Fermi gas energetics in low-dimensional metals of special geometry

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Changes in the metal properties caused by periodic indents in the metal 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 inside the low-dimensional metal 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, 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 low-dimensional metal increase, and consequently, the work function decreases. In the experiment, the magnitude of the effect is limited by the roughness of the metal surface. A rough surface causes scattering of the de Broglie waves and compromises their interference. Recent experiments demonstrated a reduction of work function in thin metal films having periodic indents in the surface. Experimental results are in good qualitative agreement with the theory. This effect could exist in any quantum system comprising fermions inside a potential-energy box of special geometry. [DOI: 10.1116/1.2753852]

I. 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, and others[1] based on the wave properties of the electrons. In this article, we discuss what happens when regular indents, which cause interference of de Broglie waves, are fabricated on the surface of a thin metal film. We will study the free electrons inside a rectangular potential-energy box with indented 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 low-dimensional metals (thin metal films). The experimental possibility of fabricating such indents on the surface of a thin metal film was studied. Practical recommendations regarding dimensions and shape of the indents are given. In addition, the influence of non-regularities of thin metal films, such as the presence of granules inside the film and the roughness of surface of the film, was studied.

II. ELECTRONS IN A POTENTIAL-ENERGY BOX WITH AN INDENTED 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 Fig. 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 indents on the wall have the shape of strips having depth a and width w. Let us name the box shown on Fig. 1 as indented potential-energy box (IPEB) 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

$$\nabla^2\Psi + (2m/\hbar^2)E\Psi = 0. \tag{1}$$

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,

$$(\nabla^2 + k^2)\Psi = 0, \tag{2}$$

where k is wave vector, $k=\sqrt{2mE}/\hbar$.

Once the indent depth a in our particular case is supposed to be much less than the thickness of the metallic film $a \ll L_x$, 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 Fig. 1 can be divided in two, as shown in Fig. 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,

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