Lateral electron localization by the induced surface charge

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We investigate the problem of the electron interacting with the charge induced on the metal or dielectric surface. We show that the interaction between the electron and the induced surface charge leads to the lateral confinement of the electron. As a result the electron propagates parallel to the surface not as a plane wave but as a wave packet of a Gaussian shape. The electron moving together with the induced charge can be treated as a new quasi-particle, which we call inducton. We discuss a possible experimental evidence for inductons in semiconductor nanostructures, metal-vacuum, and dielectric-vacuum interfaces.

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The electron interacting with the charge induced on the metal (dielectric) surface was a subject of many experimental papers and theoretical papers. In semiconductor nanostructures, the induced potential leads to a screening of the electron-electron interaction and a modification of the potential confining the carriers in the quantum wells, wires, and dots. The classical image-charge potential was applied to study the electron localization in the direction normal to the metal surface. The lateral localization of the electron, i.e., parallel to the metal surface, has been observed by the time-resolved two-photon photoemission experiment.

In the present Letter we study the electron moving near the surface of the metal or dielectric. We show that the interaction with the induced charge leads to the lateral confinement potential acting on the electron. In the existing literature, e.g., papers, the classical potential has been overlooked due to the neglect of the dependence of the induced charge distribution on the electron wave function.

We first formulate a two-dimensional (2D) model for a typical metal-semiconductor planar structure. Next, we extend the model to the three-dimensional (3D) system and compare the results of calculations with the available experimental data. We show that the observed lateral electron localization can be explained by the effect of the induced surface charge without a necessity of taking into account neither the surface corrugation nor the electron-dipol coupling.

We consider a planar structure, in which an electron is confined in the quasi-2D quantum well separated from the metal by a blocking barrier of thickness d. We assume that the quantum well and the barrier are characterized by the same dielectric constant ε. We focus on the properties that are essentially independent of the specific atomic and crystal structure of the materials. Therefore, we assume the idealized model of the metal, which consists of a positive background charge and an arbitrary number of nearly free electrons, and its surface is the infinite plane. The single electron generates the Coulomb field, which induces the positive charge on the metal surface, which in turn acts on the electron changing its quantum state. For our model structure the interaction of the electron with the induced charge can be calculated by the image charge method. We assume that the electron is strongly confined within the quantum well in the normal-to-plane (vertical) direction z and the image charge distribution is a mirror reflection of the electron charge distribution with respect to the metal surface plane (z = 0).

The potential energy of the interaction of the electron with the charged surface can be expressed as

$$W = \frac{\kappa}{2} \int d^3r d^3r' \frac{\varrho_-(r) \varrho_+(r')}{|r - r'|},$$

where prefactor 1/2 accounts for the self-interaction character of the electron-image charge interaction and \(\kappa = 1/4\pi\varepsilon_0\varepsilon\). In Eq. (1), there appear the two spatially separated charge densities: the electron charge density \(\varrho_-(r) = -e|\psi(x, y)|^2\delta(z - d)\) and the image charge density \(\varrho_+(r) = q|\psi(x, y)|^2\delta(z + d)\), where \(e > 0\) is the elementary charge, \(\psi(x, y)\) is the wave function of the electron, and \(q = e\).\)

First, in the framework of the simple 2D model, we perform the variational calculation with the trial wave function chosen in the form

$$\psi(x, y) = (1/\pi^{1/2}l) \exp[-(x^2 + y^2)/2l^2],$$

where variational parameter \(l\) determines the radius of electron localization. For the Gaussian charge densities we can apply the effective interaction potential \(W\) when calculating the potential energy [Eq. (1)]. Expression \(W\) takes on the form (cf. Eq. (19) in Ref. [19])

$$W(l) = -(1/2)(\sigma e q/l) (\pi/2)^{1/2} \text{erf} \text{c}(2^{1/2} d/l).$$

Using wave function \(\psi\) we calculate the expectation value of the total energy \(E(l) = \hbar^2/(2m_l^2) + W(l)\), where \(m_l^2\) is the effective electron mass. Function \(E(l)\),
displayed in Fig. 1 for \( d = a_D \), possesses the pronounced minimum for finite radius of electron localization \( l = 3.61a_D \) with \( E_{\text{min}} = -0.158R_D \), where \( R_D = m_e\hbar^2e^4/(2\hbar^2) \) is the effective donor rydberg and \( a_D = \hbar^2/(m_e\kappa e^2) \) is the effective Bohr radius. The results of Fig. 1 show the existence of the bound state with the lateral electron localization. The electron moves parallel to the interface not as a plane wave but as a wave packet of finite spatial extension in lateral directions. In order to conveniently picture this motion, we find it useful to introduce a new quasi-particle, which we call inducton, since the confinement potential, which forms this wave packet, is generated by the induced charge.

For the stationary states the Hamiltonian of the inducton can be derived from the condition \( \delta((\psi^* T | \psi) + W) / \delta \psi = 0 \), where \( T \) is the kinetic energy operator and \( W = W[\psi^* , \psi] \) is given by (1). We obtain the Hamiltonian of the form \( H = -\hbar^2 \nabla^2 / (2m_e) + U(r||, d) \), where

\[
U(r||, d) = -\kappa eq \int d^2 r' \left| \psi(r') \right|^2 \left[ \frac{1}{[(r|| - r')^2 + 4d^2]^{1/2}} \right] \tag{4}
\]

and \( r|| = (x, y) \). Let us discuss the physical content of Hamiltonian \( H \). Quantity \( U \) [Eq. (4)] is the Hartree potential energy due to the charge induced on the metal (dielectric) surface, but is not the potential energy of the electron, which absolute value is two times smaller [cf. Eq. (1)]. As a result, eigenfunctions \( \psi_n \) of Hamiltonian \( H \) can be identified with the electron wave functions in the inducton states, but the eigenvalues of \( H, E_n \), do not determine the total energy of the system. Instead \( E_n \) possess the same interpretation as the one-electron energies in the self-consistent method, e.g., Hartree-Fock method. We note that one can obtain the same Hartree potential using the quantum linear response theory.

Due to the interaction with the induced charge the electron is not an isolated particle. During the transition between quantum states the induced charge can either transfer its energy to the electron (the transition with full relaxation) or release it partly or fully into the metal (the transitions with partial relaxation or without relaxation). In the first case, we can observe the total energy of the inducton, while in the last case, we can measure the one-particle energy, similarly as in the many-electron system described by the Hartree-Fock method under condition that the Koopmans theorem is satisfied. Figure 2 displays the one-electron lowest energy level, total energy, and radius \( l \) of the inducton. We note that the inducton radius is comparable with \( d \).

The results depicted in Figs. 1 and 2 have been obtained with Gaussian trial wave function (2). In order to check the validity of our choice of wave function (2), we have solved the eigen equation of \( H \) by the numerical self-consistent method on the one-dimensional radial mesh. In the present paper, we limit our attention to the s-like solutions with the rotational symmetry. The numerical procedure yields the results, which can be treated as "exact". We have found (cf. inset of Fig. 1) that the ground-state wave function obtained by the self-consistent procedure is almost the same as the optimum trial wave function [Eq. (2)], which means that the exact ground-state wave function can be very well approximated by the Gaussian of form (2). This proves the consistency of our Gaussian model based on Eq. (2).

The electron motion parallel to the interface can be
described by a plane wave, but then the induced charge density is zero, total energy \( E \geq 0 \), and the inducton states are not formed. In the inducton states with \( E < 0 \), in which the electron wave function is localized, potential \( U \) [Eq. (11)] does not vanish and is attractive. In these states, the momentum of the electron is not defined. The inducton can move in the lateral direction with the non-zero momentum but the electron wave function in the inducton state is a wave packet.

The inductons considered so far were formed in the quantum well; so, they were described as the 2D systems. Let us generalize our approach to the 3D systems. For this purpose we abandon the assumption of the quantum-well confinement and consider the electron moving in the half-space outside the blocking barrier. The electron induces the charge on the metal surface and due to the interaction with the induced charge the 3D wave packet is formed. The system is described by the corresponding 3D Hamiltonian, which has the form of its 2D counterpart with potential energy \( U(\mathbf{r}) = U(\mathbf{r}_\parallel, z) \) resulting from the charge induced on the metal surface and potential of the blocking barrier, i.e., \( U(\mathbf{r}) = \infty \) for \( 0 < z \leq d \), and \( U(\mathbf{r}) \) is given by the 3D version of formula (14) for \( z > d \). The image charge density is the mirror reflection of the electron charge density in the \( z = 0 \) plane, i.e., \( \varrho_{+,n}(\mathbf{r}) = q|\psi_n(x, y, -z)|^2 \).

We expect that the quasi-2D inductons can occur in planar semiconductor nanostructures, which contain the quantum-well layer and are covered by the metal layer. The largest binding energy of the inducton should be observed in semiconductors with small dielectric constant and large electron band mass. Due to the larger valence band mass, the hole inducton should be more stable than the electron inducton.

The 3D inductons can appear in semiconductor structures of the type of the field effect transistor with the isolated gate. Due to the increase of the binding energy with the decreasing blocking barrier thickness, the inductons formed in the structures containing the thin blocking barrier will be the most strongly bound. A possible experimental evidence of such inducton states is within the reach of modern experimental setups.

FIG. 3: Wave functions of the three lowest-energy s-like states plotted as functions of cylindrical coordinates \( r\parallel \) and \( z \).

Assuming the cylindrical symmetry, we solve the corresponding 3D eigenproblem on the 2D mesh \((r\parallel, z)\) by the self-consistent procedure. Figure 3 depicts the s-like wave functions, which correspond to the lowest-energy levels. The ground-state wave function \((n = 1)\), as a function of \( r\parallel \), has the Gaussian shape. The excited-state wave functions \((n = 2, 3)\) clearly exhibit the non-separability of variables \( r\parallel \) and \( z \).

Figure 4 shows that with the increasing blocking barrier thickness the energy levels shift upwards and the interlevel separations decrease. This feature is in a qualitative agreement with the experimental data [8]. We note that the energy levels do not form the hydrogen-like Rydberg series.

However, the so-called image-potential electron states [9] were observed near the metal-vacuum interface. The theoretical interpretation of these states is based upon the notion of Rydberg states [8]. In this interpretation [8], the potential energy of the interaction of the electron with its image charge is assumed in the form \( U_{\text{image}}(z) = -\kappa_{\text{eq}}/(4z) \), which is valid for the classical point charge. In quantum mechanics, the charge density of the electron is determined by a wave function. The image of the spread-out charge is also spread out. The potential energy of the electron should be calculated according to Eq. (11) and the induced potential should depend on lateral position \( r\parallel \) [cf. Eq. (14)]. Potential \( U_{\text{image}} \), used in Refs. [8, 9], corresponds to either the classical particle or the quantum particle with the lateral wave function given by a Dirac delta function. In spite of

FIG. 4: One-electron s-like energy levels calculated with \( \varepsilon = 1 \) as functions of thickness \( d \) of the blocking layer. Inset: Fourier transform of the ground-state inducton wave function (solid curve) vs \( k\parallel \) (in Å\(^{-1}\)). Dots correspond to the experimental data taken from Fig. 4(A) of Ref. [8] for time delay 266 fs.
this the authors use the plane wave for the lateral motion of the electron, which is a serious inconsistency. If the electron travels in the motion of the electron, which is a serious inconsistency. If the electron travels in the $x-y$ plane as the plane wave (cf. Fig. 1 for $l \rightarrow \infty$), its image charge is completely delocalized and the induced potential is zero. This inconsistency is repeated in all the other papers on this subject, e.g., [7, 8].

Based on the results of the present paper, we propose an alternative interpretation of the states observed in Refs. [3, 5]. According to our proposition these findings can be treated as the experimental evidence for the formation of the inducton. To support this interpretation we have calculated the Fourier transform of the ground-state wave function of the inducton. The results (inset of Fig. 4) very well agree with the experimental data. Using the results of Fig. 4 for $d = 0$, we have calculated the energy differences $\Delta_{mn} = E_m - E_n$ between the one-particle energy levels and compared them with the experimental data. The calculated (measured) energy differences are $\Delta_{21} = 0.41 (0.43)$ eV, $\Delta_{41} = 0.49 (0.50)$ eV, and $\Delta_{41} = 0.54 (0.56)$ eV (energy separation $\Delta_{21}$ estimated from Ref. [3] is 0.45 eV). We see that the agreement with experiment is very good. The fact that the one-particle energy levels are observed in experiments can result from the slow relaxation of the induced charge during the photoemission. We note that the present model is valid if the electron does not penetrate the metal, i.e., if the metal surface is covered by a thin dielectric layer. This condition is satisfied in the experiments.

In summary, we have shown that the charge induced on the metal (dielectric) surface by the nearby electron creates the lateral confinement potential, which in turn leads to the lateral localization of the electron. The collective electron-induced-charge motion can be conveniently described with the help of the new quasi-particle, the inducton. According to the reinterpretation we have proposed the localized states observed near the metal surface are the inducton states. The electron described by the plane wave does not generate any induced charge potential. The plane-wave states can only be created if the excitation energy is larger than the continuum-energy threshold. The electron localization in the vertical direction is only possible if the lateral electron localization occurs. Electrons states which are not laterally localized cannot be bound to the metal surface.

We expect the inducton states to be universal for the charge carriers moving near the metal or dielectric surfaces and should observed at the metal-vacuum and dielectric-vacuum interfaces as well as in semiconductor nanostructures.

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