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Chapter 1

QUANTUM STATE DEPRESSION IN A QUANTUM WELL OF SPECIAL GEOMETRY

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ABSTRACT

Changes in the quantum well properties caused by periodic ridges in the surface were studied within the limit of quantum theory of free electrons. The authors show that due to destructive interference of de Broglie waves, some quantum states become quantum mechanically forbidden for free electrons. Wave-vector density in k space is reduced dramatically.

At the same time the number of free electrons does not change considerably, as the metal remains electrically neutral. Because of the Pauli exclusion principle, some free electrons must occupy quantum states with higher wave numbers. The Fermi vector and Fermi energy of quantum well increase, and consequently, the work function decreases. Resent experiments are in qualitative agreement with the presented theory.

This effect could exist in any quantum system comprising fermions inside a potential-energy box of special geometry.

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1. INTRODUCTION

Recent developments of nanoelectronics enable the fabrication of structures with dimensions comparable to the de Broglie wavelength of a free electron inside a solid. This new technical capability makes it possible to fabricate some microelectronic devices such as resonant tunneling diodes and transistors, superlattices, quantum wells (QW), and others [1] based on the wave properties of the electrons. In this article, we discuss what happens when regular ridges, which cause interference of de Broglie waves, are fabricated on the surface of a QW layer. We will study the free electrons inside a rectangular potential-energy box with ridged wall and compare the results to the case of electrons in a box with plane walls. We have shown that modifying the wall of a rectangular potential-energy box leads to an increase of the Fermi energy level. Results obtained for the potential-energy box were extrapolated to the case of QW layers.

2. ELECTRONS IN A POTENTIAL-ENERGY BOX WITH A RIDGED WALL

We begin with the general case of electrons inside a potential-energy box. Assume a rectangular potential-energy box with one of the walls modified as shown in Figure 1. Let the potential energy of the electron inside the box volume be equal to zero, and that outside the box volume be equal to infinity. The ridges on the wall have the shape of strips having depth a and width w. Let us name the box shown on Figure 1 as ridge potential-energy box RPEB to distinguish it from the ordinary potential-energy box PEB having plane walls. The time independent Schrödinger equation for electron wave function inside the PEB has the form

$$\nabla^2\Psi + (2m/\hbar^2)E\Psi = 0 \qquad (1)$$

Here, Ψ is the wave function of the electron, m is the mass of the electron, and E is the energy of the electron. Let us rewrite Eq. (1) in the form of the Helmholtz equation,

$$(\nabla^2 + k^2)\Psi = 0 \qquad (2)$$

where k is wave vector, $k = \sqrt{2mE}/\hbar$. Once the ridge depth a in our particular case is supposed to be much less than the thickness of the metallic film $a << L_x$, we can use the volume perturbation method to solve the Helmholtz equation [2].

The idea is as follows: The whole volume is divided in two parts, the main volume MV and the additional volume AV. The MV is supposed to be much larger than the AV, and it defines the form of solutions for the whole composite volume. Next, solutions of the composite volume are searched in the form of solutions of the MV. The method is especially effective in the case where the MV has a simple geometry, for example, a rectangular geometry, allowing separation of the variables. In our case, the whole volume in Figure 1 can be divided in two, as shown in Figure 2. We regard the big rectangular box as the MV and the total volume of strips as the AV. The MV has dimensions L_x, L_y, and L_z. The solutions of Eq. (2) for such a volume are well known. Because of the rectangular shape, solutions are found by using the method of separation of variables. The solutions are plane waves having a discrete spectrum,

$$\mathrm{k}_n^{mx} = \pi n / L_x,\ \mathrm{k}_j^{my} = \pi j / L_y,\ \mathrm{k}_i^{mz} = \pi i / L_z \qquad (3)$$

Here, k^{mx}, k^{my} and k^{mz} are the x, y, and z components of wave vectors of the MV and n,m, i=1,2,3,... In the same manner the spectrum of the single strip of the AV is the following:

$$\mathrm{k}_p^{ax} = \pi p / a,\ \mathrm{k}_q^{ay} = \pi q / w,\ \mathrm{k}_i^{az} = \pi i / L_z \qquad (4)$$

k^{ax}, k^{ay} and k^{az} are components of wave vectors of one strip of AV, p,q=1,2,3,..., and a and w are dimensions of the strip, as shown on Figure 2. Analysis conducted in [3] shows that wave vector spectrum of RPEB is

$$\mathrm{k}^{x}{}_{p}=\pi p/a,\ \mathrm{k}^{y}{}_{q}=\pi q/w,\ \mathrm{k}^{z}{}_{i}=\pi i/L_z \qquad (5)$$

and is equal to the spectrum of a single strip Eq. (4). In the Eq. (5), we skip some working indices used in this section to simplify the presentation.

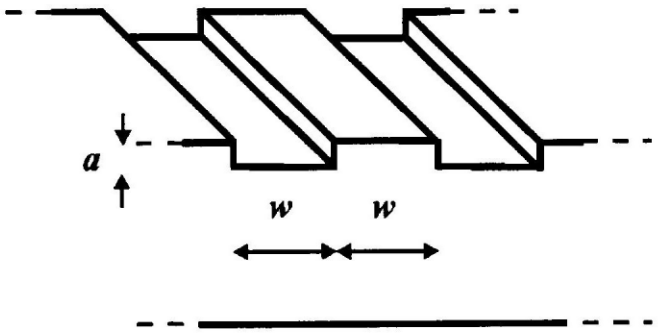

Figure 1. 3D view of ridged potential-energy box.

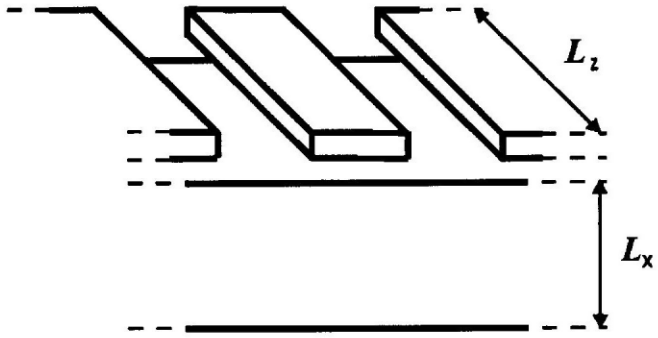

Figure 2. Potential-energy box with ridged wall divided into two volumes.

Equation 5 is obtained using the volume perturbation method for solving of the Helmholtz equation. This method assumes that the AV is much less than the MV $(a/2L_x)<<1$. Special attention should be paid to the limit of very low a and w. The case a, $w\rightarrow 0$ has the following physical interpretation. Standing waves in the MV ignore the AV because of wave diffraction on it. If we assume that the wave ignores nonregularities with dimensions less than its wavelength, we must make the following corrections in Eq. (5). It is valid for $k^x > 2\pi/a$ and $k^y > 2\pi/w$ for p, q=2, 3, 4.... For the range $0<k^x<2\pi/a$ and $0<k^y<2\pi/w$, Eq. (3) should be used for RPEB instead of Eq. (5). In practice, dimensions a, w are such that only the first few k should be added to Eq. (5).

For the case of large $a/2L_x$, other methods were used. The general solution of Eq. (2) in such a complicated geometry exhibits several problems. A complicated surface shape does not allow to find an orthogonal coordinate system that will allow to separate the variables. Therefore, boundary conditions may be written only in the form of piecewise regular functions. A

general solution of Eq. (2) usually contains infinite sums. However, there are methods [2] that allow one to obtain a dispersion equation and to calculate the wave vector. The Helmholtz equation is frequently used for calculating the electromagnetic field in electromagnetic resonator cavities, waveguides, and delay lines. We found the following similarities between the electron wave-function inside the RPEB and electromagnetic field inside electromagnetic delay lines. First, our geometry matches the geometry of a corrugated waveguide delay line [4] . Second, the same Eq. (2) is used to describe both cases. Third, the boundary condition for the electromagnetic wave inside the corrugated waveguide ϵ=0 (here, ϵ is the electric component of the electromagnetic wave) for walls of a conductive waveguide exactly matches the boundary condition for electrons, Ψ=0 outside the metal. Fourth, any wave can be presented as the sum of plane waves in both cases. We also found that similar analogies are described in the literature [5]. Therefore, for the case of high a, we used the method of solving the Helmholtz equation inside the corrugated waveguides. This method is based on solving a transcendental equation. We found numerical solutions for the transcendental equation for high $a/2L_x$ and obtained the same result, namely, the reduction of the spectrum density for RPEB relative to PEB.

For very thin layers $L_z >> L_x$, w, it is expected that our structure will not exhibit quantum features in the Z direction. Therefore, it is reasonable to consider a model of the electron motion in a two-dimensional (2D) region delimited by the line X=0 from one side, and a periodic curve on the opposite side. In that case, we can consider the 2D Helmholtz equation and use special methods to solve. Specifically, we used the Boundary Integral Method (BIM), which is especially effective for the low-energetic part of the spectrum and has been widely employed for studying 2D nano systems [6].

The BIM method implies consideration of an appropriate integral equation instead of the Helmholtz equation. We have applied the corresponding numerical algorithm [7] to a finite number of periods and calculated the lowest few ten energy levels. We note that computation of higher energy levels with reasonable accuracy demands rapidly increasing machine-time. The obtained spectrum of transverse wave vectors also shows a reduction in spectral density.

At the end of this section, it is worth to note that the above-discussed effect of the energy-spectrum reduction is closely related to the so-called Quantum Billiard Problem. The 2D system studied represents a modification of the quantum billiard problem. Unlike the circle and rectangular billiards, the corrugated boundary makes the system under consideration non-integrable. This means that the number of degrees of freedom exceeds the number of

constants of motion. Such billiards constitute chaotic systems. The distinction between the spectra of chaotic and non-chaotic (regular) systems is exhibited by an energy level spacing distribution [7, 8]. Namely, consecutive energy levels are likely to attract each other in the case of an integrable system, whereas they repel each other in the case of a chaotic system.

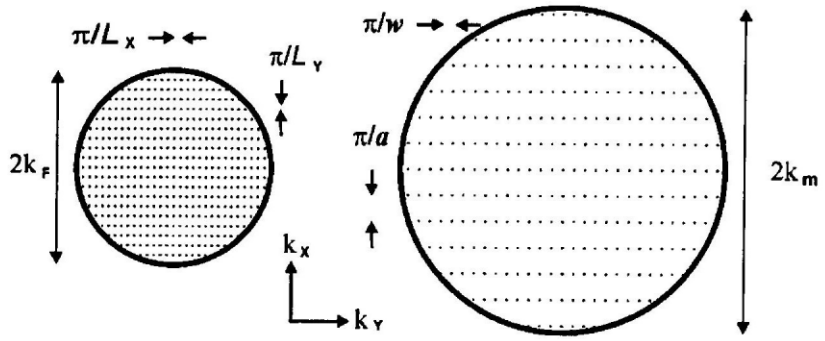

Figure 3. Section of Fermi sphere is *k* space for PEB (left) and RPEB (right). Points denote quantum states for free electron.

3. Free Electrons in Metal Layer with Ridged Surface

To investigate how periodic ridges change quantum states inside the thin metal layer, we will use a quantum model of free electrons. Free electrons inside the metal form a Fermi gas. Cyclic boundary conditions of Born-Carman,

$$k^x{}_n = 2\pi n/L_x,\ k^y{}_j = 2\pi j/L_y,\ k^z{}_i = 2\pi i/L_z, \qquad (6)$$

are used instead of Eq. (3). Here, $n, j, i=0, \pm1, \pm2, \pm3...$ The result of the theory is a Fermi sphere in k space. All possible quantum states are occupied below k_F at T=0. However, for T>0, there are two types of free electrons inside the Fermi gas. Electrons with $k \approx k_F$ interact with their environment and define the transport properties of metals such as charge and heat transport. Electrons with $k << k_F$ do not interact with the environment because all quantum states nearby are already occupied by other electrons (it becomes forbidden to exchange small amounts of energy with the environment).

Such electrons are ballistic and have formally infinite mean free path. This feature allows us to regard them as planar waves, traveling between the walls of the metal (if the distance between walls is not too great). Further, we will concentrate on such ballistic electrons.

Once we work with electrons with infinite (or very long) mean free paths, we can regard the metal layer as a potential-energy box and extrapolate calculations of the previous section to it.

We start by comparing the volume of an elementary cell in k space for thin metal films with and without periodic ridges. From Eq. (5) and Eq. (6), we have:

$$dV_k=8\pi^3/(L_xL_y L_z) \text{ and } dV_{km}=8\pi^3/(awL_z) \quad (7)$$

Here, dV_k is the volume of an elementary cell in k space for a plain film, and dV_{kin} is the volume of an elementary cell in k space for an ridged film. Further, we find maximum wave vector and Fermi energy as in reference [3]

$$k_m= k_F [L_y(L_x +a/2)/(aw)]^{1/3} . \quad (8)$$

$$E_m=E_F[L_y(L_x +a/2)/(aw)]^{2/3} \quad (9)$$

If we assume $a<<L_x$, Eq. (9) can be rewritten in the following simple form:

$$E_m=E_F(L_xL_y /aw)^{2/3} . \quad (10)$$

The dimensional quantum effects in ultra-thin metal films, using a rectangular potential-box model and quantum model of free electrons, were studied in Ref. [9]. Quantum state depression in metal films was investigated experimentally in Ref. [10]. Quantum state depression in semiconductor ridged quantum well was investigated theoretically in Ref. [11].

CONCLUSIONS

To investigate a new quantum interference effect in metal layers, we studied the behavior of free electrons in the potential-energy box of special geometry. It was shown that when periodic ridges are introduced in the plain wall of a rectangular potential-energy box, the spectrum density of possible

solutions of the Schrödinger equation is reduced dramatically. Once the number of possible quantum states decreases, electrons must occupy higher energy levels because of the Pauli exclusion principle. Results obtained for electrons in the modified potential-energy box were extrapolated to the case of the free ballistic electrons inside the metal film. The electron distribution function changes. Fermi energy increases, and consequently, work function decreases. Recent experiments demonstrate quantitative agreement with the theory. Increase in the Fermi level and the corresponding decrease of the work function of the thin films will have practical use for devices working on the basis of electron emission and electron tunneling. In addition, such layers will be useful in the semiconductor industry, particularly for the structures in which contact potential difference between two layers plays an important role.

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