

# Calculation of the Fermi wave vector for thin films, quantum wires and quantum dots

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A comparison of the construction of the Fermi surface for thin films, quantum wires and quantum dots has been made within the framework of the free-electron model. The dependence of the Fermi wave vector on the confined size of low-dimensional systems has been numerically obtained for the model, with some experimental parameters corresponding to Cu structure.

Key words: *thin film; quantum wire; quantum dot; Fermi surface*

## 1. Introduction

Various physical properties of bulk materials can be illustratively and relatively simply discussed within the framework of the free-electron model [1, 2]. On the other hand, low-dimensional systems (LDS) play an important and continuously growing role in contemporary science and technology [3–6]. Therefore, in order to discuss the physical properties of LDS, i.e. thin films (TF), quantum wires (QWr), and quantum dots (QD), it is important in the first approximation to have an extension of the free-electron model for confined structures. In such considerations, the quantum-mechanical description, and in particular the concept of a quantum well, plays a crucial role [4, 7].

The aim of this paper is to perform some model calculations of the Fermi wave vector in the framework of the free-electron approximation for the low-dimensional systems (TF, QWr, and QD). In the theoretical section, the formulae suitable for numerical calculation of the Fermi wave vector  $k_F$  for TF, QWr, and QD are given. In the final section, some tentative numerical results are presented for the model LDS with the electronic density corresponding to Cu and (100)-type surface orientation. A wider presentation of the results for TF has been given elsewhere [8].

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## 2. Theoretical model

A thin film is considered to be a set of  $n$  monoatomic planes, perpendicular to the  $z$  axis, with each plane having its own thickness  $d$  dependent on crystallographic orientation. As a result, the total thickness of the film is given by  $L_z = nd$ . The lateral dimensions of the film in the  $x$  and  $y$  directions are denoted by  $L_x$  and  $L_y$ , respectively, and it is assumed that these dimensions tend to infinity. Thus, the model corresponds to a 1-dimensional quantum well, in which one-electron states are described by the normalized wave function:

$$\varphi_{k_x, k_y, \tau_z}(x, y, z) = \frac{1}{\sqrt{L_x L_y}} e^{i(k_x x + k_y y)} \sqrt{\frac{2}{L_z}} \sin\left(\frac{\pi \tau_z z}{L_z}\right) \quad (1)$$

The function represents a plane wave propagating in the  $(x, y)$  plane, with quasi-continuous wave vector components  $k_x$ ,  $k_y$  and periodic boundary conditions as well as a standing wave in the  $z$ -direction that vanishes at the film surface and has a discrete wave vector  $k_z = \pi \tau_z / L_z$ , where  $\tau_z = 1, 2, \dots$  is a mode number.

In the case of quantum wires, we deal with a 2-dimensional quantum well with lateral dimensions of  $L_y = md$  and  $L_z = nd$ , and  $L_x$  tending to infinity. Thus, in such a case two components of the wave vector ( $k_y$  and  $k_z$ ) are quantised, with corresponding  $\tau_y, \tau_z = 1, 2, \dots$  and the pairs  $(\tau_y, \tau_z)$  numbering the 2-dimensional standing modes. Simultaneously, in a QWr the plane wave is propagating in the  $x$ -direction.

For a quantum dot we assume a 3-dimensional quantum well model represented by a box, having the lateral dimensions  $L_x = pd$ ,  $L_y = md$ , and  $L_z = nd$ , in which only standing waves exist. A triple of natural numbers  $(\tau_x, \tau_y, \tau_z)$  unambiguously describes a 3-dimensional standing wave mode in the quantum well.

The construction of the Fermi surface and the Fermi wave vector  $k_F$  is schematically shown in Fig. 1. In Figure 1a, the occupied electronic states for TF are shown, forming circular cross-sections from a bulk Fermi sphere, perpendicular to the  $k_z$  axis and separated by distances of  $\pi/L_z$ . In Figure 1b, the occupied electronic states for a QWr are presented by the bold segments, oriented parallel to the  $k_x$  axis and separated in the  $k_y$  and  $k_z$  dimensions by  $\pi/L_y$  and  $\pi/L_z$ , respectively. Finally, in Figure 1c the occupied electronic states for a QD are depicted by the bold points with the coordinates  $(\tau_x, \tau_y, \tau_z)$ . The points are separated by distances of  $\pi/L_x$ ,  $\pi/L_y$ , and  $\pi/L_z$ , in the  $k_x$ ,  $k_y$ , and  $k_z$  directions, respectively. All the electronic states are contained within a sphere possessing a  $k_F$  radius. The surface of the sphere has a constant energy, whereas the quantization of the wave vector and the Pauli exclusion principle are taken into account in the occupation scheme.

For a TF, the analytical formula can be derived for the Fermi wave vector  $k_F$  [8] :

$$(k_F d)^2 = 2\pi\rho \frac{n}{\tau_F} + \frac{\pi^2}{6n^2} (\tau_F + 1)(2\tau_F + 1) \quad (2)$$

where  $n$  corresponds to the thickness of the film and  $\rho$  is a dimensionless electronic density defined by the formula  $\rho = N_e d^3 / L_x L_y L_z$ , where  $N_e$  is the total number of electrons in the sample. By  $\tau_F$  in Eq. (2) we denote the largest natural number satisfying the inequality:

$$\rho \geq \pi \tau_F (\tau_F - 1) \frac{\left(2\tau_F + \frac{1}{2}\right)}{6n^3}$$

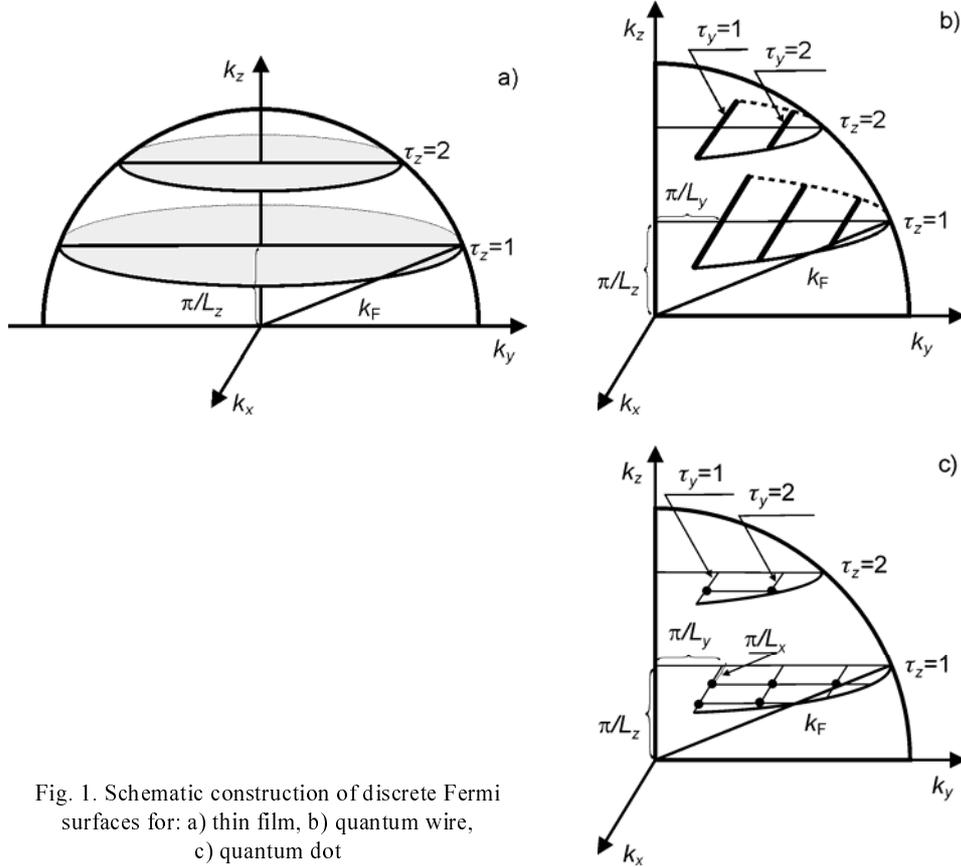


Fig. 1. Schematic construction of discrete Fermi surfaces for: a) thin film, b) quantum wire, c) quantum dot

In the case of a QWr, the Fermi wave vector is found to be of the form:

$$\pi \rho_{mn} = 2 \sum_{\tau_y} \sum_{\tau_z} \sqrt{(k_F d)^2 - \left(\frac{\pi \tau_y}{m}\right)^2 - \left(\frac{\pi \tau_z}{n}\right)^2} \quad (3)$$

where summation over the natural numbers  $\tau_y$  and  $\tau_z$  should be done numerically. When performing the summation, the upper limits for  $\tau_y$  and  $\tau_z$  are imposed by a simple requirement that the expression under the square root in Eq. (3) must not be negative.

For a QD, the formula for  $k_F$  is the following :

$$\rho p m m = 2 \sum_{\tau_x} \sum_{\tau_y} \sum_{\tau_z} 1 \quad (4)$$

where summation over the natural numbers  $\tau_x$ ,  $\tau_y$ , and  $\tau_z$  should be performed numerically with the boundary condition:  $(k_F d)^2 \geq (\pi \tau_x / p)^2 + (\pi \tau_y / m)^2 + (\pi \tau_z / n)^2$ , determining the radius of summation.

### 3. Numerical results and discussion

Numerical results have been obtained for a prototype crystalline structure and electron density corresponding to Cu, i.e.  $N_c / L_x L_y L_z = 0.085 / \text{\AA}^3$ , and a (100)-type LDS surfaces. Thus, the interplanar distance is equal to  $d = a/2 = 1.805 \text{ \AA}$ , whereas the dimensionless electronic density  $\rho$  is 0.5. The choice of copper is connected to the view that the Fermi surface for this metal is quite similar to a spherical surface [9], therefore our model is more realistic than for other metals.

The results of calculation of the Fermi wave vector  $k_F$  are shown in Fig. 2. In Figure 2a, a decreasing tendency of  $k_F$  with increasing thickness of the film  $n$  is seen ( $n$  is the number of atomic planes). The bulk value of  $k_F$  for Cu is  $1.360 \text{ \AA}^{-1}$ , being the limit for  $k_F$  when  $n \rightarrow \infty$ . The results of calculation of  $k_F$  for a QWr are presented in Fig. 2b, versus the wire width  $m$  for three selected thicknesses:  $n = 1$ ,  $n = 2$ , and  $n = 5$ . It can be seen in Fig. 2b that the most rapid changes occur for the smallest values of  $m$  and  $n$ . In Figure 2b, the limiting values of  $k_F$  for  $m \rightarrow \infty$  are also depicted by the values corresponding to the results for thin films for a given  $n$  (compare with Fig. 2a).

In turn, the Fermi wave vector  $k_F$  is plotted in Fig. 2c versus the length of the QD  $p$ . Two cases are illustrated – the upper curve (for  $m = n = 1$ ) at the  $p \rightarrow \infty$  limit corresponds to the QWr result (compare with Fig. 2b for  $m = 1$  and  $n = 1$ ), and the lower curve (for  $m = n = p$ ) describes a cubic QD. The limit for the lower curve when  $p \rightarrow \infty$  corresponds to the bulk material and has the same value as in Fig. 2a.

It follows from the calculations that this simple extension of the free electron model for LDSs leads to interesting and important results, induced only by size quantization. It has been checked that by increasing the sizes of the confined structures the results for  $k_F$  become convergent. For instance, when tending with successive sizes to infinity, the results for a QD at first approach the QWr results, which in turn tend to TF results in the limit of the next infinite size. Calculations of the Fermi wave vector should be regarded as useful, since they are necessary for obtaining information about the density of states at the Fermi level, which in turn determines the electronic properties of LDSs.

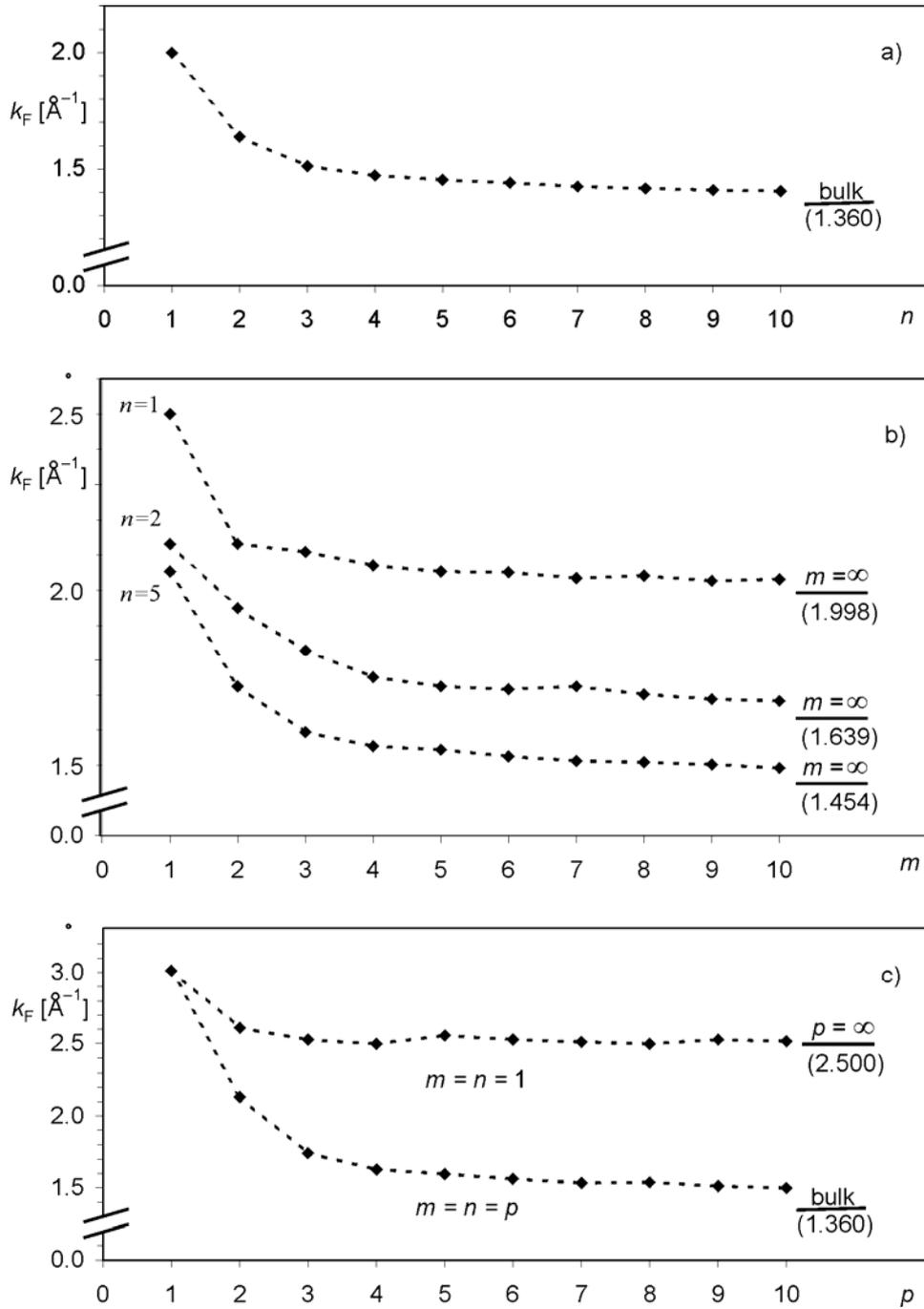


Fig. 2. The Fermi wave vector,  $k_F$ , calculated for experimental parameters corresponding to the electronic density and (100) interplanar distances of Cu: a)  $k_F$  for a TF vs. thickness  $n$ , b)  $k_F$  for a QWr vs. the wire width  $m$ , c)  $k_F$  for a QD vs. the dot length  $p$

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