - (\delta x)^2} \left[ \alpha_0 + \alpha_1 \left( \frac{\delta x}{x_0} \right)^2 \right]. \quad (4.12)
\]
\(^2\)Explicit calculation in the next to leading order in \( \delta x \) is presented in the appendix A.
\(^3\)i.e. \( \delta x/x_0 \approx 0.066 \) with (typical) parameters \( x_0 = 10A \) and \( \epsilon = 4 \).
\(^4\)The explicit calculation within the Taylor expansion is presented in the appendix A.
CHAPTER 4. BIAS AND TEMPERATURE DEPENDENCE OF THE TUNNELING CURRENT

4.2 Parabolic shape of the total barrier and the tunneling matrix element

To avoid the unphysical divergence — discussed in the chapter 3 within Simmons’ model — of the potential at metal insulator surface, we postulate the barrier to be a parabola, which starts at one metal electrode and ends on another, see figure 4.2. Parabola is the simplest form of a function, which has still a quasirealistic shape, and for which the tunneling probability and the tunneling current equations can be calculated analytically.

Here we are using scaled limits of the barrier, where the first Fermi level of the metal is located at the position $-x_0/2$ and second is — at zero bias — at position $x_0/2$. The advantage of this kind symmetric definition of the boundaries arises, when we calculate the tunneling probability within WKB approximation.

Now by applying the bias voltage across the junction the peak position is shifted from zero to the point $\delta x$. At non-zero bias voltages, the left hand side boundary of a barrier remains to be the same, but the Fermi level on the right hand side boundary is shifted by the amount of $eV$, like in figure 4.2.

Now we will construct a parabolic barrier, which is made of two separate parabolas. One with the curvature $a$ from the point $-x_0/2$ to $\delta x$ and another with curvature $a'$ from the point $\delta x$ to the $x_0/2$. The interface of these two parabolas, at the point $\delta x$, has to be continuous. This kind construction of the barrier takes into account the voltage dependence of the curvature and height of the barrier. We end up with a barrier, which has the form

$$V(x) = \begin{cases} V_1(x), x \in [-x_0/2, \delta x] \\ V_2(x), x \in (\delta x, x_0/2] \end{cases}$$

(4.13)

The barrier height was calculated with bias voltage in the previous section. Now tunneling electrons from one electrode into another see the barrier height $V_h$ relative to the Fermi level. This means that the effective height of the barrier for the tunneling electrons is $V_h$. Note that height is relative to the Fermi-level of the left
electrode, i.e. with positive bias voltages height barrier is lower and at negative bias voltages higher in respect to the left electrode.

Now let us construct a barrier containing two parabolas $V_1(x)$ and $V_2(x)$. We need two parabolas to construct a barrier with bias dependence. Parabola $V_1(x)$ has to satisfy the following conditions: barrier has to have its maximum value at the point $x = \delta x$, and zero value\(^5\) at positions $x = -x_0/2$, i.e.

\[
V_1(x = \delta x) = V_h
\]

\[
V_1(x = -\frac{x_0}{2}) = 0
\]

\[
\frac{dV_1(x)}{dx}igg|_{x=\delta x} = 0.
\]

The parabola, which satisfies these conditions is of the form

\[
V_1(x) = V_h - \frac{V_h}{\left(\frac{x_0}{2} + \delta x\right)^2} (x - \delta x)^2.
\]

The conditions for the second part of the barrier are almost the same

\[
V_2(x = \delta x) = V_h
\]

\[
V_2(x = \frac{x_0}{2}) = -eV
\]

\[
\frac{dV_2(x)}{dx}igg|_{x=\delta x} = 0,
\]

here the shift of the Fermi level, i.e. zero energy level, is taken into account. The parabola, which satisfies these conditions has the form

\[
V_2(x) = V_h - \frac{V_h + eV}{\left(\frac{x_0}{2} - \delta x\right)^2} (x - \delta x)^2.
\]

By combining the equations (4.17) and (4.21) we end up with the barrier

\[
V(x) = \begin{cases} 
V_h - \frac{V_h}{\left(\frac{x_0}{2} + \delta x\right)^2} (x - \delta x)^2, & x \in [-\frac{x_0}{2}, \delta x] \\
V_h - \frac{V_h + eV}{\left(\frac{x_0}{2} - \delta x\right)^2} (x - \delta x)^2, & x \in (\delta x, \frac{x_0}{2}] 
\end{cases}
\]

Here we can see, that the curvature of the barrier is dependent on the bias voltage. With positive bias the left side of the barrier has bigger curvature than the right

\(^5\)Here zero energy of course means the Fermi-energy on the metal surface, i.e. we have scaled the energy zero position to $E_F$. 

34
side. When the polarity of the bias is changed, the curvature goes in the opposite way, as one might expect. The curvature of the barrier is symmetric in the voltage, i.e. \( a(V) = a'(-V) \). We also can see, that the piecewisely constructed barrier is continuous everywhere, as it, for physical reasons, has to be.

At zero temperature and bias voltage all the states at metal surface are filled only up to the Fermi level \( E_F \) of a metal. At non-zero temperatures metal electrodes have excited electrons with certain energies above the Fermi energy \( E_F \), i.e. there are levels at energy \( E \) occupied above Fermi surface, see figure 4.2. Hence the effective width of the barrier — i.e. width which the tunneling electron see — depends on the energy of the occupied level. The barrier has the value \( E \) at the point \(-x'_0/2\) and \( x'_0/2\). Therefore we end up into conditions

\[
V_1(-x'_0/2) = E \\
V_2(x'_0/2) = E .
\]

Now by substituting these conditions into definitions of \( V_1(x) \) and \( V_2(x) \), we end up into equations two values of the \( x'_0 \), corresponding the intervals \( x \in [-x_0/2, \delta x] \) and \( x \in (\delta x, x_0/2] \),

\[
\frac{x'_0}{2} + \delta x = \sqrt{\frac{V_h - E}{V_h}} \left( \frac{x_0}{2} + \delta x \right), \quad x \in [-\frac{x_0}{2}, \delta x] \tag{4.24}
\]

\[
\frac{x'_0}{2} - \delta x = \sqrt{\frac{V_h - E}{V_h}} \left( \frac{x_0}{2} - \delta x \right), \quad x \in (\delta x, \frac{x_0}{2}] \tag{4.25}
\]

The absolute square of the tunneling matrix element, i.e. the transmission probability is calculated by applying the WKB approximation\(^6\). This approximation is valid for a smooth barrier, which varies slowly within the width of the barrier. The transmission probability through the barrier is then

\[
|M(E)|^2 = \exp \left\{ -\frac{2\sqrt{2m^*}}{\hbar} \int_{-x'_0/2}^{x'_0/2} [V(x) - E]^{1/2} dx \right\}
\]

\[
= \exp \left\{ -\frac{2\sqrt{2m^*}}{\hbar} \left[ \int_{-x'_0/2}^{\delta x} [V_1(x) - E]^{1/2} dx + \int_{\delta x}^{x'_0/2} [V_2(x) - E]^{1/2} dx \right] \right\} .
\]

\(^6\)WKB approximation is introduced in section 2.2
Here $m^*$ is the effective mass of the electron in the insulator. The transmission probability with the parabolic potential, constructed of two separate parabolas, is therefore\footnote{The explicit calculation is represented in the appendix B.}

$$|M(E)|^2 = \exp \left\{ -\frac{\pi \sqrt{2m^*}}{2\hbar} \left[ \frac{x_0 + \delta x}{\sqrt{V_h}} + \frac{x_0 - \delta x}{\sqrt{V_h + eV}} \right] (V_h - E) \right\}. \quad (4.27)$$

### 4.3 Tunneling current — the three dimensional model

In this section we will derive the fully three dimensional model of the tunneling current in NIN tunnel junctions. Here we assume that the electrodes are made of similar metals and tunneling dominates only near of the fermi level — this is a valid approximation when temperature is much lower than Fermi temperature and with
small bias voltages, hence the density of states (DOS) is constant in tunneling. From
the tunneling current equation we obtain the bias and the temperature dependence.

We treat electrons as free three-dimensional Fermi gas on the electrodes. Therefore
the energy distribution of the electrons at the temperature $T$ is given by the
Fermi–Dirac statistics \[ f(E) = \frac{1}{\exp[(E - E_F)/(k_B T)] + 1}, \]
where $E_F$ is the Fermi energy of the metal.

The total number of electrons per unit volume — i.e. the electron density — in
electrode is therefore given by \[ n = \frac{1}{8 \pi^3} \int_{\mathbb{R}^3} f(k) d^3k \]
\[ = \frac{2m^3}{h^3} \int_{\mathbb{R}^3} f(v) d^3v. \] (4.29)

Here first integration is over the whole $k$ space. We can transform this integration
over $k$ space over the velocity $v$ space, because $d^3k = h^{-3} d^3p = (m/h)^3 d^3v$. The
factor of two in the coefficient comes from the two-fold spin degeneracy of the
electrons.

At zero temperature the Fermi–Dirac distribution (4.28) is a step function
\[ f(v) = \begin{cases} 1, & |v| \leq v_F, \\ 0, & |v| > v_F, \end{cases} \] (4.30)
where $v_F = \sqrt{2E_F/m}$ is the Fermi velocity of the metal. This has the effect, that
the electron density in the equation (4.29) at zero temperature depends only on
Fermi velocity
\[ n(T = 0) = \frac{2m^3}{h^3} \int_{|v|=0}^{v_F} d^3v = \frac{8\pi m^3}{3h^3} v_F^3. \] (4.31)

Let us next assume, that the tunneling from electrode 1 to electrode 2 is strictly
a one dimensional event. Here we take the $x$ direction for the tunneling. Therefore
only the $x$ component of the velocity $v$ is responsible for tunneling. We divide
the velocity into two components: the perpendicular component $v_x$ and parallel component $v_r$ to the barrier. Here $v_r^2 = v_y^2 + v_z^2$.

In polar coordinates the electron density with velocity $v_x$ in the x direction is then

$$n(v_x) = 2m^3 \frac{2\pi}{h^3} \int_0^{2\pi} d\theta \int_0^\infty f(v)v_r dv_r$$

$$= \frac{4\pi m^3}{h^3} \int_0^\infty f(v)v_r dv_r.$$  \hspace{1cm} (4.32)

Here the coefficient $v_r$ in integrand comes from the Jacobian in the coordinate transform: $v_y = v_r \sin(\theta)$ and $v_z = v_r \cos(\theta)$. Hence the Jacobian is

$$J = \begin{vmatrix} \frac{\partial v_y}{\partial v_r} & \frac{\partial v_y}{\partial \theta} \\ \frac{\partial v_z}{\partial v_r} & \frac{\partial v_z}{\partial \theta} \end{vmatrix} = v_r.$$ \hspace{1cm} (4.33)

Expressing the velocity distribution as the energy distribution we change the variables $E_r = mv_r^2/2$ and $dE_r = mv_r dv_r$. Therefore the density of the electrons in the x direction is given by the relation

$$n(E_x) = \frac{4\pi m^2}{h^3} \int_0^\infty f(E)dE_r.$$ \hspace{1cm} (4.34)

The number of particles tunneling per area per second from the electrode 1 to the electrode 2 is then

$$\Gamma_{1\rightarrow 2} = \int_0^\infty v_x n(v_x)[1 - f(E + eV)]|M(E_x)_{1\rightarrow 2}|^2 dv_x$$

$$= \frac{1}{m} \int_0^\infty n(E_x)[1 - f(E + eV)]|M(E_x)_{1\rightarrow 2}|^2 dE_x$$

$$= \frac{4\pi m}{h^3} \int_0^\infty \int_0^\infty f(E)[1 - f(E + eV)]|M(E_x)_{1\rightarrow 2}|^2 dE_x dE_x.$$ \hspace{1cm} (4.35)

Here $v_x n(v_x)$ is the number of electrons in the differential velocity interval $dv_x$ and factor $[1 - f(E + eV)]$ corresponds the probability, that there is a free state for the tunneling electron on the other side of the barrier, i.e. on the electrode 2.
There are also electrons flowing from electrode 2 to electrode 1, therefore for biased junction, we get similar result

$$\Gamma_{2\rightarrow1} = \frac{4\pi m}{\hbar^3} \int_0^\infty \int_0^\infty f(E + eV)[1 - f(E)]|M(E_x)_{2\rightarrow1}|^2 dE_r dE_x. \quad (4.36)$$

We assume, that the tunneling matrix is symmetric, i.e. $|M(E_x)_{1\rightarrow2}|^2 = |M(E_x)_{2\rightarrow1}|^2 = |M(E_x)|^2$. Hence the total electron transmission per area is

$$\Gamma = \Gamma_{1\rightarrow2} - \Gamma_{2\rightarrow1} = \frac{4\pi m eA}{\hbar^3} \int_0^\infty \int_0^\infty [f(E) - f(E + eV)]|M(E_x)|^2 dE_r dE_x. \quad (4.37)$$

Consequently the tunneling current is

$$I = eA\Gamma = \frac{4\pi m eA}{\hbar^3} \int_0^\infty \int_0^\infty [f(E) - f(E + eV)]|M(E_x)|^2 dE_r dE_x. \quad (4.38)$$

Next we do the integration over $E_r$ in equation (4.38) to reduce the two dimensional integration into the one dimensional one

$$i := \int_0^\infty [f(E) - f(E + eV)]dE_r$$

$$= \int_0^\infty \left[ \frac{1}{1 + \exp[\beta(E_r + E_x - E_F)]} - \frac{1}{1 + \exp[\beta(E_r + E_x + eV - E_F)]} \right] dE_r \quad (4.39)$$

$$= \frac{1}{\beta} \int_0^\infty \left[ \frac{1}{1 + e^{(\beta E_r)e(-\beta E)}} - \frac{1}{1 + e^{(\beta E_r)e(\beta eV - \beta E)}} \right] d(\beta E_r),$$

where $E = E_F - E_x$ and $\beta = (k_B T)^{-1}$. This integral gives

$$i := \frac{1}{\beta} \log \left\{ \frac{1 + e^{\beta(E_F - E_x)}}{1 + e^{\beta(E_F - E_x) - eV}} \right\}. \quad (4.40)$$

Substituting this result into equation (4.38), the three dimensional tunneling current becomes

$$I(V, T) = \frac{4\pi eA k_B T}{\hbar^3} \int_0^\infty |M(E_x)|^2 \log \left\{ \frac{1 + e^{(E_F - E_x)/(k_B T)}}{1 + e^{(E_F - E_x - eV)/(k_B T)}} \right\} dE_x. \quad (4.41)$$

\textsuperscript{8}Explicit integration is done in the appendix C.
Next we substitute the transmission probability from equation (4.27) into equation (4.41), this results

$$I(V, T) = \frac{4\pi e A k_B T}{\hbar^3} e^{-B V h} \int_0^\infty e^{B(E_x - E_F)} \log \left\{ \frac{1 + e^{(E_F - E_x)/T}}{1 + e^{(E_F - E_x - eV)/T}} \right\} dE_x ,$$  \hspace{1cm} (4.42)

here we have denoted the inverse energy in tunneling matrix element by $B$, hence

$$B := \frac{\pi \sqrt{2m^*}}{2\hbar} \left[ \frac{2\delta x + \delta x}{\sqrt{V_h}} + \frac{2\delta x - \delta x}{\sqrt{V_h + eV}} \right]. \hspace{1cm} (4.43)$$

As discussed before in the derivation of the transmission probability the zero level of the energy was set to the Fermi level, hence the energy with Fermi energy is $E = E_x - E_F$.

Next we consider the integral in the equation (4.41), for simplicity we use units where $k_B = 1$

$$\int_0^\infty e^{B(E_x - E_F)} \log \left\{ \frac{1 + e^{(E_F - E_x)/T}}{1 + e^{(E_F - E_x - eV)/T}} \right\} dE_x. \hspace{1cm} (4.44)$$

Here it is justified to extend the lower limit of the integration to $-\infty$ because the logarithm term is finite in this case, i.e.

$$\lim_{E_x \to -\infty} \log \left\{ \frac{1 + e^{(E_F - E_x)/T}}{1 + e^{(E_F - E_x - eV)/T}} \right\} = \frac{eV}{T} \hspace{1cm} (4.45)$$

and the exponential term goes to zero in this limit. Hence the integral is

$$\int_{-\infty}^\infty e^{B(E_x - E_F)} \log [1 + e^{(E_F - E_x)/T}] dE_x - \int_{-\infty}^\infty e^{B(E_x - E_F)} \log [1 + e^{(E_F - E_x - eV)/T}] dE_x . \hspace{1cm} (4.46)$$

These two integrals can be calculated separately by partial integration, let us do this next to the first integral in previous equation. First we take

$$f' = e^{B(E_x - E_F)} \hspace{1cm} ; \hspace{1cm} f = \frac{1}{B} e^{B(E_x - E_F)} \hspace{1cm} (4.47)$$

$$g' = -\frac{1}{T} \frac{e^{(E_F - E_x)/T}}{1 + e^{(E_F - E_x)/T}} \hspace{1cm} ; \hspace{1cm} g = \log \left( 1 + e^{(E_F - E)/T} \right) \hspace{1cm} (4.48)$$
Therefore the first integral in the equation (4.46) is within the partial integration and previous notations

$$\int_{-\infty}^{\infty} f'(E_x) g(E_x) dE_x = \left[ f(E_x) g(E_x) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f(E_x) g'(E_x) dE_x .$$

Therefore we obtain within the partial integration

$$\int_{-\infty}^{\infty} e^{B(E_x-E_F)} \log \left[ 1 + e^{(E_F-E_x)/T} \right] dE_x$$

$$= \left[ \frac{1}{B} e^{B(E_x-E_F)} \log \left( 1 + e^{(E_F-E_x)/T} \right) \right]_{-\infty}^{\infty} + \frac{1}{BT} \int_{-\infty}^{\infty} \frac{e^{B(E_x-E_F)}}{1 + e^{(E_x-E_F)/T}} dE_x$$

$$= \frac{1}{BT} \int_{-\infty}^{\infty} \frac{e^{B(E_x-E_F)}}{1 + e^{(E_x-E_F)/T}} dE_x .$$

Here we have integrand over Fermi–Dirac distribution multiplied by a smooth function. Hence at low temperatures $T \ll T_F$ we can apply the Sommerfeld expansion\footnote{The Sommerfeld expansion is valid, when if multiplying function vanishes as $E \to -\infty$ and diverges no more rapidly than some power of $E$ when $E \to \infty$.} into this integral. Here Sommerfeld criterions are fulfilled, if $B < T^{-1}$, because exponential prefactor vanishes as $E \to -\infty$ and Fermi function vanishes more rapidly than exponential factor diverges in the limit $E \to \infty$.

Within the Sommerfeld expansion this results

$$\frac{1}{BT} \int_{-\infty}^{\infty} \frac{e^{B(E_x-E_F)}}{1 + e^{(E_x-E_F)/T}} = \frac{1}{B^{2T}} \left( 1 + \sum_{n=1}^{\infty} a_n T^{2n} B^{2n} \right) ,$$

where $a_n = (2 - 1/2^{(2n-1)}) \zeta(2n)$, $\zeta(2n)$ is the Riemann’s zeta function \cite{41}.

The previous procedure can be applied also to the second integral in equation (4.46). By doing this we obtain

$$\int_{-\infty}^{\infty} e^{B(E_x-E_F)} \log \left[ 1 + e^{(E_F-E_x-EV)/T} \right] dE_x = \frac{e^{-BEV}}{B^2T} \left( 1 + \sum_{n=1}^{\infty} a_n T^{2n} B^{2n} \right) .$$

Now by calculating the equations (4.51) and (4.52) in the second order ($n = 1$), as
is usual procedure, and substituting these into equation (4.44) we obtain

\[ \int_0^\infty e^{B(E_x - E_F)} \log \left\{ \frac{1 + e^{(E_F - E_x)/T}}{1 + e^{(E_F - E_x - eV)/T}} \right\} dE_x = \frac{1}{B^2T} (1 - e^{-BeV}) \left( 1 + \frac{\pi^2B^2}{6}T^2 \right). \] (4.53)

Hence the tunneling current in equation (4.42) is

\[ I(V, T) = \frac{4\pi meAk_BT}{\hbar^3} e^{-B_{Vh}} \left( 1 - e^{-BeV} \right) \left( 1 + \frac{\pi^2B^2}{6}T^2 \right). \] (4.54)

Now by substituting the barrier height \( V_h \) from equation (4.12) and the numerical values of \( \alpha_0 \) and \( \alpha_1 \) into this, we finally have the explicit tunneling current equation in the three dimensional model

\[ I(V, T) = \frac{8\pi meA}{B^2\hbar^3} \exp \left[ -B \left( \phi'_0 + \frac{1}{33.72} \frac{x_0}{K(eV)^2} \right) \right] \times \sinh \left( \frac{BeV}{2} \right) \left[ 1 + \left( \frac{T}{T_0} \right)^2 \right], \] (4.55)

where

\[ \phi'_0 = \phi_0 - 1.386 \frac{K}{x_0} \] (4.56)

is the effective work function, i.e. barrier height without bias voltage but image forces included, and

\[ T_0^2 = \frac{6}{(\pi k_B B_0)^2} \] (4.57)

is the material dependent temperature parameter,

\[ B(V) = \frac{\pi \sqrt{2m^*}}{2\hbar} \left[ \frac{x_0}{2} + \delta x \right] \left[ \frac{x_0}{2} + \frac{x_0}{2} - \delta x \right] \left[ \sqrt{\phi'_0} + \frac{eV}{2} + \frac{1}{33.72} \frac{x_0}{K(eV)^2} \right] \left[ \sqrt{\phi'_0} - \frac{eV}{2} + \frac{1}{33.72} \frac{x_0}{K(eV)^2} \right]^2 \] (4.58)

is the inverse energy parameter and \( B_0 = B(V = 0) \) is \( B \) at zero bias voltage, i.e.

\[ B_0 = \frac{\sqrt{2m^*}}{2\hbar} \frac{x_0}{\sqrt{\phi'_0}}. \] (4.59)
By taking the derivative of equation (4.55) we obtain the tunneling conductance:

\[ G(V, T) = \left\{ -\frac{2}{B} \frac{dB}{dV} - \frac{Be\phi_0}{16.86K} eV + \frac{dB}{dV} eV \left( \frac{1}{2\tanh \left( \frac{BeV}{2} \right)} + \frac{Be}{2} \tanh \left( \frac{BeV}{2} \right) \right) \right\} I(V, T), \]

(4.60)

this results into zero bias conductance

\[ G_0 := G(V = 0, T) = \frac{4\pi me^2 A}{\hbar^3 B_0} e^{-B_0\phi_0} \left[ 1 + \left( \frac{T}{T_0} \right)^2 \right]. \]

(4.61)

### 4.4 Predictions from the model

From the derived equations of the tunneling current (4.55) and conductance (4.60) we can predict the bias voltage dependence of the tunneling events. We can see from the tunneling current equation, that it is symmetric and odd function of the bias. The conductance is therefore even and symmetric function with respect to the bias voltage. The shape of the barrier determines, how strong is the voltage dependence of the tunneling current and conductance. The inverse energy parameter \( B \) contains the information about the shape of the barrier and is voltage dependent. \( B \) is also symmetric in respect to the sign of the applied bias.

Model predicts square dependence of the temperature for tunneling current and tunneling conductance, this can be seen from equations (4.55) and (4.61). By combining equations (4.57) and (4.59) one can see, that the temperature parameter \( T_0 \) is proportional to the square root of a 'effective' work function \( \phi_0 \) and inversely proportional to the barrier thickness. Therefore by lowering for example the work function of a barrier or by decreasing the barrier thickness we can decrease \( T_0 \). By decreasing \( T_0 \) the temperature dependence of a tunneling conductance becomes stronger. The temperature dependence of the tunneling conductance and current originates only from the Fermi–Dirac statistics, which electrons obey. The bias dependence of the tunneling is purely quantum effect and is dominated by the shape of the tunneling barrier.

This model also predicts, that from the temperature dependence and zero bias

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10Derivation is presented in the appendix D.
dependence junction parameters $x_0$ and $\phi'_0$ can be derived. Actually all junction parameters — height of the barrier $\phi_0$, barrier thickness $x_0$ and dielectric constant of insulator $\epsilon$ — can be determined from experiments. This can be done by measuring the Coulomb blockade dip of tunneling conductance in addition to $G_0$ and $T_0$ at known temperature. Because relation (2.43) gives the relation in between $\epsilon$ and $x_0$. Hence we have three unknown variables and three equations and therefore all three parameters can be solved.
Chapter 5

Experiments

5.1 Fabrication of planar tunnel junctions

Submicron sized tunnel junctions are fabricated by electron beam lithography and vacuum evaporation techniques. In lithography process electron beam is used instead of UV light to reach narrower linewidth: de Broglie wavelength of electrons is smaller than the wavelength of UV light. Tunnel junctions are usually made with double angle evaporation method. Double angle evaporation technique is presented in figure 5.1.

For two angle evaporation two layers of positive resist is spread on silicon oxide (SiO$_2$) substrate, thickness of these layers are usually few hundred nanometers. The resist is a polymer, which is sensitive to the electron beam. First layer consists of 9% P(MMA-MAA) copolymer and upper layer 3% PMMA resist. PMMA polymer resist is sensitive to electron beam; impacting electrons cut the polymer molecules in the resist layer. Resist layer has to be uniform and homogenous, therefore it is spread with spinner. The angular velocity of the sample in spinner determines the thickness of the layer. After spinning the resist layer has to be hardened, because all the solvent chemicals have to be evaporated away. Resist polymer is usually dissolved in the chlorobenzene. To harden the resist layer, it has to be baked.

After spreading the thin polymer layer the chip can be patterned by an electron beam lithography. This is done with SEM (Scanning Electron Microscope). De-
signed structure, which one wants to pattern, is first drawn with a CAD program. The resolution in patterning is usually determined by a current of electrons: larger patterning current makes larger line width.

Patterned regions on upper resist layer are etched away with a developer. For double angle evaporation there has to be a cavity under the top resist layer, this is obtained by exposing the chip to another developer, which etches copolymer. After etching the exposed areas away and creating the cavity, deposition of the metal is done with the vacuum evaporation technique.

Metal layers in nanostructures have to be pure and uniform, therefore metal is deposited in the UHV (Ultra High Vacuum) chamber, which is equipped with electron beam gun. Electron beam gun is used for heating up the metal in the crucible. In double angle technique of making tunnel junctions, the first layer is deposited on one angle. Then oxide layer is made by natural oxidation in situ and other layer is deposited with opposite angle compared to the first. The cross over of two metal layers in between the thin oxide layer forms a tunnel junction.
The thickness of the oxide layer reached with natural oxidation is about $8 - 20\text{Å}$. In natural oxidation there is an upper limit due to the saturation of the oxide layer. The aluminum layer can absorb only a limited amount of oxygen, i.e. oxygen atoms with aluminum form aluminum oxide layer only on the surface. After metal deposition the resist layers are lifted off with acetone.

### 5.2 Measurement setup

The measured quantities in experiments were the tunneling conductance and the tunneling current versus the bias voltage at different temperatures. The tunneling conductance, i.e. differential conductance, was measured by two methods: with technique based on lock-in amplifier and with a commercially available CBT electronics [26].

Measurement setup with lock-in amplifier is shown in figure 5.2. In lock-in based measurements the low frequency ($\sim 20$ Hz) AC excitation signal was summed up to DC bias voltage. $\pm4$ V DC bias was obtained from the sweep box, which had an adjustable sweep rate. The AC component was fed as a reference signal to the lock-in. The current through the sample was amplified with a current amplifier. The current was measured and fed to lock-in, which picked up the AC signal and took the ratio of AC components of current and the bias voltage. This differential conductance $dI/dV$ and the DC components of the current and bias voltage were recorded with a computer. The AC excitation voltages used were about $\sim (0.5 - 1)$ mV/junction. To obtain the narrower spectrum, signal to the sample was divided with a voltage divider. DC signal from AC was separated by a low pass filtering.

In addition to the lock-in technique, we performed experiments with commercially available CBT electronics: CBT Monitor 400 R [26]. With this setup we measured Coulomb Blockade, i.e. the voltage regime about $\pm15$ mV. CBT monitor setup is shown in figure 5.3.

The main difference in between lock-in and CBT monitor measurements is, that the CBT monitor injects current through the sample and measures the voltage drop,
i.e. sample is current biased. In lock-in measurements we used voltage bias instead. With lock-in technique one can measure higher voltage regime than with CBT electronics and therefore to measure bias voltage dependence of tunneling current or tunneling conductance the lock-in technique is preferred for our purpose. The Coulomb blockade can be measured in both setups, in lock-in setup one has to divide the bias voltage by a voltage divider to obtain about ±15mV voltage regime to separate Coulomb blockade from the rest of the spectrum. We mainly used CBT monitor instead of lock-in setup in Coulomb blockade measurements, because CBT electronics is optimized for that purpose.

We measured samples in the temperature range from liquid helium temperature 4.2K up to room temperature ~ 295K. Samples were attached to the sample holder on the dip stick and cooled down in the helium transport dewar. Temperature ranges between 4.2K and room temperature were obtained by positioning the dipstick between the level of liquid helium and the neck of the dewar. At cool down we approached helium level step by step: we lowered the dip stick few centimeters at the time and let the sample to get into thermal equilibrium with the environment.
The same procedure was repeated usually in warming up.

Temperatures were measured with Cernox resistor CX-1070-SD-4L [43], which was calibrated to the temperature range from 4.00K up to 325K. Sample and Cernox thermometer were glued with varnish to the sample holder. The sample stage itself was made out of copper to obtain a good thermal contact between the thermometer and the sample. Good thermal contact in these experiments is very important, because one has to be sure that measured temperature of sample and thermometer is the same. We even increased the thermal contact by putting extra copper strip from thermometer to the sample. Connection pads of the sample were attached to the pads of the sample holder by bonding them in ultra sonic bonder with narrow wire, diameter of the bonding wire is about 100μm. Schematic view of the sample holder is shown in the figure 5.4. Resistance of thermometer at each temperature was measured as a four probe measurement with AVS-47 resistance bridge[44].
We made experiments on a number of Al–AlO$_x$–Al tunnel junction matrices, containing 20 junctions in series and 5 in parallel. The junction area was measured with SEM (Scanning Electron Microscope), there were two types of samples according to the area. First type had junction area on average 0.088 $\mu$m$^2$ (350nm×250nm) and other type 0.17 $\mu$m$^2$. The oxide layer on the top of the aluminum was grown naturally in situ under pure oxygen pressure in the loading chamber of the UHV evaporator.

The measured quantities, with setups introduced in the previous section, were Coulomb blockade at 4.2K and the tunneling conductance and the current at different temperatures in the temperature range from 4.2K up to 295K. From these measurements we extracted the temperature dependence of the zero bias conductance, i.e. we resolved parameter $T_0$ for each sample. From measured coulomb blockade data the charging energy $E_C$ and the capacitance $C$ were calculated by assuming a parallel plate geometry of the tunnel junction.

Figure 5.4: Schematic view of a sample stage. Right hand side (A) represents side view and left hand side (B) top view of the sample holder.
Chapter 6

Results and Conclusions

In this chapter we will show results from the experiments, introduced in the previous chapter, and explain the main features of the junctions within our new model described in the chapter 4. We measured ten Al–AlO$_x$–Al tunnel junction samples, the main results are collected into the table 6.1. In the table Coulomb dip of the conductance and zero bias conductance for all samples are 4.2K values.

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<th>Sample</th>
<th>$\Delta G/G_T$ (%)</th>
<th>$T_0$ (K)</th>
<th>$G_0$ ($\mu$S)</th>
<th>$A$ ($\mu$m$^2$)</th>
<th>$\epsilon$</th>
<th>$x_0$ (Å)</th>
<th>$\phi_0$ (eV)</th>
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<td>14.6</td>
<td>1.11</td>
</tr>
<tr>
<td>06092002</td>
<td>2.12</td>
<td>746</td>
<td>31.2</td>
<td>0.17</td>
<td>3.19</td>
<td>14.5</td>
<td>1.13</td>
</tr>
<tr>
<td>20092002</td>
<td>1.92</td>
<td>710</td>
<td>32.2</td>
<td>0.17</td>
<td>3.60</td>
<td>14.8</td>
<td>1.05</td>
</tr>
</tbody>
</table>

Table 6.1: Statistics on measured samples. Coulomb blockade dip $\Delta G/G_T$ and the zero bias conductance per junction $G_0$ were measured at 4.2K.
6.1 Temperature dependence of the tunneling conductance

The measured temperature dependence of the zero bias conductance for ten samples is represented in the figure 6.1. Different symbols correspond to individual samples. All zero bias conductances are normalized with the zero bias conductance at 4.2K after substracting the Coulomb blockade dip away. Inset shows the temperature dependence of typical sample, showing how well experimental data fits to the predicted $T^2$ dependence. Temperature parameter $T_0$ for each of ten samples is shown in the table 6.1, resulting $T_0 = 753K$ on average. Figure 6.3 shows the tunneling conductance spectra of a typical sample on each temperature. From the table 6.1 we can see, that $T_0$ varies from 710K up to 780K. This variation is not surprising, because $T_0$ is not expected to be a constant of nature, but should depend on the sample parameters $\phi'_0$ and $x_0$. Figure 6.2 shows $T_0$ dependence of the tunneling conductance per area $g_0$. Similar temperature dependence of the tunneling conductance is also observed experimentally before [6], but there has not been a good solid explanation for such $T^2$ dependence.

In the derivation of the tunneling current equation (4.55), in the previous chapter, we applied the Sommerfeld expansion into the integral over Fermi function. Sommerfeld expansion is valid, if the inverse energy parameter $B$ is smaller than the inverse temperature $(k_BT)^{-1}$. This condition is now satisfied in the temperature range $(4.2 - 300)K$, which we used in the experiments. For average value of $T_0 = 753K$ we obtain $B_0 = 12(eV)^{-1}$ and inverse temperature varies from $37(eV)^{-1}$ up to $2763(eV)^{-1}$ in the temperature range we used. Hence the Sommerfeld criterions are fulfilled in our analysis.
Figure 6.1: Temperature dependence of the zero bias conductance of Al–AlO$_x$–Al tunnel junction matrices. Different symbols correspond to different samples, all conductances are normalized with 4.2K value, when Coulomb blockade was subtracted from original data. Inset shows an example of the temperature dependence of a typical sample.

### 6.2 Voltage dependence of the tunneling conductance

We calculated the tunneling current at the bias regime ±100mV, the tunneling conductance was calculated by taking a numerical derivative of the calculated current spectrum. Calculated and measured conductance curves are shown in the figure 6.4.

By comparing the shape of the calculated and measured curve, we see that the
shape of the conductance versus bias is pretty much the same. We have also observed the deviations from the parabolic shape of the conductance versus bias curves, like in the figure 6.5. So far, we cannot completely explain where this deviation in the shape arises. There probably have to be contributions in the tunneling conductance, that depend on the absolute value of the applied bias voltage.

Calculated curve in the figure 6.4 shows, that the calculated bias dependence is about six times stronger than measured one. This feature we cannot yet explain. To obtain the factor of six probably requires some fine tuning in our model. Part of this strong bias dependence can be because we have all the time assumed, that effective mass of electron in the insulator is equal to one free electron mass, i.e.
Some experiments have shown that effective mass can be $0.75m$ [38]. Smaller effective mass reduces the strength of the voltage dependence by reducing the parameter $B$. Band structure calculations have shown even smaller values of effective mass, down to $0.33m$ [45]. For a thin oxide layer it is very inconvenient to do such calculations; the oxide layer is probably amorphous, not crystallized and therefore it has no well determined band structure. The calculation of the tunneling conductance vs. bias voltage with two different effective masses, $m^* = m$ and $m^* = 0.33m$, is presented in the figure 6.6. Calculations show that with the smaller effective mass the bias dependence of the tunneling conductance is reduced.

In addition to the parabolic barrier, we calculated the conductance versus bias
Figure 6.4: Tunneling conductance versus bias voltage. Red line corresponds to the calculated from the model and black line is measured. Each spectrum is normalized with the maximum value of the conductance.

curves for two different types of a barrier: trapezoidal and Simmons’ barrier\(^1\). The trapezoidal barrier represents the case, where image charge effects are completely neglected, i.e. \( \epsilon \rightarrow \infty \). In the numerical calculation we used the same junction parameters for all barriers\(^2\). Results of the calculations are shown in the figure 6.7. From this figure one can see, that the more square barrier results into the smaller bias dependence.

\(^1\)See the eq. (3.1).

\(^2\)Ofcourse in the calculation of the trapezoidal barrier there was no dielectric constant, because image charge effects were neglected.
Figure 6.5: Example of the conductance spectrum, which deviates from the parabolic shape in respect to the bias voltage. Here conductance is normalized with the maximum value of the conductance.

6.3 Absolute measurements of junction parameters

We can see from the model, that it makes possible the absolute measurement of the junction parameters: all junction parameters can be determined just by measuring the tunneling spectra. Measured quantities, which are required to determine the fundamental junction parameters, are the zero bias conductance and the Coulomb blockade at a known temperature, the temperature dependence of the zero bias conductance and the area of the junction. Fundamental junction parameters, which
Figure 6.6: Calculated tunneling conductance vs. bias voltage with two different values of effective electron mass $m^*$. The solid line represents value $m^* = m$ and dashed line $m^* = 0.33m$, both tunneling conductances are normalized with the maximum value. It can be seen, that the smaller effective mass reduces the bias dependence of the tunneling conductance.

can be determined, are the barrier height $\phi_0$, the dielectric constant of the insulator $\epsilon$ and the barrier thickness $x_0$. From $T_0$ in equation (4.57) the inverse energy parameter at zero bias, $B_0$, can be determined. From equation (4.61) $\phi'_0$ can be determined by knowing the $T_0$. Hence from these two relations we get $x_0$ and $\phi'_0$. By knowing the junction area $A$ and barrier thickness $x_0$, the dielectric constant $\epsilon$ can be determined from equation (2.43) by assuming the parallel plate geometry of tunnel junction.

Hence we end up to the problem with four unknowns and four equations, (4.56),
Figure 6.7: Calculated conductance vs. bias voltage curves for three different barriers with the same junction parameters. The solid line represents parabolic barrier due to our model, dashed line is the trapezoidal barrier and dotted line Simmons’ approximative image potential, see eq. (3.1).

\[(4.59), (4.61) \text{ and } (2.43):\]

\[
\phi_0' = -\frac{1}{B_0} \ln \left\{ \frac{h^3 B_0}{4\pi m e A} \left[ 1 + \left( \frac{T}{T_0} \right)^2 \right]^{-1} G_0 \right\} \quad (6.1)
\]

\[
x_0 = \frac{2hB_0}{\pi \sqrt{2m^*}} \sqrt{\phi_0'} \quad (6.2)
\]

\[
\epsilon = \frac{N - 1}{6N} \frac{e^2}{\epsilon_0 A} \left( \frac{\Delta G}{G_T} \right)^{-1} \frac{x_0}{k_B T} \quad (6.3)
\]

\[
\phi_0 = \phi_0' + \frac{1.386 e^2}{8\pi \epsilon_0} \frac{1}{e\epsilon x_0} \quad (6.4)
\]

Here the $\phi_0'$ is obtained from the temperature dependence of the zero bias conduc-
tance, i.e. \(G_0(T)\), and absolute value of the zero bias conductance \(G_0\) at some known temperature. Parameters \(x_0\) is therefore calculated from \(\phi_0\) and temperature dependence. Dielectric constant \(\epsilon\) is obtained from the charging energy measurement, i.e. by measuring the Coulomb blockade, at known temperature. Work function \(\phi_0\) is then obtained from known variables \(\phi_0',\ \epsilon\) and \(x_0\).

Parameters we obtained from measured quantities are represented in the table 6.1. Here we can see, that the barrier height is rather constant, on average \(\phi_0 = 1.12\text{eV}\), varying from 1.0eV up to 1.2eV, hence the relative variation is about 17%. Thickness of the barrier is on average value \(x_0 = 14.1\text{Å}\) and dielectric constant \(\epsilon = 3\). Thickness of the barrier is also rather constant, varying from 13.8Å to 14.8Å, which corresponds to the relative variation about 7%. Dielectric constant seems to variate more that other junction parameters: from 2.17 up to 4.51, about 50%.

Small variations in the junction thickness can be explained by sample making procedure: oxide layer is made with the natural oxidation of the aluminum. In natural oxidation aluminum can absorb only certain amount of oxygen and this leads to the saturation of the oxide layer on aluminum surface. Probably thicker layers can be made by artificial deposition of oxide. Oxide layer made within this procedure of course leads to the less uniform layer, which can disturb the tunneling process itself.

Changes in dielectric constant can probably be due to formation of the oxide layer. Oxide layer is not probably completely crystallized, but is more like amorphous structure. Therefore its dielectric properties can differ from oxidation to oxidation. Differences in the work function are probably also due to the surface formation.

Junction parameters, calculated from experimental data, are consistent with recent measurements of the barrier height [38] and thickness[46, 47, 39]. The barrier height can be measured for example by BEEM (Ballistic Electron Emission Microscopy) [38] and barrier thickness by TEM (Transmission Electron Microscopy) [46].
6.4 Conclusion

We have developed a model, which avoids the unphysical divergence of the potential barrier on the metal–insulator surface. This model explains the temperature dependence of the tunneling conductance. There are still some problems, which have to be solved to understand completely the observed bias dependence of the tunneling conductance. The calculated tunneling conductance has stronger bias dependence than the measured one, and therefore some fine tuning into the model has to be done in the future.

We have also obtained a completely new method to measure the fundamental junction parameters — $\phi_0$, $\epsilon$ and $x_0$ — just by measuring the tunneling spectra. Three quantities — $T_0$, Coulomb dip and $G_0$ at a known temperature — have to be measured to determine these parameters.

For future, the results from the temperature dependence can be used for wide range thermometry with arrays of normal metal tunnel junctions. We predict, that by lowering the work function of an electrode material stronger temperature dependence, i.e. smaller $T_0$ can be obtained. This means that a more sensitive wide range thermometer is obtained with smaller $T_0$. Hence the future experiments should be extended to other materials like niobium, Nb, which has smaller work function than aluminum [48]. We have already started these experiments. Results with niobium have already shown some surprises.

In addition to the experiments, it would be very interesting to make a completely quantum mechanical model of tunnel junction structures with the density functional theory (DFT). In a quantum mechanical model the continuity of the potential at the metal–insulator surface does not have to be postulated, but it comes automatically due to the spill out of electrons, as discussed in section 2.5.

Results due to our model — for example explanation of the temperature dependence and absolute measurement of the junction parameters — are mainly new, even yet unpublished, and have scientific importance in understanding the physics beyond tunnel junctions. At the publication date of this thesis, an article about the
model and results was still under preparation.
Bibliography


Appendix A

Next to the leading order calculation of $\delta x$ and barrier height

A.1 Calculation of $\delta x$

At the position $x = x_0/2 + \delta x$ the barrier has its maximum value $V_h$, i.e.

$$\left. \frac{dV(x)}{dx} \right|_{x = x_0/2 + \delta x} = 0. \quad (A.1)$$

Expression for the derivative of the potential $V(x)$ is

$$\frac{dV}{dx} = -\frac{eV}{x_0} - Kx_0 \left[ \frac{f'(x)}{x(x_0 - x)} - \frac{f(x)}{x^2(x_0 - x)} + \frac{f(x)}{x(x_0 - x)^2} \right] \quad (A.2)$$

Now by we take $f(x)$ as a second order polynomial, hence

$$f \left( \frac{x_0}{2} + \delta x \right) = \alpha_0 + \frac{\alpha_1}{x_0^2} (\delta x)^2$$

$$f' \left( \frac{x_0}{2} + \delta x \right) = -\frac{2\alpha_1}{x_0} \left( \frac{1}{2} - \frac{x}{x_0} \right), \quad (A.3)$$

here $f'$ is the derivative of the $f(x)$ in respect to $x$.

Now by substituting results from the eq. (A.3) into eq. (A.2), we obtain

$$\left. \frac{dV(x)}{dx} \right|_{x = x_0/2 + \delta x} = -\frac{eV}{x_0} - Kx_0 \left[ \frac{2\alpha_1}{x_0^2} \frac{(\delta x)^2}{(\frac{x_0}{2} + \delta x)^2 (\frac{x_0}{2} - \delta x)^2} + \frac{\alpha_0}{x_0} \frac{\alpha_1}{x_0^2} \frac{(\delta x)^2}{(\frac{x_0}{2} + \delta x)^2 (\frac{x_0}{2} - \delta x)^2} \right]. \quad (A.4)$$
Let us now calculate all terms in the brackets in the next to the leading order, i.e.
we within expanding those in order of \( [\delta x/(x_0/2)]^2 \). These terms are in the next to
the leading order of \( x_0 = 2 \).

\[
\begin{align*}
2\alpha_1 & \frac{x_0^2}{(x_0^2 + \delta x)(x_0^2 - \delta x)} \frac{\delta x}{x_0^4} = 8\alpha_1 \frac{\delta x}{x_0^4} \left\{ 1 + \left( \frac{\delta x}{x_0/2} \right)^2 + \mathcal{O} \left[ \left( \frac{\delta x}{x_0/2} \right)^4 \right] \right\} \\
& = 4\alpha_0 \frac{\delta x}{x_0^3} \left\{ \left( \frac{\delta x}{x_0/2} \right) + \mathcal{O} \left[ \left( \frac{\delta x}{x_0/2} \right)^3 \right] \right\} \\
& = \frac{\alpha_0}{x_0^3} \left( \frac{\delta x}{x_0/2} \right) \left( \frac{1}{x_0^2} + 2 \left( \frac{\delta x}{x_0/2} \right)^2 + \mathcal{O} \left[ \left( \frac{\delta x}{x_0/2} \right)^3 \right] \right) \\
& = \frac{\alpha_0}{x_0^3} \left( \frac{\delta x}{x_0/2} \right)^2 + \mathcal{O} \left[ \left( \frac{\delta x}{x_0/2} \right)^3 \right] \\
\end{align*}
\]

(A.5)

Now by substituting these expansions into eq. (A.4) we obtain the relation in
the next to the leading order

\[
\left. \frac{dV(x)}{dx} \right|_{x=x_0/2+\delta x} = -\frac{eV}{x_0} - \frac{4K(\alpha_1 + 4\alpha_0)}{x_0^2} \left( \frac{\delta x}{x_0/2} \right),
\]

(A.10)

and by requiring this to be equal to zero, we obtain \( \delta x \)

\[
\delta x = -\frac{eV}{8K(\alpha_1 + 4\alpha_0)}.
\]

(A.11)

**A.2 Barrier height \( V_h \)**

Next we calculate the barrier height, i.e. value of the potential at the point \( x = x_0/2 + \delta x \). The barrier has the form

\[
V(x) = \phi_0 - \frac{eV}{x_0} - \frac{Kx_0}{x(x_0 - x)} \left[ \alpha_0 + \alpha_1 \left( \frac{x}{x_0} - x \right)^2 \right].
\]

(A.12)
Now by substituting the $x = x_0/2 + \delta x$ we obtain

$$V_h = V(x = x_0/2 + \delta x) = \phi_0 - \frac{eV}{2} - \frac{\delta x}{x_0}eV - \frac{Kx_0}{2} - (\frac{\delta x}{x_0})^2 \left[ \alpha_0 + \alpha_1 \left( \frac{\delta x}{x_0} \right)^2 \right].$$

(A.13)

Now by expanding this into second order with respect to the $\delta x/(x_0/2)$ we obtain

$$V_h = \phi_0 - \frac{eV}{2} - \frac{\delta x}{x_0}eV - \frac{4K}{x_0} \left\{ 1 + \left( \frac{\delta x}{x_0/2} \right)^2 + \mathcal{O} \left[ \left( \frac{\delta x}{x_0/2} \right)^4 \right] \right\} + \alpha_0 + \alpha_1 \left( \frac{\delta x}{x_0/2} \right)^2.$$

(A.14)

By substituting $\delta x$ from eq. (A.11) into this we obtain in the second order of $\delta x/(x_0/2)$

$$V_h = \phi_0 - \frac{eV}{2} - \frac{4K\alpha_0}{x_0} + \frac{x_0}{16K(\alpha_1 + 4\alpha_0)}(eV)^2.$$

(A.15)
Appendix B

Tunneling matrix element calculation for a parabolic barrier

The tunneling probability in the WKB approximation for the barrier, constructed of two parabolas, is

$$|M(E)|^2 = \exp \left\{ -\frac{2\sqrt{2m^*}}{\hbar} \left[ \int_{-x_0'}^{x_0'} [V_1(x) - E]^{1/2} dx + \int_{x_0'}^{x_0''} [V_2(x) - E]^{1/2} dx \right] \right\},$$

(B.1)

where potentials $V_1(x)$ and $V_2(x)$ are defined as

$$V_1(x) = V_h - \frac{V_h}{(\frac{x_0}{2} + \delta x)^2} (x - \delta x)^2$$

(B.2)

$$V_2(x) = V_h - \frac{V_h + eV}{(\frac{x_0}{2} - \delta x)^2} (x - \delta x)^2$$

(B.3)

and $x_0'$ has the form

$$\frac{x_0'}{2} + \delta x = \sqrt{\frac{V_h - E}{V_h}} (\frac{x_0}{2} + \delta x) , x \in [-x_0/2, \delta x]$$

(B.4)

$$\frac{x_0'}{2} - \delta x = \sqrt{\frac{V_h - E}{V_h + eV}} (\frac{x_0}{2} - \delta x) , x \in (\delta x, x_0/2]$$

(B.5)
Now let us calculate integrals separately in the equation (B.1). The left hand side integral is

\[ I_1 := \int_{-x_0'/2}^{x_0'/2} [V_1(x) - E]^{1/2} dx \]

\[ = \int_{-x_0'/2}^{x_0'/2} \left[ V_h - E - \frac{V_h}{(x_0 + \delta x)^2} (x - \delta x)^2 \right]^{1/2} dx \]

\[ = \sqrt{V_h - E} \int_{-x_0'/2}^{x_0'/2} \left[ 1 - \frac{V_h}{V_h - E} \left( \frac{x - \delta x}{x_0 + \delta x} \right)^2 \right]^{1/2} dx . \] \hspace{1cm} (B.6)

Now we see, that the coefficient of the term \( x - \delta x \) is actually the term in eq. (B.4) squared. Hence

\[ I_1 = \sqrt{V_h - E} \int_{-x_0'/2}^{x_0'/2} \left[ 1 - \left( \frac{x - \delta x}{x_0' + \delta x} \right)^2 \right]^{1/2} dx . \] \hspace{1cm} (B.7)

By changing the variable

\[ y := \frac{x - \delta x}{x_0' + \delta x} \] \hspace{1cm} (B.8)

we obtain

\[ I_1 = \sqrt{V_h - E} \left( \frac{x_0'}{2} + \delta x \right) \int_{-1}^{0} \left[ 1 - y^2 \right]^{1/2} dy \]

\[ = \frac{\pi}{4} \sqrt{V_h - E} \left( \frac{x_0'}{2} + \delta x \right) \] \hspace{1cm} (B.9)

\[ = \frac{\pi V_h - E}{4 \sqrt{V_h}} \left( \frac{x_0}{2} + \delta x \right) . \]

The other integral in the equation (B.1) can be calculated in completely similar way resulting

\[ I_2 := \int_{-x_0'/2}^{x_0'/2} [V_2(x) - E]^{1/2} dx \]

\[ = \int_{-x_0'/2}^{x_0'/2} \left[ V_h - E - \frac{V_h + eV}{(x_0 + \delta x)^2} (x - \delta x)^2 \right]^{1/2} dx \]

\[ = \frac{\pi V_h - E}{4 \sqrt{V_h + eV}} \left( \frac{x_0}{2} - \delta x \right) . \] \hspace{1cm} (B.10)
Therefore the total integral in the tunneling probability is

\[ I_1 + I_2 = \frac{\pi}{4} \left[ \frac{x_0 + \delta x}{\sqrt{V_h}} + \frac{x_0 - \delta x}{\sqrt{V_h + eV}} \right] (V_h - E) \]  \hspace{1cm} (B.11)

and the tunneling probability in the WKB

\[ |M(E)|^2 = \exp \left\{ \frac{\pi \sqrt{2m^*}}{2\hbar} \left[ \frac{x_0 + \delta x}{\sqrt{V_h}} + \frac{x_0 - \delta x}{\sqrt{V_h + eV}} \right] (V_h - E) \right\} \]  \hspace{1cm} (B.12)
Appendix C

Three dimensional tunneling current integral

Let us calculate the integral

\[
i = \frac{1}{\beta} \int_{0}^{\infty} \left[ \frac{1}{1 + e^{(\beta x)e(-\beta x)}} - \frac{1}{1 + e^{(\beta x)e(\beta x - \beta x)}} \right] d(\beta x)
\]  
(C.1)

this integral appears in the tunneling current equation, when we try to integrate over an extra dimension, i.e. in reducing two dimensional integral into one dimensional.

Here we change the variables and denote

\[
x := \beta x
\]
\[
C := e^{-\beta x}
\]
\[
D := e^{\beta(x V - E)}
\]

(C.2)

Let us next calculate the first part of the integral, i.e.

\[
\int_{0}^{\infty} \frac{dx}{1 + C e^{x}}
\]  
(C.3)

by changing the variables \( y := C e^{x} \) we end up into form

\[
\int_{0}^{\infty} \frac{dy}{y(1 + y)} = \left[ \log \left( \frac{y}{1 + y} \right) \right]_{C}^{\infty}
\]  
(C.4)

\[
= \left[ \log \left( \frac{C e^{x}}{1 + C e^{x}} \right) \right]_{0}^{\infty}.
\]
In the similar way other integral becomes into form
\[
\int_0^\infty \frac{dx}{1 + D e^x} = \left[ \log \left( \frac{D e^x}{1 + D e^x} \right) \right]_0^\infty.
\] (C.5)

Now by substituting back the changed variables \(x, C\) and \(D\) we obtain from eq. (C.1)
\[
i = \frac{1}{\beta} \left[ \log \left( \frac{e^x}{e^{\beta E} + e^x} + e^x \right) \right]_0^\infty = \frac{1}{\beta} \left[ \log \left( \frac{e^{\beta E} + e^x}{e^{\beta (E-eV)} + e^x} \right) \right]_0^\infty.
\] (C.6)

Now in the limit \(x \to \infty\) the logarithm term results
\[
\lim_{x \to \infty} \log \left( \frac{e^{\beta E} + e^x}{e^{\beta (E-eV)} + e^x} \right) = \log(1) = 0
\] (C.7)

and in the other limit \(x = 0\) we obtain
\[
\log \left( \frac{e^{\beta (E-eV)} + 1}{e^{\beta E} + 1} \right),
\] (C.8)

therefore the tunneling integral (C.1) results
\[
i = \frac{1}{\beta} \log \left\{ \frac{1 + e^{\beta E}}{1 + e^{\beta (E-eV)}} \right\} = \frac{1}{\beta} \log \left\{ \frac{1 + e^{\beta (E_F - E_x)}}{1 + e^{\beta (E_F - E_x - eV)}} \right\}.
\] (C.9)

Let us check, what happens at the low temperature limit, i.e. limit of \(T \to 0\), which is equal as limit \(\beta \to \infty\). We can divide this into three parts with respect to the energy \(E_x\):

\[
E_x < E_F - eV : i \sim eV \quad (C.10)
\]

\[
E_F - eV < E_x < E_F : i \sim E_F - E_x \quad (C.11)
\]

\[
E_x > E_F : i \sim 0.
\] (C.12)
Appendix D

Tunneling conductance

The tunneling current is of the form
\[
I(V,T) = \frac{8\pi meA}{B^2h^3} \exp\left[-B\left(\phi'_0 + \frac{x_0}{33.72K} (eV)^2\right)\right]
\times \sinh\left(\frac{BeV}{2}\right)\left[1 + \left(\frac{T}{T_0}\right)^2\right].
\]
(D.1)

Now the conductance is the derivative of the tunneling current in respect to the bias voltage
\[
G \equiv \frac{dI}{dV} = -\frac{2}{B} \frac{dB}{dV} I + \frac{dV}{dV} \left\{-B\left(\phi'_0 + \frac{x_0}{33.72K} (eV)^2\right)\right\} + I\left(\frac{dB eV}{dV} \frac{Be}{2} \cosh(BeV/2) \sinh(BeV/2)\right) \frac{1}{dV} \left\{-2 \frac{dB}{B} - \frac{Bex_0}{16.86K} eV + \frac{dB eV}{dV} \frac{1}{2 \tanh\left(\frac{BeV}{2}\right)} + \frac{Be}{2} \frac{1}{\tanh\left(\frac{BeV}{2}\right)}\right\} I(V,T).
\]
(D.2)

Now we see from the previous form and substituting \(I(V,T)\), that only term, which is non-zero at zero bias \(V = 0\) is \(\frac{Be}{2 \tanh\left(\frac{BeV}{2}\right)}\), and therefore zero bias conductance is
\[
G_0 := G(V = 0, T) = \frac{4\pi meA}{h^3B_0} e^{-B_0\phi'_0} \left[1 + \left(\frac{T}{T_0}\right)^2\right],
\]
(D.3)
where \(B_0 \equiv B(V = 0)\).