Effect of Friedel oscillations on Capacity of Tunnel Junction

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Abstract

Effect of long range charge density oscillations on capacity of tunnel structure is studied within random phase approximation (RPA). Using this approximation we obtain expressions for the short and the long distance behavior of the self-consistent screened potential. We demonstrate that long range density oscillations, commonly referred to as Friedel oscillations, lead to decreasing of total electrostatic capacity. Particular emphasis has been placed on influence of an external magnetic field is applied perpendicular to the barrier plane on the capacity of a structure. It is shown that increasing of magnetic field implies an increase of quantum correction to capacity due to Friedel oscillations.

1 Introduction

Response of tunneling structures on an external dc bias plays an important role in a number of tunneling phenomena, such as zero-bias anomaly and Coulomb blockade. Besides only the fundamental physical interest, it can have a pronounced effect on performances of electronic devices, based on semiconductor tunnel junctions.

It is well known that the presence of a potential barrier leads to the long-range oscillation of electron density, which are commonly referred to as the Friedel oscillations. In the contrast to the three-dimensional case where the electron density oscillations around an impurity decays as $\cos(2k_FR)$ (where $r$ is the distance from the impurity and $k_F$ is Fermi wave vector) in the case of metal surface this oscil-
lations decays only as $\frac{\sin(2k_F z)}{z^2}$, here $z$ is the distance from the surface [1]. In [2] was shown that in one 1D tunneling structure, charge density oscillations decay only as $\frac{\cos(2k_F z)}{z^2}$ and this induces a singularity in differential conductance. This singularity originates from the electron scattering on the Friedel oscillations. It is well-known that the motions of three-dimensions electrons in an external magnetic field are quasi one-dimensional and it is possible to expect that in a strong fields the long-range behaviour of electron density will be similar to those of one-dimensional systems.

In this paper we investigate effect of Friedel oscillations on capacity of barrier structure, it will be shown, that long-range electron density oscillations lead to decreasing of electrostatic capacity of the structure and this effect plays more important role with increasing external magnetic field, which is perpendicular to the barrier plane.

Formally, the goal is to find a self-consistent distribution of a total electrostatic potential $\Phi(r)$, since the knowledge of this potential is sufficient to calculate capacity of a structure. Self-consistent potential is calculated within RPA approximation, using this approach we obtained the short- and the long-distance behaviour of electrostatic potential.

2 General formulation

Here we briefly summarize the standard self-consistent analysis, which allows to write an expression for potential $\Phi(r)$ . In linear response theory the induced charge density is given by

$$\rho(r) = \int_{-\infty}^{\infty} dr' \Pi(r, r') \Phi(r')$$

(1)

here the polarization kernel $\Pi(r, r')$ is given by

$$\Pi(r, r') = \sum_{k, k'} \frac{f_{k'} - f_k}{E_{k'} - E_k + i0} \Psi_k^*(r') \Psi_{k'}(r') \Psi_{k'}^*(r) \Psi_k(r).$$

(2)

Hence $f_k$ is the Fermi distribution function (below we will assume that the temperature is zero), $\Psi_k$ is wave functions.

The potential $\Phi(r)$ is also related to the charge density by Poisson’s equation which can be written as

$$\Phi(r) = -4\pi \int G(r, r') \rho(r'),$$

here $G(r, r'')$ is a Green function of Laplas equation.

Combining (1) with (2) gives us an integral equation for electrostatic potential.
\[ \Phi(r) = \int dr' F(r, r') \Phi(r'), \]  

(3)

here

\[ F(r, r') = \int dr'' G(r, r'') \Pi(r'', r'). \]

as it was mentioned in introduction, the goal of the present work is to calculate the the self-consistent response of tunnel structure on external bias, because formally the knowledge of potential is sufficient to calculate capacity of a structure.

The model we use for a tunnel structure consists two semiconductor half-spaces \( z < -d/2 \) and \( z > d/2 \), separated by a potential barrier of width \( d \). A uniform compensating positive background extending through semiconductors, so electrostatic potential \( \Phi(r) \) doesn’t depend on lateral (x-y) coordinates. Below we will assume that:

(i) transparency of the barrier is zero, so electrostatic potential is a linear function inside a potential barrier.

(ii) \( \Phi(z) \) is an odd function in z direction.

This assumptions allow to transform the task to the problem of an electrical field \( E \) penetration at the surface of semiconductor [3], [4]. However in the difference from the case of surface of semiconductor, where \( E \) had a fixed value, in our case the electrical field depends on external dc bias \( V \) as well as induced electrostatic potential. The total electrical field \( E \) in the barrier structure can be written as a sum of two terms \( E(z) = E_{\text{ext}}(z) + E_{\text{ind}}(z) \), where \( E_{\text{ext}}(z) \) is discontinous function which is equal to a constant \( E_{\text{ext}} \) inside the barrier and zero in semiconductor leaders, \( E_{\text{ind}}(z) \) is the field induced by electron systems and it is discontinous function too. The fact, that a total electrical field should be continues function along the structure, bring us to the boundary condition for \( E_{\text{ind}} \) at \( (z = d/2 + 0) \)

\[ E \left( \frac{d}{2} \right) = \frac{2\Phi(d/2) + V}{d}. \]  

(4)

It was mentioned that self-consistent potential is calculated within RPA approximation, which is valid if \( r_s \ll 1 \). Where

\[ r_s = \left( \frac{9\pi}{4} \right)^{1/4} \frac{1}{k_F a_B}, \]

here \( a_B \) is Bohr radius In this study we ignore considerations of exchange and correlation interactions between electrons.

3 Self-consistent potential of tunnel structure

In this section, we present calculations of the self-consistent potential for a tunneling structure.
The case of zero magnetic field

In this case electrons are described by a normalized eigenfunction

\[ \Psi(r) = \frac{1}{2\pi} e^{i\mathbf{k}_|| \cdot \mathbf{r}_||} \psi_{k_z}(z), \]

where \( \mathbf{k}_|| \) and \( \mathbf{r}_|| \) are two-dimensional vectors laying in the x-y plane parallel to the barrier layers and \( z \)-dependent part of wave function is \( \psi_{k_z} = \frac{1}{\sqrt{2\pi}} \sin k_z z \). On substituting this wave functions in Eq.(3) we obtain

\[ \Phi(z) = \int_{d/2}^{\infty} dz' [\Lambda(z - z') + \Lambda(z + z' - d)] \Phi(z') dz' - \int_{d/2}^{\infty} K(z, z') \Phi(z') dz' \quad z > d/2 \]

\[ \Phi''(z) = 0 \quad |z| < d/2 \]

here

\[ \Lambda_q(z) = 4\pi e^2 \int_{-\infty}^{\infty} \frac{dk_||}{(2\pi)^2} \int_{0}^{\infty} \frac{dk}{(2\pi)^2} \left( \frac{e^{i(k-k')z} + \text{c.c.}}{(k-k')^2 + q^2} \right) \frac{f_{k',k||+q} - f_{k,k||}}{E_{k',k||+q} - E_{k,k||} + i0} \]

\[ K_q(z, z') = 4\pi e^2 \int_{-\infty}^{\infty} \frac{dk_||}{(2\pi)^2} \int_{0}^{\infty} \frac{dk}{(2\pi)^2} \left( \frac{f_{k',k||+q} - f_{k,k||}}{E_{k',k||+q} - E_k + i0} \right) \frac{e^{i(k-k')z} e^{-i(k-k')z'} + e^{i(k+k')z} e^{i(k-k')z'} + \text{c.c.}}{(k-k')^2 + q^2} \frac{e^{i(k+k')z} e^{i(k-k')z'} + e^{-i(k+k')z} e^{-i(k-k')z'} + \text{c.c.}}{(k+k')^2 + q^2}, \]

here \( q = (q_x, q_y, 0) \) is 2D wave vector in the plane of barrier. As far as \( \Phi \) doesn’t depend on lateral coordinates, we will consider the case \( q = 0 \).

Making Fourier transforming Eq.(5) with respect to the variable and some algebra we obtain

\[ \Phi(\zeta) = -\frac{1}{2\pi} \int_0^{\infty} d\eta \int_{-\infty}^{\infty} dq_z \frac{e^{iq_z \zeta}}{q_z^2 \epsilon(q_z)} K(q_z, \eta) \Phi(\eta) \quad \zeta > 0, \]

here \( \zeta = z - d/2, \eta = z' - d/2, \epsilon(q_z, 0) \) is the Lindhard dielectric function

\[ \epsilon(q_z, q) = 1 - \int_{-\infty}^{\infty} dz e^{-i q_z z} \Lambda_q(z), \]

\[ K_q(\zeta, q_z) = \int_{-\infty}^{\infty} d\eta e^{-i q_z \eta} \tilde{K}_q(\zeta, \eta). \]

Integral equation (7) can be considered as a generalization of well-known Shafra- nov’s equation [5] to the case of non-uniform electron gas.
After integrating over $k_\parallel$ and $k$, we obtain the following expression for the integral kernel

$$K(q_z, \eta) = -\frac{2k_{TF}^2 k_F}{|q_z|} \left\{ (1 - |q_z|^2) (Ci|2k_F\eta + q_z\eta| - Ci|2k_F\eta - q_z\eta|) + \frac{q_z}{2k_F^2 \eta} \sin 2k_F\eta \cos q_z\eta + \frac{\sin 2k_F\eta \sin q_z\eta}{2k_F^2 \eta^2} - \frac{\cos 2k_F\eta \sin q_z\eta}{k_F \eta}, \right.$$  \hspace{1cm} (8)

where $k_{TF}$ is Thomse-Fermi wave vector. In the long wavelength limit ($q_z \ll k_F$) RPA dielectric function and integral kernel $K$ can be simplified as

$$\epsilon(q_z) = 1 + \frac{k_{TF}^2}{q_z^2}$$

$$K(q_z, \eta) = -2k_{TF}^2 \frac{\sin(2k_F\eta)}{2k_F\eta} \cos q_z\eta.$$  

In this limit the integral over $q_z$ in (7) is done by closing the integration contour in the upper half plane and picking up the pole at $q_z = ik_{TF}$ and Eq.(7) can be transformed to

$$\Phi'' - k_{TF}^2 (1 - \frac{\sin(2k_F\zeta)}{2k_F\zeta})\Phi = 0$$  \hspace{1cm} (9)

with boundary conditions

$$\frac{d\Phi}{d\zeta} \bigg|_{\zeta=0} = E \quad \frac{d\Phi}{d\zeta} \bigg|_{\zeta=\infty} = 0$$  \hspace{1cm} (10)

In deriving of Eq.(9) we used the following expression

$$\frac{d^2}{dx^2} e^{-a|x|} = -2a\delta(x)e^{-a|x|} + a^2 e^{-a|x|}$$

Here we emphasize that under our assumption (i) electron density must be zero at interface semiconductor-potential barrier $\zeta = 0$ and as it easy to see that solution of Eq.(9) satisfies this condition. It describes the behaviour of the screened Coulomb potential if $\zeta \sim \lambda_{TF}$ and it exponentially decays at large distances $\zeta \gg \lambda_{TF}$.

Here we would like to repeat that Eq.(9) was obtained with account of pole in $\epsilon$, however apart from the pole, the dielectric function has branch point at $q_z = 2k_F$ and this singularity generates long-range oscillations in charge density (Friedel oscillations). At large distances $\zeta \gg \lambda_F$ this oscillations plays the dominant role in distribution of induced charge. Asymptotic solution of Eq.(7) can be presented as

$$\Phi(\zeta) \sim \frac{k_{TF} \sin 2k_F\zeta}{k_F (2k_F\zeta)^2}$$

Here we emphasize that under our assumption (i) electron density must be zero at interface semiconductor-potential barrier $\zeta = 0$ and as it easy to see that solution of Eq.(9) satisfies this condition. It describes the behaviour of the screened Coulomb potential if $\zeta \sim \lambda_{TF}$ and it exponentially decays at large distances $\zeta \gg \lambda_{TF}$.
Thus behaviour of electrostatic potential across the structure is

\[
\Phi(\zeta) = \begin{cases} 
\Phi(0)e^{-k_T \int_0^\zeta dx \sqrt{1 - \frac{\sin 2k_F x}{2k_F x}}} & \zeta < \zeta_c \\
\Phi(0) \frac{k_F \sin 2k_F \zeta}{k_F (2k_F \zeta)^2} + o(k_T/k_F) & \zeta > \zeta_c 
\end{cases}
\]  

(11)

According to [4] parameter \( \zeta_c \) can be estimated as

\[
z_c = \lambda_T \ln \left( \frac{k_F}{k_T} + \alpha \right),
\]

where \( \alpha > 1 \).

**The case of finite magnetic fields**

In this section we consider the response of barrier structure on external bias in the presence of magnetic fields perpendicular to the planes of the barrier. Under the Landau gauge with vector potential \( A = (-Hy, 0, 0) \) the wave functions and corresponding energy levels can be specified by the set of quantum numbers \((n, k_z)\) as

\[
\Psi_\alpha(r) = \frac{1}{2\pi} e^{ik_z x} \psi_{k_z}(z) \phi_n(y - y_0),
\]

\[
E_n(k_z) = \hbar \omega_c (n + 1/2) + \frac{(\hbar k_z)^2}{2m}.
\]

Here \( n \) is a number of Landau level, \( \omega_c = \frac{eH}{mc} \) is the cyclotron frequency and \( \phi_n(y) \) is the normalized harmonic-oscillator wave function with Landau state index.

As was mentioned above, applied magnetic field reduces the effective dimensionality of charge from 3D to 1D, in other words electron gas in semiconductor can be considered as a set of 1D gases and every one dimensional gas is specified by partial Fermi wave vector \( k_F^p \). In the case of sufficiently weak fields \( k_F^p l_H >> 1 \), the partial Fermi wave vector can be defined as

\[
k_F^p = k_F \sqrt{\left(1 - \frac{2}{(l_H k_F)^2}(n + 1/2)\right)}.
\]

Using together with the expression for polarization operator and we get an equation for self-consistent potential in external magnetic field.

\[
\Phi(\zeta) = -\frac{1}{2\pi} \int_0^\infty d\eta \int_{-\infty}^{\infty} dq_z e^{iq_z \zeta} K_H(q_z, \eta) \Phi(\eta),
\]

(12)

where \( \epsilon_H(q_z) \) is dielectric function in the presence of magnetic field.

\[
\epsilon_H(q_z) = 1 + \sum_n \frac{4}{a_0^2 q_z^3} \ln \left| \frac{2k_F^n + q_z}{2k_F^n - q_z} \right|,
\]

(13)
\[ K_H(q_z, \eta) = - \sum_n \frac{8}{a_B q_z l_H^2} (C_1 |2k_F^n \eta + q_z \eta| - C_1 |2k_F^n \eta - q_z \eta|). \]

In the long-wave limit \( q_z \ll k_F^n \) the expression for \( \epsilon_H \) can be transformed to

\[ \epsilon_H(q_z, 0) = 1 - \frac{\sum_n k_s^n}{q_z^2}, \quad (14) \]

here \( k_s^n = \frac{2}{\pi a_B l_H^2 k_F^n} \), \( k_s^2 = \sum_n k_s^n \) and summation is performed over all Landau levels where \( k_s^n \ll k_F^n \). It is evident that this condition isn’t valid for all levels, however using numerical modeling of (13) it is possible to demonstrate that in a case of weak-magnetic fields expression (14) is a quite good approximation of (13), even though the summation is performed over all occupied Landau levels. It is easily seen that in the zero-magnetic-field limit \( k_s \) transforms to well-known expression for Thomas-Fermi vector.

In a similar to the zero-field case, in the long-wave limit the integral equation (12) can be transformed to

\[ \Phi'' - (k_s^2 - \sum_n k_s^n \cos 2k_F^n \zeta) \Phi = 0. \quad (15) \]

This equation describes behaviour of electrostatic potential at \( \zeta \sim \lambda_s \), here \( \lambda_s \) is Thomas-Fermi length in magnetic field. It is possible to show (using Poisson summation formula) that in the limit of zero magnetic field Eq.(15) can be transformed to Eq.(9).

Similarly to the case \( H = 0 \), long-range behaviour of \( \Phi \) is conditioned by branch points in the dielectric function and at \( \zeta \gg \lambda_{TF} \) charge density oscillations have the following asymptotic

\[ \rho(\zeta) = \Phi(0) \sum_n k_s^n k_F^n \cos \frac{2k_F^n \zeta}{2k_F^n \zeta}. \quad (17) \]

Every term in this sum decays as \( 1/\zeta \) and it is typical for one-dimensional systems. The same behaviour was obtained in [6], however in that article authors used exponential parametrization of self-consistent potential, where unknown parameter determined while functional minimization process. In the case \( l_H k_F \gg 1 \), summation in (17) can be fulfilled using Poisson formula

\[ \rho(\zeta) \sim k_{TF} k_F \frac{\cos \frac{2k_F \zeta}{(2k_F \zeta)^2}}{(2k_F \zeta)^2} + \frac{\sqrt{2}}{k_s a_B \zeta l_H^2} \text{Re} \sum_{k=1}^{\infty} (-1)^k \frac{e^{i \pi (k_F l_H)^2}}{\sqrt{k}} e^{-i \zeta^2 / \pi k l_H^2}. \quad (18) \]

The first term in this expression corresponds to density oscillations without magnetic field and it is in an agreement with Eq.(11), the second term depends on
magnetic field.
In the magnetic quantum limit, when only the lowest Landau level is partially filled, we have

$$\varrho(\zeta) = \Phi(0)k_sk_F\frac{\cos(2k_F\zeta)}{2k_F\zeta} \quad (19)$$

here we need to mention that in quantum limit, $k_F$ can’t be calculated using expression presented above.

4 Electrostatic capacity of the barrier structure

It is well-known that the differential capacitance per unit area is $C = dQ/dV$ where

$$Q = \int_{d/2}^{\infty} dz \varrho(z)$$

is a total charge over semiconductor lead. Substituting distribution of self-consistent electron density $\varrho(z)$ into the definition for electrostatic capacity we will obtain an expression for $C$. In the case of zero magnetic fields it expressed as

$$C = \frac{1}{4\pi} \frac{1}{(d + 2\lambda_{TF} + 2\lambda_q)}, \quad (20)$$

where

$$\lambda_q = r_s \ln^{-1}\left(\frac{1}{\sqrt{r_s}}\right)\lambda_{TF}.$$

Accounting of Friedel oscillations in electron density produce a shift of charge center mass towards and away from the surface semiconductor-dielectric, what leads to decreasing capacity of the structure. We wish to separate the classical term in the total capacity, which depends on the barrier width and classical screening length from quantum one which depends on long-range oscillations of charge density

$$\frac{1}{C} = \frac{1}{C_g} + \frac{1}{C_s} + \frac{1}{C_q},$$

here $C_g$ is the geometrical capacity of the structure, $C_s = \frac{1}{8\pi \lambda_{TF}}$ is contribution to capacity due to Thomas-Fermi screening in semiconductor regions. The expression for $C_q$ coincides with result obtained within semiclassical approach [7], which was based on solution of Boltzmann equation for electron distribution function. $C_q = \frac{1}{8\pi \lambda_q}$ is quantum correction to tunnel capacity due to long-range behaviour of
charge density. As we mentioned in the introduction, in this study we assumed that $r_s \ll 1$, so quantum contribution is smaller than the classical one

$$\frac{C_s}{C_q} = \frac{r_s}{\ln \frac{k_F}{k_{TF}}} \ll 1. \quad (21)$$

In the case of finite magnetic fields Friedel oscillations decay slower than in the case $H = 0$ and this fact brings to increasing to penetration length of electric field in semiconductor lead. For this case the expression for capacity has the form

$$C_H = \frac{1}{4\pi} \frac{1}{d + 2\lambda_s + \sum \frac{n^2}{k_s^2} \lambda_F^n}. \quad (22)$$

Under the condition $k_F l_H \gg 1$ we have

$$C_H = \frac{1}{d + 2\lambda_{TF} + \lambda_q + 2\lambda_{TF} \sqrt{r_s} \sin \frac{\pi k}{(k_F l_H)^2}} \sum \frac{(-1)^k}{\pi k} \sin \pi k (k_F l_H)^2. \quad (23)$$

Thomas-Fermi screening length also depends on $H$, but in a weak magnetic fields it is approximately equal to $\lambda_{TF}$.

$$\frac{C_s}{C_q(H)} \sim \frac{\sqrt{r_s}}{(k_F l_H)^2} \quad (24)$$

As it is easy to see that $\frac{C_s}{C_q(H)}$ is still small however in difference from the previous case this ratio $\sim \sqrt{r_s}$. Quantum contribution in the total capacity will play more significant role with increasing of magnetic field.

5 Conclusions

Within RPA approximation expressions for self-consistent electrostatic potential are obtained. It is shown, that long-range electron density oscillations lead to decreasing of structure capacity and this effect plays more significant role with increasing external magnetic field.

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References

[1] N.D.Lang, W.Konh, Phys.Rev., B1 (1970) 4555
[2] D.Yue, L.I. Glazman, K.A. Matveev, Phys. Rev., B49 (1994) 1966
[3] A.M.Newns, Phys. Rev., B1 (1970) p 3304
[4] Yu.I.Balkarey, V.B.Sandomirsky Zh.Eksp.Teor.Fiz, 54, (1968), 808
[5] V.D.Shafranov Zh.Eksp.Teor.Fiz, 34, (1958), 1475
[6] J.A.Appelbaum, G.A.Baraff Phys.Rev.B 4, (1971) 1235
[7] S.A Mikhailov, V.A. Volkov, Sov. Phys. JETP Lett., 61 (1995) p.524