

Charging effects in a quantum wire with leads

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We investigate the distribution of the electron density and the potential in a quantum wire coupled to reservoirs, treating this structure as a unified quantum system and taking into account the Coulomb interaction of electrons. The chemical potential difference that exists between a decoupled, isolated quantum wire and the reservoirs gives rise to charge transfer in the coupled system. We show that the quantum wire can be charged positively or negatively or remain neutral as a whole, depending on such factors as the wire radius and the background charge density in the wire. The magnitude of the charge and its sign are to a large extent determined by the exchange interaction of the electrons in the wire. Using a Hartree-Fock approach, we develop a model of a quantum wire which includes the reservoirs. This model allows us to find the self-consistent distribution of the electron density and the potential in the wire both at equilibrium and in the presence of transport. The linear conductance is investigated as a function of the chemical potential. The nonadiabatic transition from the reservoirs to the wire leads to conductance oscillations caused by multiple scattering of electron waves. The period of the oscillations depends on the charge acquired by the wire and the exchange energy. We find that the exchange interaction strongly enhances the Friedel oscillations near the contacts. However, they do not noticeably suppress the conductance because the wire has a finite length and is charged. Under far from equilibrium conditions, which appear when the applied voltage exceeds the Fermi energy in the wire, the system becomes unstable with respect to fluctuations of the electric potential and the electron density. The instability results in the appearance of multistable electron states.

I. INTRODUCTION

Electron transport in quantum wires (QWs) now attracts considerable interest because of the fundamental importance of the electron-electron (e - e) interaction in one-dimensional (1D) systems.^{1,2} In addition, it is expected that the e - e interaction may produce important effects in the transport that would be attractive for applications. However, up to now there is no clear and unambiguous knowledge of which effects of e - e interaction are observable under the realistic conditions of a QW with leads and what the reasons are for the deviations from conductance quantization (observed experimentally³), and very little is known about the electron transport under far from equilibrium conditions.

In order to understand the transport properties, it is necessary to know the spatial distribution of the electric potential and the electron density in the structures under investigation. Many arguments and facts⁴⁻⁸ show that the leads play an essential role in the conductance, if the transport is investigated by measuring the electric current in an external circuit and by measuring the voltage drop between the leads. It is obvious that the interaction of the QW with the leads is not weak.

In the present paper we investigate this interaction, considering the QW and the leads as a unified system. An important problem that arises is how the electric field and the

electron density are distributed at equilibrium (i.e., in the ground state), and how they are redistributed when an external voltage is applied. We show that even in the equilibrium state the QW acquires a charge and a contact potential difference between the QW and the leads. This phenomenon is similar to the well known contact potential difference in classical conductor systems. The essential difference between the low-dimensional system under consideration and classical conventional 3D conductors is that the contact potential is not screened over a finite length but spreads over a length determined by the geometrical size of the structure.⁹ The contact potential difference is determined by the difference in the chemical potentials $\Delta\mu$ of electrons in the QW and in the leads, when these subsystems are considered independently. By analyzing the chemical potentials we find that three cases are possible, depending on the wire radius and the background charge density: (i) the QW is charged positively, (ii) the QW acquires a negative charge, or (iii) the QW remains neutral as a whole.

We develop a model of a QW with leads in which the lead-wire interaction is taken into account. It is based on a Hartree-Fock approach for the electrons in the QW and the representation of leads (which are considered as electron reservoirs) in a way that takes into account their 3D nature, but requires only a 1D calculation. Using this model we investigate the distribution of the electron density and the electric

potential at equilibrium, as well as under far from equilibrium conditions. In particular, we emphasize the role of the exchange interaction effect on these quantities. If in the absence of coupling the chemical potential of the wire exceeds that of the reservoir, $\Delta\mu > 0$, the coupled system expels electrons from the QW into the leads, when equilibrium is established. As a result a potential well appears in the QW. The wire acts as a charge donor to the reservoir. If $\Delta\mu < 0$, electrons are attracted by the wire, and a potential barrier arises between the QW and the leads. The wire acts in this case as an acceptor. In the case where $\Delta\mu = 0$, the electron density is redistributed only within the QW and only Friedel oscillations arise near the contacts. The Friedel oscillations appear in all cases; however, they are superimposed on a much more slowly varying potential created by the acquired charge. The slowly varying potential has an amplitude that is large compared to the Friedel oscillations and thus dominates the scattering processes. The exchange interaction strongly affects the potential shape and somewhat enhances the Friedel oscillation amplitude.

When an external voltage is applied, the chemical potentials in the electron reservoirs are shifted relative to each other, disturbing the electron flows in the QW. As this takes place, the electron density, the potential, and the exchange energy are changed self-consistently. The importance of the electrostatic potential distribution in quantum wires with leads, especially for the investigation of time-dependent transport, and for nonlinear transport, has been emphasized previously,¹⁰ but quantitative calculations have to our knowledge not been reported thus far.

Under far from equilibrium conditions, when the applied voltage exceeds the Fermi energy in the QW, the electron density is substantially redistributed between the QW and the reservoirs, giving rise to a very strong variation in the potential landscape. In turn the potential produces a variation in the electron density. The connection between the electron density and the potential is very important for the understanding of nonlinear transport. The need of a self-consistent treatment has been emphasized by Landauer.¹¹ Within the scattering approach, in the weakly nonlinear regime, it has been investigated by Christen and one of the present authors¹² and by Ma, Wang, and Guo.¹³ The calculation of the present paper allows us to investigate the strongly nonlinear transport in the system under consideration. If the applied voltage is high enough, the self-consistent connection of charge and potential gives rise to an instability of the electron density distribution and ultimately leads to multistability of the electron states in the QW. This means that several stable states with different spatial distributions of the electron density and the potential are possible at a given applied voltage.

The paper is organized as follows. In Sec. II the chemical potential difference between the decoupled QW and the 2D electron reservoir is analyzed. Section III describes the model of the QW with leads. Section IV contains the results of the numerical calculations of the electron density and potential distribution in the QW with leads. In Sec. VI the multistability of the electron states is described that appears for far from equilibrium conditions.

II. CONTACT POTENTIAL DIFFERENCE

To be specific we consider a QW connecting two regions of a 2D electron gas. We assume that there are no nearby gates and that all electric field lines emanate and terminate either on the wire or on the 2D electron gas. QW structures of this kind are produced by etching of heterostructures with a 2D electron gas. Such structures are widely used in experiments.^{14–18}

First we investigate such a QW separately from 2D electron reservoirs. The uncoupled wire is charge neutral. The electron charge is concentrated inside the QW, while the compensating positive charge of the impurities is really located in the immediate vicinity of the QW or at its surface. The decoupled QW and the electron reservoir have their own chemical potentials μ_{1D} and μ_{2D} , which are generally not equal each other. We are interested in the chemical potential difference $\Delta\mu$ between the QW and the reservoir.

According to Seitz's theorem¹⁹ the chemical potential in the QW is determined by the Fermi energy of noninteracting electrons and the self-energy $\Sigma(k_F)$ which takes into account the e - e interaction,

$$\mu_{1D} = \varepsilon_0 + \varepsilon_F + \Sigma(k_F). \quad (1)$$

Here $\varepsilon_0 \approx \pi^2 \hbar^2 / (2ma^2)$ is the first subband energy caused by transverse confinement (a is the QW radius, m is the effective mass of electrons). $\Sigma(k_F)$ contains the contributions arising from the exchange and correlation interaction as well as from the electron interaction with the positive background charge. The exchange and correlation energy was investigated in the recent paper of Calmels and Gold²⁰ using the self-consistent theory of Singwi, Tosi, Land, and Sjölander²¹ for the case where only the lowest subband is occupied. The Hartree energy is easily estimated if we assume that the positive charge is located at the surface of the QW. These calculations lead to the following expression for the chemical potential μ_{1D} of the QW in terms of the dimensionless parameters $r_s = 1/(2a_B n)$ and $\beta = a_B/a$ (with a_B the effective Bohr radius and n the 1D electron density):

$$\frac{\mu_{1D}}{R_y} \approx \frac{\pi^2}{2} \beta^2 + \frac{\pi^2}{16r_s^2} + \frac{\Sigma_{xc}}{R_y} - \frac{B_H}{r_s}, \quad (2)$$

where R_y is the effective Rydberg. In Eq. (2) the first term is the lowest subband energy, the second term is the kinetic energy, and the third term represents the exchange and correlation energy. There are two expressions for the exchange-correlation term depending on whether $r_s < 1$ or $r_s > 1$:

$$\frac{\Sigma_{xc}}{R_y} \approx -\beta \frac{5.57\pi - 4\beta r_s}{2\pi^2} \quad \text{if } r_s < 1$$

and

$$\frac{\Sigma_{xc}}{R_y} \approx -\frac{1.84}{r_s} \left[\ln \frac{2\beta r_s}{\pi} + 0.7115 \right] \quad \text{if } r_s > 1.$$

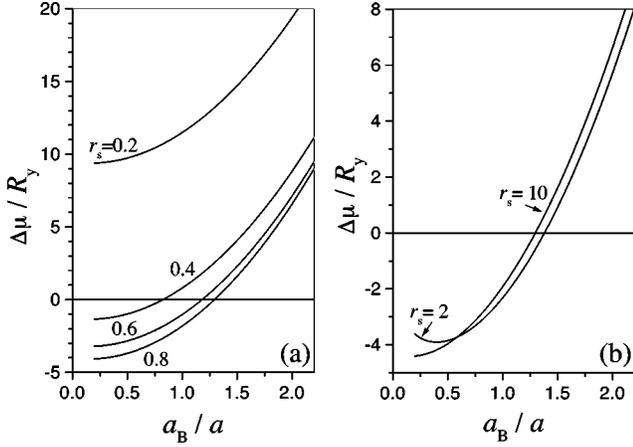


FIG. 1. Dependence of the chemical potential difference $\Delta\mu$ between the decoupled QW and the 2D electron reservoir on the wire radius a (in units of the Bohr radius) for various density parameters: (a) $r_s < 1$, (b) $r_s > 1$. The calculations were done with the following parameters of the 2D layer: $d = 2a$, $R_s = 0.5$.

The last term in Eq. (2) is the Hartree energy of the electron interaction with the positive background; B_H is a numerical factor that depends on the radial distribution of the electron density. If the electron density is distributed uniformly, $B_H \approx 1/3$.

The chemical potential in the 2D reservoir can easily be obtained from the known expression²⁵ for the electron energy as a function of the density parameter $R_s = (\pi a_B^2 N_{2D})^{-1}$ (where N_{2D} is the 2D electron density). In the high density case, $R_s < \sqrt{2}$, one obtains

$$\frac{\mu_{2D}}{R_y} = \left(\frac{\pi a_B}{d}\right)^2 + 2R_s^{-2} - 1.80R_s^{-1} - 0.38 - 0.0863R_s \ln R_s + 0.519R_s, \quad (3)$$

where d is the thickness of the 2D layer.

Using Eqs. (2) and (3), the chemical potential difference $\Delta\mu = \mu_{1D} - \mu_{2D}$ is calculated as a function of the QW radius and the density parameter r_s . The results of these calculations are illustrated in Fig. 1, where the $\Delta\mu$ dependence on the wire radius a is shown for various values of r_s . Here we consider r_s as an independent parameter because the background charge density depends on external factors, such as the charge absorbed at the wire surface. Figure 1 shows that in sufficiently thin wires the chemical potential is higher than in the reservoir. However, with increasing radius of the QW the chemical potential in the wire can become lower than in the reservoir.

The chemical potential difference $\Delta\mu$ is caused by all energy components contributing to the chemical potentials in the QW and in the reservoir. As an example it is instructive to consider the estimations for the specific case where the QW diameter is equal to the 2D layer thickness, $d = 2a$, and the background charge density per unit area, N_{2D} , is the same in the reservoir and in the QW. The latter means that $n = 2aN_{2D}$. In this case the energies contributing to the chemical potentials are estimated as follows. The confinement energy in the QW is approximately twice that in the reservoir. Hence the confinement energy causes μ_{1D} to rise

with respect to μ_{2D} . The ratio of kinetic energy in the QW to that in the reservoir is $\varepsilon_{F1}/\varepsilon_{F2} \sim an$. Since the QW is supposed to be a 1D system, the product an must be small. Hence the Fermi energy ε_{F1} in the QW is noticeably smaller than the Fermi energy ε_{F2} in the reservoir. This results in lowering μ_{1D} relative to μ_{2D} . The ratio of the exchange-correlation energies in the case of $r_s < 1$ is estimated as $\varepsilon_{xc1}/\varepsilon_{xc2} \sim (an)^{-1/2}$. The exchange-correlation energy in the QW is seen to be larger than that in the reservoir. Taking into account that the exchange-correlation energy is negative, we conclude that it lowers μ_{1D} with respect to μ_{2D} .

If the wire is now coupled to the 2D reservoir, we can distinguish three cases. For $\Delta\mu > 0$, electrons are transferred from the QW to the reservoir, so that the positive background charge dominates the electron charge in the wire. If $\Delta\mu < 0$, the reservoir supplies electrons to the QW producing an excess negative charge. When $\Delta\mu = 0$, the electron density is not redistributed between the wire and reservoir.²²

The electron density redistribution continues until an equilibrium state is attained in the whole system such that there exists a uniform electrochemical potential. As this takes place, a charge and a built-in electric field E_0 appear in the QW. If the reservoir conductivity is high, the built-in field satisfies the condition $e \int_0^\infty dx E_0(x) = \Delta\mu$. Such a charge transfer is similar to what happens when a contact potential difference appears in classical 3D systems. However, an essential difference is in the distance over which the contact field is screened. In the 3D case the contact field is screened over a finite length (e.g., the Debye length or the Thomas-Fermi screening length). In the mesoscopic structure considered here, the contact field is produced by the charge, one part of which is situated in the 1D wire and the other on the surface of the reservoir adjacent to the wire. One can easily see that, owing to the 3D nature of the electric field, any distribution of charges in a QW cannot screen the contact field over a finite distance. Thus the question arises of how the charge density and the electric field are distributed in the QW and over the reservoir surface. In the case of a high enough electron density, the interaction effects are not strong, and this problem can be solved analytically using the Thomas-Fermi approximation.²⁶ In the present paper, we study this problem using a numerical solution of the Schrödinger equation coupled to the Poisson equation within the Hartree-Fock approximation.

III. MODEL

Finding the self-consistent electron density and the potential in a QW coupled to electron reservoirs is a rather complicated problem because the electron density redistribution between the QW and the reservoirs produces a strong variation of the electron energy in the QW. The energy variation is estimated as $\Delta\mu$, which is shown above to be of the order of the Fermi energy. In essence, the QW and the reservoirs should be considered as a unique quantum system. To our knowledge, such a problem has not been studied to date. In the present paper, we investigate it using a simplified model based on the Hartree-Fock approximation, which allows one to take adequately into account the charge accumulated in the QW both for the equilibrium state and under the far from

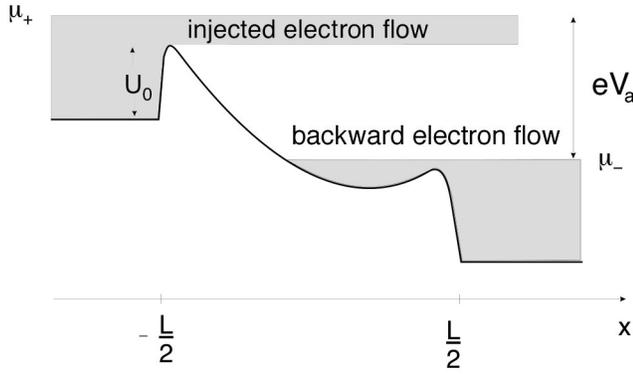


FIG. 2. Energy diagram of a QW with leads and the electron flows.

equilibrium conditions appearing when an external voltage is applied. This approach allows one also to study the exchange interaction effect on the charge accumulated and the electric potential. However, it does not take into account the electron correlation energy. The ratio of the correlation energy to the exchange energy depends on the electron density. For 1D conductors this ratio can be estimated according to Ref. 20. The correlation energy is negligible when $r_s \ll 1$. Under this condition the Hartree-Fock approximation is justified.

It is instructive to estimate numerically the number of electrons in a GaAs QW when $r_s = 0.5$. The Fermi energy and the electron density are respectively $\varepsilon_F \approx 4$ meV and $n \approx 6 \times 10^5 \text{ cm}^{-1}$. Our computation procedure works well when the QW length is not too large in comparison with the Fermi wavelength. If one puts the QW length equal to $0.3 \mu\text{m}$, the total number of electrons in the QW is estimated as about 18. Thus the system contains about ten electrons in a QW open to reservoirs. The number of electrons really existing in the wire and their density distribution is determined by the QW length, the background charge, the applied voltage, and the $e-e$ interaction energy. The parameters of the QW estimated above are realizable in experiment.

In order to investigate specific cases with different relative positions of the chemical potentials in the QW and reservoirs, we introduce a positive background charge density en_b in the QW, which is considered as a parameter of our model. By varying en_b it is possible to realize any relative position of the chemical potentials of the uncoupled system. Charges on the QW surface are not taken into account in our present consideration.

Another simplification is that only the lowest subband in the QW is considered.

A 1D sketch of the energy diagram of a QW with leads and the electron flows (in a far from equilibrium situation) is shown in Fig. 2. Here U_0 is the confinement energy in the QW and μ_{\pm} are the chemical potentials in the reservoirs.

The positions of μ_+ and μ_- relative to the conduction band bottom of the corresponding reservoirs are fixed because the electron gas in the reservoirs is incompressible. However, μ_+ and μ_- are shifted relative to each other in the presence of an applied voltage V_a .

The following energies contribute to the potential shape of the structure: the confinement energy in the QW; the potential produced by the external voltage source; the Hartree and exchange energies in the QW. In the reservoirs ($|x| > L/2$, L being the wire length) the electron density is taken to be so high that the $e-e$ interaction energy can be ignored in comparison with the kinetic energy. Moreover, the reservoirs are assumed to be ideally conducting and hence can be treated as equipotentials. Inside the QW the $e-e$ interaction potential $U(x, x')$ is determined by both the direct interaction of electrons with each other and the indirect interaction via image charges induced by electrons in the reservoirs. Because of this, the interaction potential depends on the coordinates x, x' of the interacting electrons separately, rather than simply on their difference. In the QW the one-electron wave functions $\psi_{r, k_r, s}(x)$ are characterized by quantum numbers: $r = \pm 1$ ($r = +1$ indicates electrons incident on the QW from the left reservoir and $r = -1$ corresponds to electrons incident on the QW from the right reservoir); k_r is a wave number in the left ($r = +1$) or right ($r = -1$) reservoir; s is a spin variable. In this paper we ignore changes in s and suppose that the states with opposite spins are equally occupied. The effects of possible spin polarization in a QW will be considered elsewhere.

The electron transport in the reservoirs, close to the transition between the reservoir and the QW, is modeled by a 1D Schrödinger equation without interaction. This model allows one to simulate adequately the transmission probability between the reservoirs and the QW. The value of the transmission probability calculated in this way as compared with that for a true 2D to 1D transition at the interface of the reservoir and the wire has been investigated by direct comparison of the transmission probabilities of these two geometries.²⁷ The difference depends on the energy but does not exceed 15% even close to the transmission threshold. The physical reason for the success of the purely 1D model is that near the chemical potential level, of all the electron waves in the reservoir, only those couple effectively to the wire that have a wave vector that is nearly parallel to the wire axis (collimation effect²⁸). We also emphasize that in the problem under investigation the electron density of the 1D Schrödinger problem is needed only within the wire. It is unimportant for the reservoirs because they are treated as equipotentials and therefore the calculated electron density distribution in the reservoirs does not directly affect the $e-e$ interaction in the QW. The calculated electron wave functions in the reservoirs affect only the transmission probability through the contacts.

In the reservoirs, $\psi_{r, k_r, s}(x)$ is thus

$$\psi_{r, k_r, s}(x) = \begin{cases} \exp[ik_r(rx + L/2)] + R_r \exp[-ik_r(rx + L/2)] & \text{if } rx < -L/2 \\ T_r \exp[ik'_r(rx - L/2)] & \text{if } rx > L/2, \end{cases} \quad (4)$$

where $(k'_r)^2 = k_r^2 + r \times 2meV_a/\hbar^2$, and V_a is the applied voltage.

In the QW, $\psi_{r,k_r,s}(x)$ is determined by the equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_{r,k_r,s}}{dx^2} + [U_0(x) - U_{\text{ext}}(x) + U_H(x) + \hat{H}_{\text{ex}}] \psi_{r,k_r,s} = \varepsilon_r(k_r) \psi_{r,k_r,s}. \quad (5)$$

In Eq. (5) the potential energy has the following components. $U_0(x)$ is an effective potential that simulates the electron confinement in the QW. In the simplest case, we can assume that $U_0(x) = U_0 = \text{const}$ for $|x| < L/2$ and $U_0(x) = 0$ for $|x| > L/2$. U_H is the Hartree energy,

$$U_H(x) = \int_{-L/2}^{L/2} dx' U(x, x') [n(x') - n_b], \quad (6)$$

with n_b being the positively charged background density, $n(x)$ being the electron density,

$$n(x) = \sum_{r=\pm,s} \int_0^\infty \frac{dk_r}{2\pi} f(k_r) |\psi_{r,k_r,s}|^2, \quad (7)$$

and $f(k_r)$ the electron distribution function in the reservoirs. In Eq. (6) we assume for simplicity that the radial component of the background charge density is the same as the electron density.

The e - e interaction potential $U(x, x')$ that appears in Eq. (6) depends on the spatial configuration of the leads. In what follows the numerical calculations are carried out for the case where the leads are represented as two plates perpendicular to the QW. This configuration is convenient for further calculations because in this case a relatively simple analytical expression is obtained for $U(x, x')$.^{23,24} This form of the interaction potential allows one to take into account not only the direct Coulomb interaction of electrons but also their interaction via image charges induced on the lead surfaces. The interaction potential is

$$U(x, x') = \frac{e^2}{\epsilon L} \int_0^\infty \frac{dy}{\sinh y} |\chi_y|^2 \times \begin{cases} \sinh[y(1/2 + \xi)] \sinh[y(1/2 - \xi')] & \text{if } \xi < \xi', \\ \sinh[y(1/2 - \xi)] \sinh[y(1/2 + \xi')] & \text{if } \xi > \xi', \end{cases}$$

where $\xi = x/L$ and χ_y is the Fourier transform of the radial density, which is taken to be $\chi_y = \exp[-(ay/2L)^2]$. Using the analytical expression for $U(x, x')$, instead of directly solving the 3D Poisson equation, greatly facilitates computations.

\hat{H}_{ex} is the exchange energy operator,

$$\hat{H}_{\text{ex}}(x) \psi_{r,k_r,s} = \int_{-L/2}^{L/2} dx' U(x, x') n_{\text{ex}}(x, x') \psi_{r,k_r,s}(x'),$$

where

$$n_{\text{ex}}(x, x') = \sum_{r=\pm} \int_0^\infty \frac{dk_r}{2\pi} [\psi_{r,k_r,s}^*(x') \psi_{r,k_r,s}(x)] f(k_r).$$

For the reservoir configuration that we consider here, the ‘‘external potential’’ is a linear function of x : $U_{\text{ext}} = eV_a(x/L + 1/2)$.

The energy $\varepsilon_r(k_r)$ in Eq. (5) is expressed in terms of the wave vector k_r and the applied voltage V_a ,

$$\varepsilon_r(k_r) = \frac{\hbar^2 k_r^2}{2m} + eV_a \delta_{r,-1},$$

where we assume that the energy reference is fixed at $x = -\infty$.

In addition, we require continuity of the wave functions determined by Eqs. (5) and (4) and their derivatives at the reservoir-wire interfaces $x = \pm L/2$. The distribution functions $f(k_r)$ in the reservoirs are taken in the form of the Fermi functions with the temperature T considering the fact that the Fermi level in the right reservoir is shifted down by eV_a with respect to the left one.

Inside the QW no distribution functions are assigned. The electron distribution over the energy is determined by the electron flows from the left and right reservoirs and the interaction processes inside the QW. The external voltage produces a variation of the electron flows, as a consequence of which the electron density is changed. Ultimately, this results in the self-consistent variation of both the electron states and their occupation for both the left and right moving particles.

The wave functions that we consider in this work are characterized by a continuous quantum number k_r .²⁹ Hence, ψ should be considered as a function of two variables x and k_r . Equation (5) is an integro-differential equation with respect to the variable x and an integral equation with respect to the variable k_r . We develop a numerical scheme for the solution of this equation on a grid spanning the two variables. The computation method is described in the Appendix. It is worth noting that in the case where the voltage is applied, the wave functions are found without using any expansion in terms of the undisturbed wave functions.

The numerical computations were performed using the 32-processor computer system Parsytec CC.

IV. THE EQUILIBRIUM STATE

First, we consider the equilibrium state that appears in the absence of an applied voltage $V_a = 0$. In order to realize the three cases ($\Delta\mu > 0$, $\Delta\mu < 0$, and $\Delta\mu = 0$) described in Sec. II, we vary the density of the positive background charge n_b . In doing this it is convenient to compare n_b with the characteristic density

$$n_0 = \frac{2}{\pi\hbar} \sqrt{2m(\mu_0 - U_0)}, \quad (8)$$

where μ_0 is the equilibrium level of the chemical potential in the system. This quantity has a simple physical meaning in the case where the exchange and correlation interaction is absent. It is the background density that determines which of the three cases is realized in the Hartree case. If $n_b = n_0$, electrons are not redistributed between the QW and the leads in the equilibration process, if $n_b > n_0$, electrons flow from the QW to the reservoirs, and if $n_b < n_0$, electrons are transferred from the reservoir to the QW. Of course, turning on the exchange and correlation interaction shifts the value of

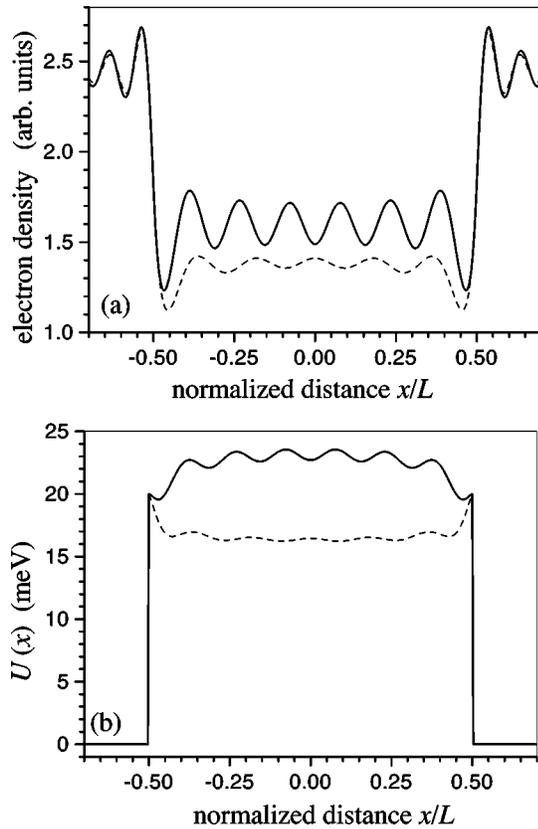


FIG. 3. (a) The electron density distribution and (b) the potential energy shape in the QW for $n_b = 1.5n_0$. The dashed lines represent the case without exchange interaction. The solid lines are obtained by taking the exchange interaction into account. The calculations were done for the parameters $a = 5 \times 10^{-7}$ cm, $L/a = 30$, $U_0 = 20$ meV, $\mu_0 - U_0 = 4$ meV, $T = 0$, and $V_a = 0$.

the background density at which electrons are not redistributed. Nevertheless, as a reference, the value n_0 remains convenient.

The electron density distribution $n(x)$ for the three cases is illustrated in Figs. 3, 4, and 5. Shown here are also the graphs of the potential energy $U(x)$ that includes the confinement energy and the Hartree energy,

$$U(x) = U_0 + U_H,$$

but not the exchange energy. The exchange energy is not included in $U(x)$ because it is a functional of ψ rather than a direct function of x . It is useful to note that U_H essentially coincides with the electric potential.

Let us consider first the case where the exchange interaction is not taken into account. It is illustrated by the dashed lines in Figs. 3–5. In this case $U(x)$ gives the full single-particle potential shape in the QW. If $n_b > n_0$ (this corresponds to $\Delta\mu > 0$), Fig. 3 shows that the potential shape lies below the U_0 energy and hence the interaction energy is negative. This means that a positive charge is accumulated in the QW. It is responsible for the appearance of a potential well.

The case $\Delta\mu < 0$ is realized when $n_b < n_0$. The electron density distribution and the potential shape are shown in Fig. 4. The interaction energy is seen to be positive and the potential shape in the QW lies above U_0 . This means that a

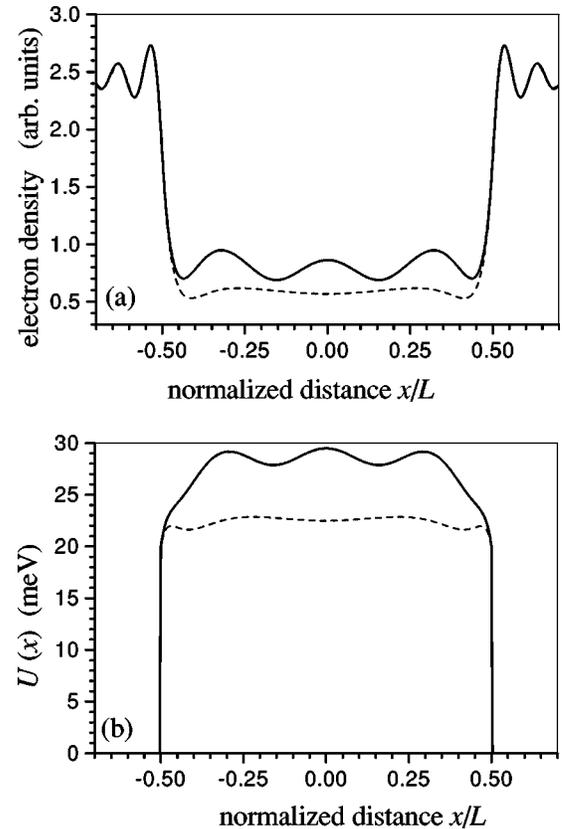


FIG. 4. The same as in Fig. 3 but for $n_b = 0.5n_0$.

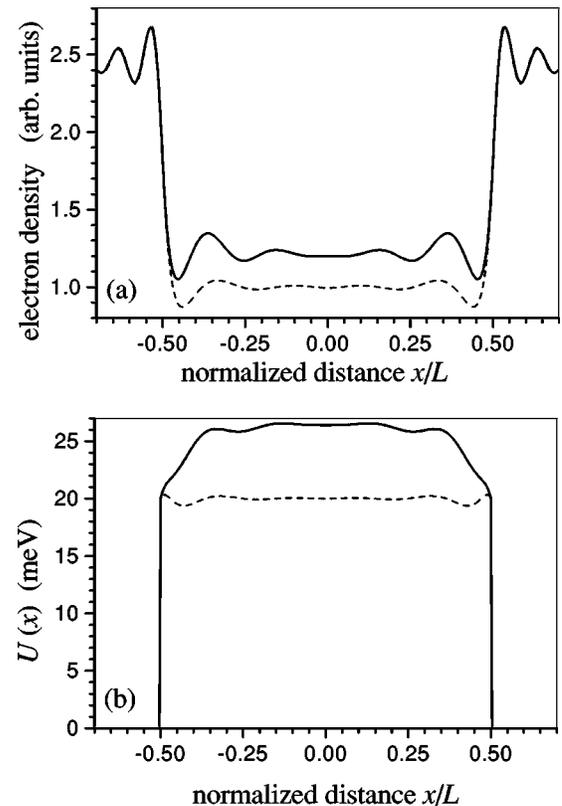


FIG. 5. The same as in Fig. 3 but for $n_b = 1.0n_0$.

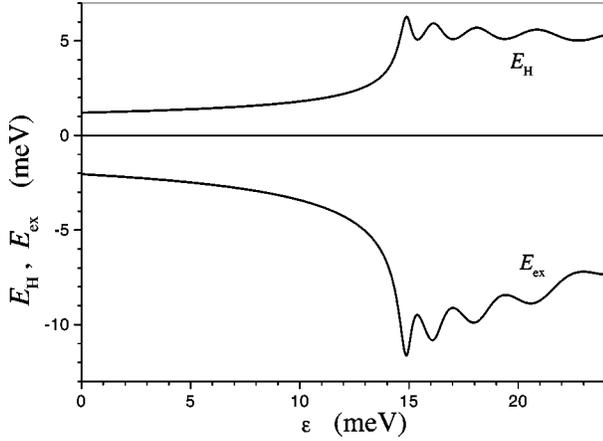


FIG. 6. Average exchange and Hartree energies of electrons incident on the QW with the energy ε . The calculations are for the parameters $a=5 \times 10^{-7}$ cm, $L/a=30$, $U_0=20$ meV, $\mu_0-U_0=4$ meV, $n_b=1.0n_0$, $T=0$, and $V_a=0$.

negative charge is accumulated in the QW. It produces a potential barrier that hinders electrons in passing through the QW.

If $n_b=n_0$, the electron density is essentially not redistributed between the QW and the reservoirs. However, Friedel oscillations of the electron density appear near the contacts, Fig. 5. The Friedel oscillations are also observed if there is carrier transfer, but they are superimposed on the much stronger variation of the potential due to the charging of the QW.

Let us now consider the exchange interaction effect. The electron density distribution and the potential shape, calculated by taking into account the exchange interaction, are shown in Figs. 3–5 as solid lines. The exchange interaction is seen to result in an increase of the electron density. This is a consequence of the fact mentioned in Sec. II that the exchange interaction decreases the chemical potential in a QW. That is why more electrons come into the QW when the equilibrium state is established. Correspondingly, the negative charge in the QW increases, which results in the growth of the energy $U(x)$. However, this does not yet mean that the electron states with energy lower than $U(x)$ are necessarily states decaying in the QW, since the exchange interaction lowers the effective barrier between the QW and the reservoir.

Since it would be incorrect to consider the exchange energy as a function of x , we calculate an average value of the exchange energy per particle incident on the QW with the energy $\varepsilon(k_+)$ from the left reservoir,

$$E_{\text{ex}} = \frac{\langle \psi | \hat{H}_{\text{ex}} | \psi \rangle}{\langle \psi | \psi \rangle},$$

(here $\langle \dots \rangle$ denotes averaging over the QW length). The average exchange energy E_{ex} is shown in Fig. 6 as a function of $\varepsilon(k_+)$. The average Hartree energy E_H is also given in this figure. It is seen that E_{ex} exceeds E_H for all energies. Hence the joint effect of the exchange interaction and the Hartree interaction consists in an effective lowering of the barrier, so that electrons with energy below the confinement energy U_0 can transit through the QW without decay.

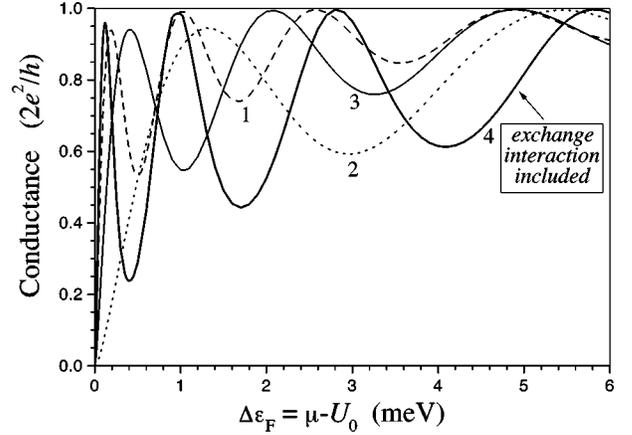


FIG. 7. Linear conductance as a function of the chemical potential μ_0 . Lines 1, 2, and 3 present the calculations within the Hartree approximation for several background densities: $n_b/n_0=1.5, 0.5, 1.0$, respectively. Line 4 is obtained by including the exchange interaction for $n_b=n_0$. The parameters used in the calculation are $a=5 \times 10^{-7}$ cm, $L/a=20$, $U_0=10$ meV, $T=0$, and $V_a=0.01$ mV.

Another effect produced by the exchange interaction is also seen from Figs. 3–5. The exchange interaction strongly enhances the Friedel oscillation amplitude. This result agrees qualitatively with the analytical calculation of the interaction effect on the transmission through a barrier in 1D systems.³⁰ In our case the Friedel oscillations are generated at the contacts of the QW with the reservoirs. Their amplitude in the potential energy is quite pronounced but smaller than the potential energy μ_0-U_0 in the QW. For the discussion which follows it is important to remark that the Friedel oscillations are superimposed on the smooth variation of the potential produced by the charge accumulated in the QW. Even if the exchange interaction is fully taken into account, this smooth component has an amplitude that is larger than that of the Friedel oscillations. Due to the smooth variation of the potential the QW becomes nonuniform.

V. LINEAR CONDUCTANCE

The model that we have developed above allows us to find the electric current arising when an external voltage is applied. The current is calculated as the sum of the partial currents of the states $\psi_{r,k_r,s}$, taking into account their occupation. The linear regime is realized when $eV_a \ll (\mu_0-U_0)$. In this case we have obtained the dc conductance as a function of the chemical potential μ_0 . The results of these calculations for zero temperature and for several densities of the background charge n_b are given in Fig. 7.

The conductance oscillations with varying chemical potential are a consequence of the nonadiabatic reservoir-wire interface. The rapid variation of the potential at this interface leads to backscattering and, if the electron wave is coherent over the entire wire length, to resonances. The oscillations have the same origin as the resonances observed in over the barrier transmission of noninteracting particles. A similar effect also appears in the transport of noninteracting electrons through a narrow, ballistic, nonadiabatic constriction in a 2D electron gas.³² Our calculations show that the $e-e$ interaction changes the effective potential barrier that electrons have to

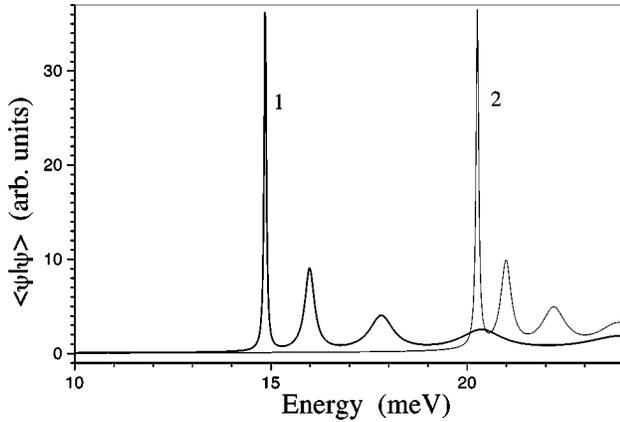


FIG. 8. Exchange interaction effect on the spectrum of the electron density $\langle \psi_k | \psi_k \rangle$. Line 1 presents the spectral density obtained by including the exchange interaction; line 2 is the spectral density without the exchange interaction. The calculations are for $a = 5 \times 10^{-7}$ cm, $L/a = 30$, $U_0 = 20$ meV, $\mu_0 - U_0 = 4$ meV, $n_b = 1.0n_0$, $T = 0$, and $V_a = 0$.

overcome in passing from one reservoir to another.

First, we discuss the results obtained within the Hartree approximation, when exchange interaction is neglected. These results are represented by the lines 1–3 in Fig. 7 for several different background densities n_b . With increasing n_b the oscillations become more frequent, which means that the effective wave number of the electrons is increased. Exactly the same behavior is demonstrated in Figs. 3–5, namely, with increasing n_b the potential in the QW is shifted downward, causing the kinetic energy to increase.

A similar effect occurs when the exchange interaction is turned on. It is demonstrated in Fig. 7 by curve 3 (obtained by ignoring the exchange interaction) and by line 4 (obtained by including exchange interaction), the background charge being the same in both cases. The exchange interaction is seen to make the conductance oscillations more frequent. The reason for this effect is that the exchange interaction results in an effective lowering of the potential energy of the electrons and consequently in an increase of their kinetic energy. In order to assess the exchange interaction effect on the effective potential, it is instructive to see how the exchange interaction affects the spectral density of electrons, i.e., $|\psi_k|^2$ integrated over the QW length. This is illustrated in Fig. 8. The exchange interaction allows the electrons with energy below the confinement energy U_0 to pass through the QW.

It is interesting to note that, despite the fact that Friedel oscillations are present in the QW, no noticeable suppression of the conductance is observed. The effect of conductance suppression by a periodic potential associated with Friedel oscillations was considered for infinite 1D systems with a δ potential in Refs. 31 and 30. This phenomenon is connected with the fact that a periodic component of the potential suppresses the transmission of the electrons with energy near the Fermi level across the QW (a gap appears at the Fermi level). The absence of this effect in our system is a consequence of two facts. First, the QW has a finite length. Second (and no less essential), the QW becomes inhomogeneous owing to the electron density redistribution between the QW and the leads. As a consequence the kinetic energy at the chemical

potential level and the Friedel oscillation period become dependent on the position in the QW. This is why the resonant interaction of electrons at the chemical potential level with the Friedel oscillations is destroyed and the electron passage is not suppressed.

VI. NONLINEAR TRANSPORT AND MULTISTABILITY

A significant redistribution of the electron density between the QW and the reservoirs occurs under far from equilibrium conditions when the applied voltage exceeds the Fermi energy. Electrons are injected from the left reservoir (cathode) while the electrons entering the QW from the positive reservoir (anode) are scattered back inside the QW. As a consequence, the electron density decreases in the QW (roughly speaking to one-half of the equilibrium density) though the positive background charge is unchanged. Because the positive charge is dominant, a potential well appears in the QW, with the potential shape being distorted by the external potential, as illustrated in Fig. 2. Therefore the kinetic and potential energies are greatly changed. The change in the potential energy produces variations in the wave functions (including even a possibility for resonant states to appear) and the electron density distribution. In this way feedback arises between the electron density and the potential in the QW, which is an important mechanism in nonlinear transport. It is that mechanism which is realized in the model proposed.

A complete numerical analysis of the nonlinear transport properties in the wide range of applied voltages within the Hartree-Fock approximation meets some difficulties caused by the long computation time. In this paper we restrict our consideration to the Hartree approximation, which is reasonable at high enough voltage because the exchange energy decreases when the kinetic energy of electrons is increased.³³ The calculations were carried out using the method of pseudotime evolution to the steady solution³⁴ described in the Appendix. It turns out that in some range of applied voltage an instability of the evolution process appears. The instability origin is not connected with the computation process but is caused by real behavior of the system.

The mechanism of the instability is as follows. When the applied voltage is high enough (compared to the Fermi energy), the electron flow injected from the negatively charged reservoir is the only flow in the QW. Let a velocity fluctuation appear in some portion of the wire. To be definite, let us assume that the velocity is increased above its stationary value. Since the total electron flow is limited by the contact, it is not disturbed by this fluctuation. Hence, the continuity of the current requires that the electron density decreases. This leads to a growth of the positive (net) charge, because electrons cannot completely neutralize the background charge. The excess positive charge causes the potential energy of the electrons to decrease. Under the condition of ballistic transport, this results in a new increase of the velocity, and so on until some nonlinear process stabilizes this instability. In our model this is achieved by a redistribution of the overall electron density and a reshaping of the potential distribution in the QW. In such a way the potential shape is switched from one state to the other under the condition that both states are characterized by the same potential difference across the QW ends.

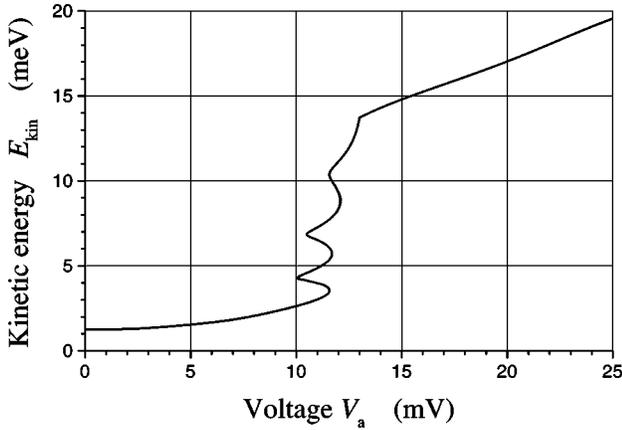


FIG. 9. Dependence of the average kinetic energy of electrons on the applied voltage. The calculations are for the following parameters: $a = 5 \times 10^{-7}$ cm, $L/a = 20$, $U_0 = 10$ meV, $\mu_0 - U_0 = 3$ meV, $n_b/n_0 = 1.0$, and $T = 0$.

In order to describe the transition from one shape to the other as a continuous process it is necessary to characterize the nonequilibrium state of the system by a parameter other than the applied voltage. This parameter should distinguish states with different potential shapes and the same potential difference across the ends. As such a parameter, the mean kinetic energy E_{kin} of electrons in the QW can be used,

$$E_{\text{kin}} = \frac{\sum_{r=\pm} \int dk_r \langle k_r | \hat{T} | k_r \rangle}{\int_{-L/2}^{L/2} dx n(x)},$$

where \hat{T} is the kinetic energy operator.

This conclusion is similar to what is known in the theory of hot electron instabilities in semiconductors. The electron heating by the electric field results in S- and N-shaped current-voltage characteristics. Under these conditions, the electron temperature uniquely determines the state of the system.³⁵ In our case the kinetic energy of the electrons is a direct analog of the electron temperature.

We have developed the algorithm that allows one to solve our problem in the case where the mean kinetic energy is fixed rather than the applied voltage. This algorithm is described in the Appendix. In this computation scheme all quantities (including V_a) are determined by E_{kin} . We have found that this algorithm gives stable results and the nonequilibrium state of the system under investigation is uniquely determined by E_{kin} . In particular, the dependence of E_{kin} on the applied voltage is shown in Fig. 9. The kinetic energy is seen to have several values for a given voltage V_a , while V_a is uniquely defined by E_{kin} . Correspondingly, several nonequilibrium states, with different distributions of the electron density and the potential, are possible at a given voltage. It is obvious that the states are not all stable with respect to time-dependent fluctuations.

The multistability, and in particular bistability, phenomenon described above may be useful for understanding the negative differential conductance observed in quantum wires.³⁶

VII. CONCLUSIONS

In this paper a QW of a finite length coupled to reservoirs is considered as a unified system. We have found that the electron density is substantially redistributed between the wire and the electron reservoirs when this system is formed. As a consequence of this process, a QW can acquire a net charge. The charging of the wire is caused by the chemical potential difference between the wire and the leads which exists if these two subsystems are decoupled. This phenomenon is similar to the contact potential difference in a classical multiconductor system. The structures of the charge density and the electric potential distributions differ according to the chemical potential difference: (i) a positive charge is accumulated in the wire and a potential well is developed there; (ii) the wire is charged negatively giving rise to a potential barrier; (iii) the wire remains uncharged as a whole. In all cases, Friedel oscillations are present which are generated at the nonadiabatic contacts of the QW with reservoirs. They are superimposed on the relatively smooth profile of the potential produced by the charge accumulated in the wire. This smooth potential has a large amplitude. The Friedel oscillation amplitude is strongly enhanced if the exchange interaction is included.

Variation of the electron density in a QW due to electron redistribution between the wire and the reservoirs produces a significant effect on dc conductance. This effect is connected with the change of the kinetic energy of the electrons due to two factors: (i) the variation of the accumulated charge and the potential variation associated with this charge; (ii) the variation of the exchange energy. The exchange energy substantially lowers the effective potential barrier that electrons have to overcome when passing from one reservoir to another.

The Friedel oscillation potential does not suppress the conductance because the QW becomes inhomogeneous as a consequence of the electron density redistribution between the QW and the leads. The electron density variation due to the voltage applied across the leads and the change of the effective potential shape, associated with this variation, in the wire is an important mechanism for nonlinear transport.

The most interesting consequence of the charging effect in the wire is the instability that arises under a high enough applied voltage. The instability shows itself as a spontaneous increase of the kinetic energy of the injected electrons at a given applied voltage. In a QW with a nonadiabatic connection to the reservoirs, the development of instabilities results in the appearance of multistable states, i.e., in the existence of several stable states at a given voltage.

We conclude by emphasizing that the charging effect analyzed here is a general phenomenon that might be important in many mesoscopic systems containing electronically different compounds. Examples of current interest are carbon nanotubes,³⁷ hybrid normal-superconducting systems, and atomic quantum point contacts.

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APPENDIX: THE COMPUTATION METHOD

The problem of finding the wave functions for a QW coupled to reservoirs can be reduced to the solution of Eq. (5) in the inner region $-L/2 \leq x \leq L/2$ and matching $\psi_{r,k,s}$ and its derivative at the boundaries $x = \pm L/2$ to the wave functions (4) in the outer regions. Combining the matching equations for $\psi_{r,k,s}$ and $\psi'_{r,k,s}$, one can exclude the coefficients R_r and T_r to get finally the following nonuniform boundary conditions for $\psi_{r,k,s}$:

$$\psi'_{r,k_r,s} = \begin{cases} ik_r(2 - \psi_{r,k_r,s}), & rx = -L/2 \\ ik'_r \psi_{r,k_r,s}, & rx = L/2, \end{cases} \quad (\text{A1})$$

where k_r and k'_r are defined in Eq. (4)

The wave functions $\psi_{r,k_r,s}$ are considered as functions of two continuous variables: the space coordinate x and the energy $\varepsilon_r = \hbar^2 k_r^2 / 2m$. Thus $\psi_{r,k_r,s} = \psi_{r,s}(x, \varepsilon_r)$, where x and ε_r are varied respectively in the regions $-L/2 \leq x \leq L/2$ and $0 < \varepsilon_r \leq \varepsilon_M$, with the upper boundary ε_M being equal to $\mu_0 + 3k_B T$ (k_B is the Boltzmann constant, T is the temperature). In this region the uniform grid $\{x_i, \varepsilon_j\}_{i=0, N_1; j=0, N_2}$ is constructed.

The equation for $\psi_{r,k,s}(x_i, \varepsilon_j)$ on the grid is obtained from Eq. (5) with use of the integro-iterpolative method for the node presentation on x_i and the trapezium formula when calculating the integrals on k_r for the nodes on ε_j . This results in a set of nonlinear finite-difference equations that can be symbolically presented in the form

$$\hat{\mathbf{M}}[\Psi]\Psi = \mathbf{F}, \quad (\text{A2})$$

where Ψ is the wave function vector to be found and $\hat{\mathbf{M}}[\Psi]$ is the nonlinear operator. The matrix equation (A2) is inhomogeneous as a consequence of the boundary conditions (A1).

The equations (A2) are solved by the iteration method. However, the commonly used successive approximation scheme ($\hat{\mathbf{M}}[\Psi^{(l)}]\Psi^{(l+1)} = \mathbf{F}$, with l being the iteration number) turns out to be badly convergent. We use the method of pseudotime evolution to the steady solution.³⁴ More specifically, we use the two-layer iteration scheme of this method. In this scheme the approximating matrix $\hat{\mathbf{M}}^{(l)}$ is introduced, which is calculated with the use of the iteration process

$$\frac{\hat{\mathbf{M}}^{(l+1)} - \hat{\mathbf{M}}^{(l)}}{\tau_l} = \hat{\mathbf{M}}[\Psi^{(l)}] - \hat{\mathbf{M}}^{(l)}, \quad l = 0, 1, 2, \dots, \quad (\text{A3})$$

where τ_l is a pseudotime parameter. The choice of τ_l allows one to attain the best convergence of the iteration process. As the starting value of $\hat{\mathbf{M}}^{(0)}$ we use $\hat{\mathbf{M}}[\Psi = 0]$, i.e., the $\hat{\mathbf{M}}$ matrix for noninteracting electrons. During the iteration process, $\Psi^{(l)}$ is calculated with the use of the equation

$$\hat{\mathbf{M}}^{(l)}\Psi^{(l)} = \mathbf{F}.$$

The pseudotime τ_l is determined by the $\hat{\mathbf{M}}^{(l)}$ operator spectrum. The optimal convergence is attained when

$$\tau_l = \frac{2}{\lambda_{\min}(\mathbf{M}^{(l)}) + \lambda_{\max}(\mathbf{M}^{(l)})},$$

where λ_{\min} and λ_{\max} are the lowest and highest eigenvalues of $\hat{\mathbf{M}}^{(l)}$. The iteration process is ended when the following condition is fulfilled:

$$\max \left| \frac{m_{ij}^{(l+1)} - m_{ij}^{(l)}}{m_{ij}^{(l)}} \right| \leq \delta,$$

where $m_{ij}^{(l)}$ is an element of the $\mathbf{M}^{(l)}$ matrix. In the present paper, δ was chosen to be 10^{-6} .

The above method is successful when the system under investigation has a unique solution. However, at some fixed values of the applied voltage the computation shows an instability. In the course of the pseudotime evolution process the calculated quantities (such as the potential, the electron density, the kinetic energy) are randomly switched between several values. This is connected with the fact that the state of the system is not uniquely determined by the calculation scheme where the applied voltage is fixed.

A unique description of the system is achieved by using the mean kinetic energy E_{kin} of the electrons as the parameter that defines the nonequilibrium state of the system. We have developed a computation algorithm that allows one to vary E_{kin} continuously; in other words, we solve the problem using E_{kin} as the fixed parameter instead of the applied voltage.

An essential question appearing in this algorithm is how the applied voltage V_a should be defined when E_{kin} is given. The equation defining V_a is obtained from Eq. (5). Multiplying this equation by $\psi_{r,k_r,s}^*$, integrating it over k_r and over x , and summing over r one gets an equation of the following form:

$$E_{\text{kin}} - eV_a A[\Psi] = B[\Psi], \quad (\text{A4})$$

where $A[\Psi]$ and $B[\Psi]$ are functionals of the electron wave functions. Solving this equation with respect to V_a one gets V_a as a functional of Ψ , with E_{kin} being a parameter,

$$V_a = \Phi_{E_{\text{kin}}}[\Psi]. \quad (\text{A5})$$

When solving the problem with E_{kin} as a parameter, Eq. (A5) should be taken into account together with Eq. (A3). This system of equations is solved using the above pseudotime evolution method and two-layer iteration scheme. The set $V_a^{(l)}$ approximating V_a is defined as

$$\frac{V_a^{(l+1)} - V_a^{(l)}}{\tau_l} = \Phi_{E_{\text{kin}}}[\Psi^{(l)}] - V_a^{(l)}, \quad l = 0, 1, 2, \dots$$

As the starting value of the $V_a^{(l)}$ set, the arbitrary value of V_a in the stability region close to the instability threshold can be used. In this generalized procedure the pseudotime τ_l is chosen taking into account the spectral properties of the total matrix $\hat{\mathbf{M}}^{(l)} \oplus V_a^{(l)}$.

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