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CONNECTION BETWEEN THE DISPERSION RELATION, SURFACES OF CONSTANT ENERGY, AND ENERGY BANDS IN SOLIDS

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Connection Between the Dispersion Relation, Surfaces of Constant Energy, and Energy Bands in Solids

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ABSTRACT

The aim of this paper is to exhibit the relationship, for free electrons in two dimensions, between the dispersion relation $\varepsilon = \varepsilon(\underline{k}) = (\hbar^2/2m)(k_x^2 + k_y^2)$, the contours of constant energy, and energy band structures in various directions. It has been found that these results, while well known, are not usually interconnected and presented together for the student.

I. INTRODUCTION

Students in solid state physics courses usually are exposed to energy-wave vector relations $\varepsilon = \varepsilon(\underline{k})$ for electrons in solids, to constant energy surfaces (particularly the Fermi surface) and to energy band structures. However, it is sometimes not clear to the students what the connection between these concepts is, and how the information contained in the various results fits together.

In teaching a one-quarter course in introductory solid state physics in this Department, the author prepared a few pages of notes whose aim was the explanation of the interconnection of these concepts. Although the material in these notes is well known, it is not usually presented to the student in one place, and the connections between the various concepts are not usually emphasized. In particular, Figure 1, while of obvious content, does not appear in any text known to the author; this figure has proved very useful to students in the course.

II. FREE ELECTRONS IN TWO DIMENSIONS

For simplicity and clarity of presentation, the results displayed are limited to the simple case of free electrons in a two dimensional square lattice of lattice constant a.

For a two-dimensional free electron gas, the relation between energy and wave vector (the dispersion relation) is given by

$$\varepsilon(\underline{k}) = (\hbar^2/2m)(k_x^2 + k_y^2). \quad (1)$$

In equation (1), ε is the electron energy, m is the free electron mass, $\hbar$ is Planck's constant divided by 2π, (k_x,k_y) are the cartesian components of the two-dimensional wave vector

$$\underline{k} = k_x\hat{k}_x + k_y\hat{k}_y , \quad (2)$$

and $\hat{k}_x$ and $\hat{k}_y$ are orthogonal unit vectors in the two-dimensional k-space under consideration.

If one plots Equation (1) in a three-dimensional space whose coordinates are (ε,k_x,k_y), the result is a circular paraboloid as shown in Figure 1. This figure shows the (k_x,k_y) plane with $\varepsilon(\underline{k})$plotted as a function of k_x and k_y. The basal plane, in which the k_x and k_y axes lie, is the plane of zero energy $\varepsilon = 0$. The first Brillouin Zone of the square lattice

$$(-\pi/a) \leqslant k_y \leqslant (\pi/a); \; (-\pi/a) \leqslant k_x \leqslant (\pi/a), \quad (3)$$

is a square of side $(2\pi/a)$ in (k_x,k_y) space and is shown drawn on the basal plane $\varepsilon = 0$. The second Brillouin Zone is also drawn on the basal plane. In Figure 1, any plane normal to the ε-axis is a plane of constant energy. The curve which is the intersection of any plane

$$\varepsilon = \text{constant} \equiv \varepsilon_1$$

with the circular paraboloid

$$\varepsilon = (\hbar^2/2m)(k_x^2 + k_y^2)$$

is a contour of constant energy. These contours are the two-dimensional analogs of the surfaces of constant energy for a three-dimensional lattice. For this free electron case, the contour of constant energy $\varepsilon = \varepsilon_1$ is a circle whose equation is

$$\varepsilon_1 = (\hbar^2/2m)(k_x^2 + k_y^2)$$

or, alternatively,

$$k_x^2 + k_y^2 = (2m\varepsilon_1/\hbar^2).$$

The circle marked A in Figure 1 is such a contour of constant energy, and has a radius $k_1 = (2m\varepsilon_1/\hbar^2)^{1/2}$.

If the plane of constant energy is the particular plane whose equation is

$$\varepsilon = \varepsilon_F ,$$

where ε_F is the Fermi energy, then the resulting contour of constant energy is the circle whose equation is

$$k_x^2 + k_y^2 = (2m\varepsilon_F/\hbar^2).$$

This circle is the two-dimensional Fermi "surface" in the problem, and is the analog of the familiar Fermi sphere for free electrons in three dimensions. The radius of the Fermi circle is the Fermi wave vector

$$k_F = (2m\varepsilon_F/\hbar^2)^{1/2}.$$

Figure 1 also shows the first and second Brillouin Zones drawn on the plane $\varepsilon = \varepsilon_F$, which is parallel to the basal plane $\varepsilon = 0$. We may look at three circles of constant energy which are the intersections of three different planes of constant energy with the dispersion relation paraboloid $\varepsilon = (\hbar^2/2m)(k_x^2 + k_y^2)$. Figure 2 shows, within and without the first Brillouin Zone, circles of constant energy $\varepsilon = 0$, $\varepsilon = \varepsilon_1$, and $\varepsilon = \varepsilon_F$. The constant energy circle for $\varepsilon = 0$ is (Figure 2(a)) a single point, that at which the dispersion relation paraboloid is tangent to the basal plane. The circle of constant energy $\varepsilon = \varepsilon_1$ (Figure 2(b)) has a radius k_1, and lies completely within the first Brillouin Zone. However, the Fermi circle of radius k_F is seen to overlap into the second Brillouin Zone, the boundaries of which are drawn in Figure 2(c).

The energy bands for this system of free electrons in two dimensions are the curves of intersection of the dispersion relation

$$\varepsilon = (\hbar^2/2m)(k_x^2 + k_y^2)$$

with any plane containing the energy ε axis. Such a plane P will be normal to the planes of constant energy. The curve of intersection of the dispersion relation will be a curve $\varepsilon = \varepsilon(\underline{k}')$, where $\underline{k}'$ is parallel to the plane P. The curve $\varepsilon = \varepsilon(\underline{k}')$ is called the energy band structure in the direction $\underline{k}'$.

For example, the plane $k_y = 0$, which is parallel to the k_x-axis and contains the energy axis, intersects the dispersion relation paraboloid in the curve

$$\varepsilon = (\hbar^2/2m)k_x^2 , \qquad (4)$$

as shown in Figure 3. In this example, the plane P is the plane $k_y = 0$ and the direction $\underline{k}'$ is the k_x direction. The curve given by equation (4) and shown in Figure 3 exhibits the energy ε as a function of k_x and is the energy band structure, for two dimensional free electrons, in the k_x direction, as displayed in the extended zone scheme.

If we examine the intersection of the dispersion relation with another plane containing the energy axis, we obtain the energy band structure in another direction. Figure 4 shows the intersection of the dispersion relation paraboloid with the plane $k_x = 0$, giving the curve

$$\varepsilon = (\hbar^2/2m)k_y^2$$

as the energy band structure in the k_y direction as shown in the extended zone scheme.

A final example is given by the intersection of the dispersion relation parabaloid with the plane, specified by $k_x = k_y$, which contains a diagonal of the first Brillouin Zone. Let

$$\underline{k}_o = k_o \hat{k}_o$$

be the wave vector in the direction specified by $k_x = k_y$, where

$$\hat{k}_o = \frac{1}{\sqrt{2}} (\hat{k}_x + \hat{k}_y)$$

is a unit vector in that direction. Then the magnitude

$$k_o = k_x\sqrt{2} = k_y\sqrt{2}.$$

The equation of the curve of intersection, on substituting $k_x = k_y = (k_o/\sqrt{2})$ into the dispersion relation $\varepsilon = (\hbar^2/2m)\ (k_x^{\ 2} + k_y^{\ 2})$, is

$$\varepsilon = (\hbar^2/2m) k_o^{\ 2}.$$

The edge of the Zone in the $\underline{k}_o$ direction is the point

$$k_x = (\pi/a);\ k_y = (\pi/a),$$

which, as shown in Figure 6, is a corner of the first Zone. The magnitude of the wave vector at a Zone corner is $k_o = (k_x\sqrt{2}) = (\pi\sqrt{2}/a)$, as indicated in Figure 5.

For this case of free electrons, the energy bands in all directions (i.e., intersections of the dispersion relation paraboloid with all planes containing the energy axis) are parabolas. The energy is parabolic in the wave vector for all directions. For free electrons, the energy bands are always parabolic.

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FIGURE CAPTIONS

Figure 1: The dispersion relation paraboloid $\varepsilon = (\hbar^2/2m)(k_x^2 + k_y^2)$ intersecting planes of constant energy to give constant energy contours.

Figure 2: Contours of constant energy for several values of the energy ε: (a)$\varepsilon = 0$; (b)$\varepsilon = \varepsilon_1$; (c)$\varepsilon = \varepsilon_F$.

Figure 3: The band structure in the k_x direction is the curve $\varepsilon = (\hbar^2/2m)k_x^2$, which is the intersection of the plane $k_y = 0$ with the dispersion relation paraboloid.

Figure 4: The band structure in the k_y direction is the curve $\varepsilon = (\hbar^2/2m)k_y^2$, which is the intersection of the plane $k_x = 0$ with the dispersion relation paraboloid.

Figure 5: The band structure in the direction $k_o = k_x\sqrt{2} = k_y\sqrt{2}$ is the curve $\varepsilon = (\hbar^2/2m)k_o^2$, which is the intersection of the plane specified by $k_x = k_y$ with the dispersion relation paraboloid.

Figure 6: First Brillouin Zone of the square lattice of lattice constant a.

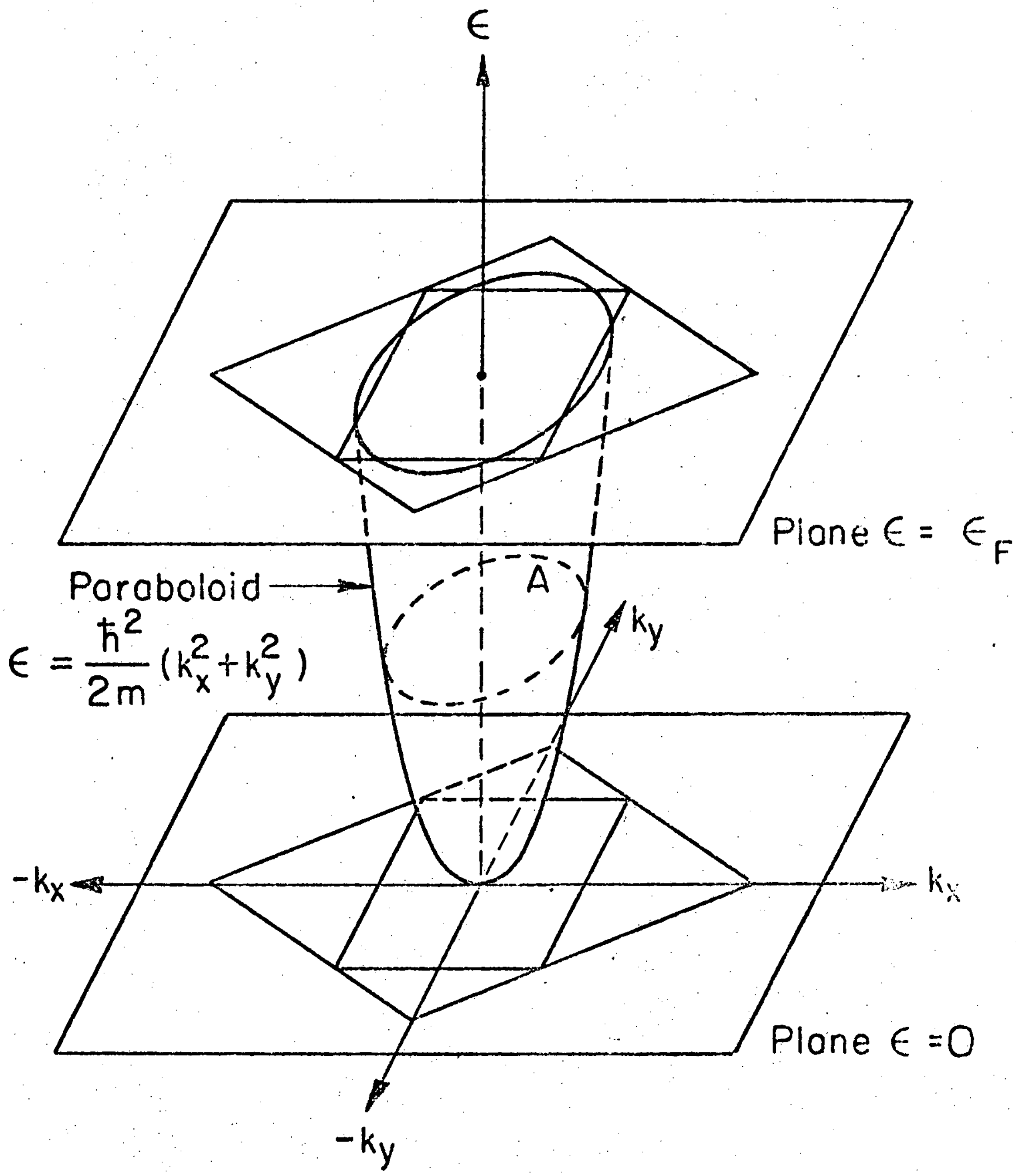

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Fig. 1

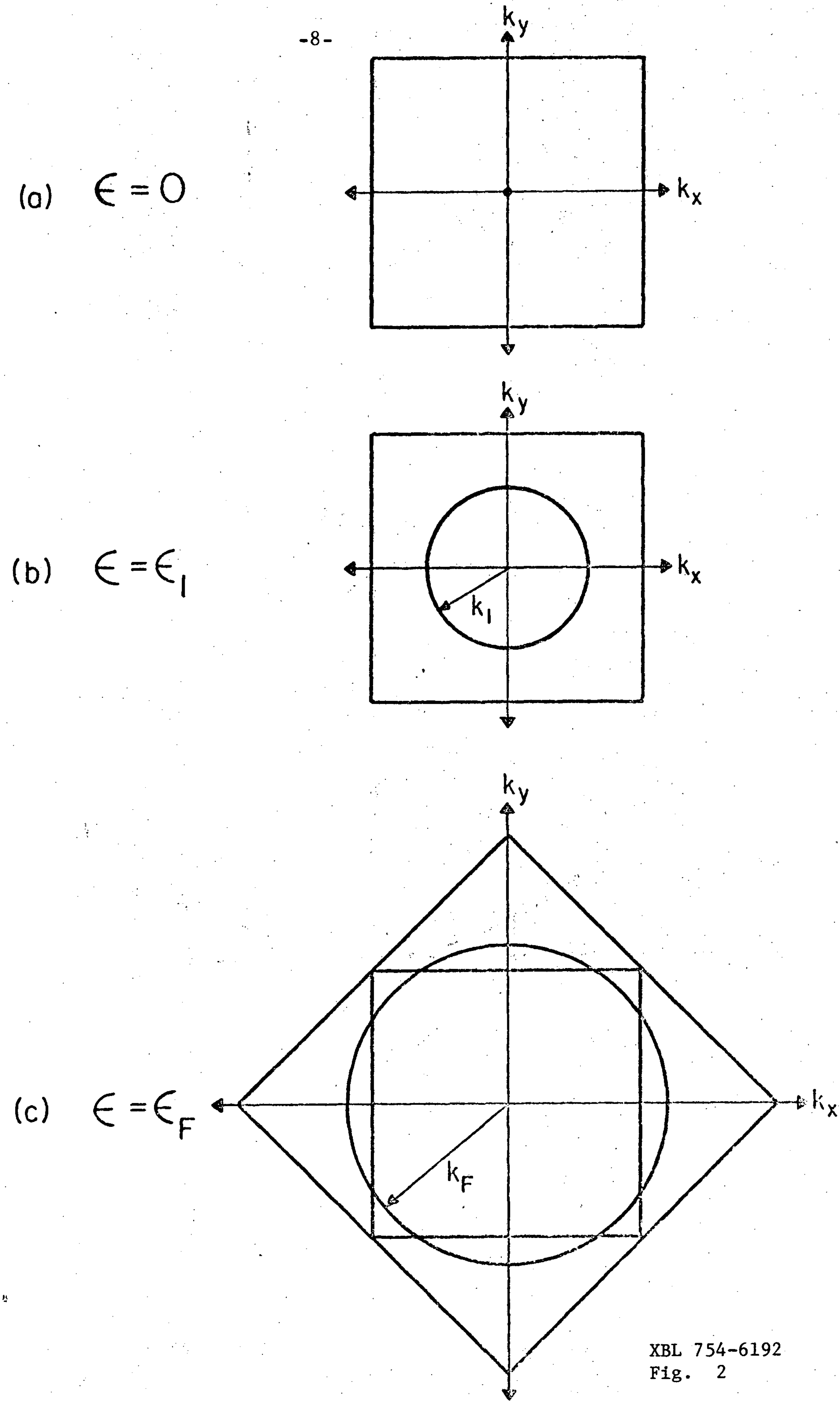

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Fig. 2

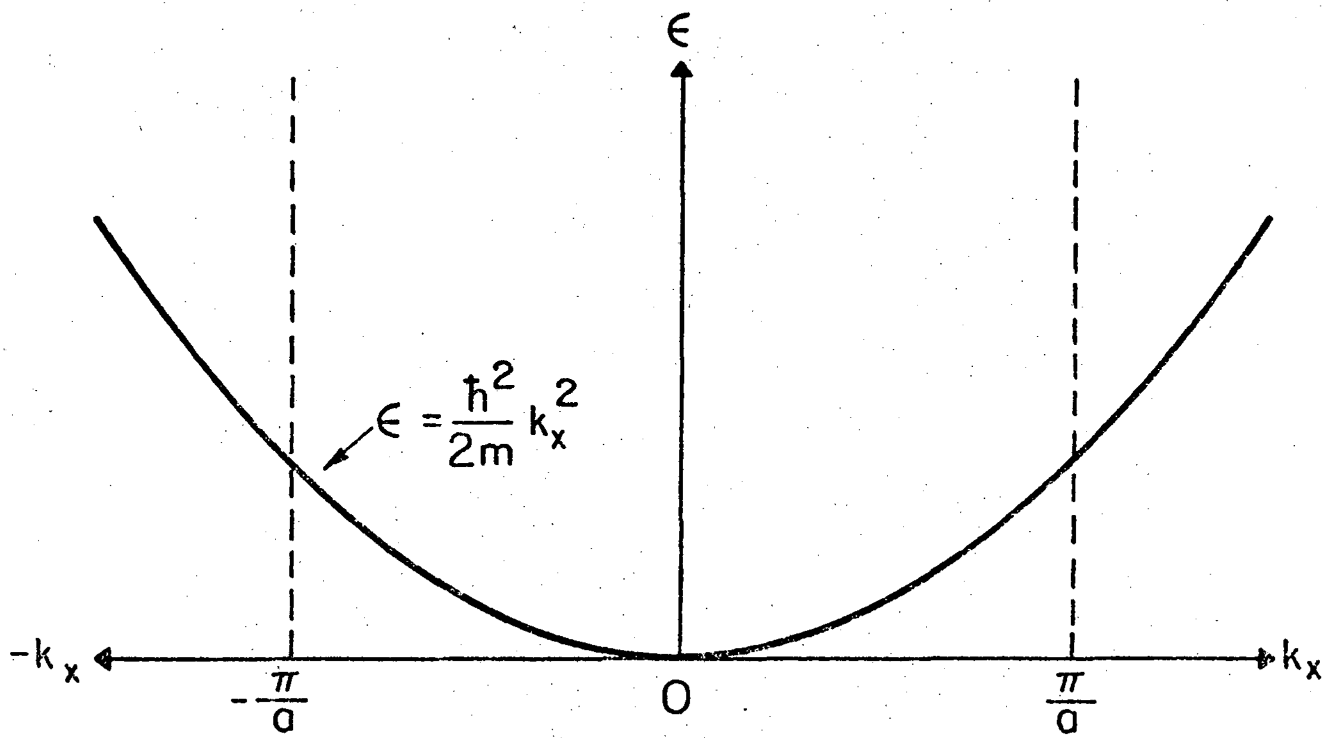

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Fig. 3

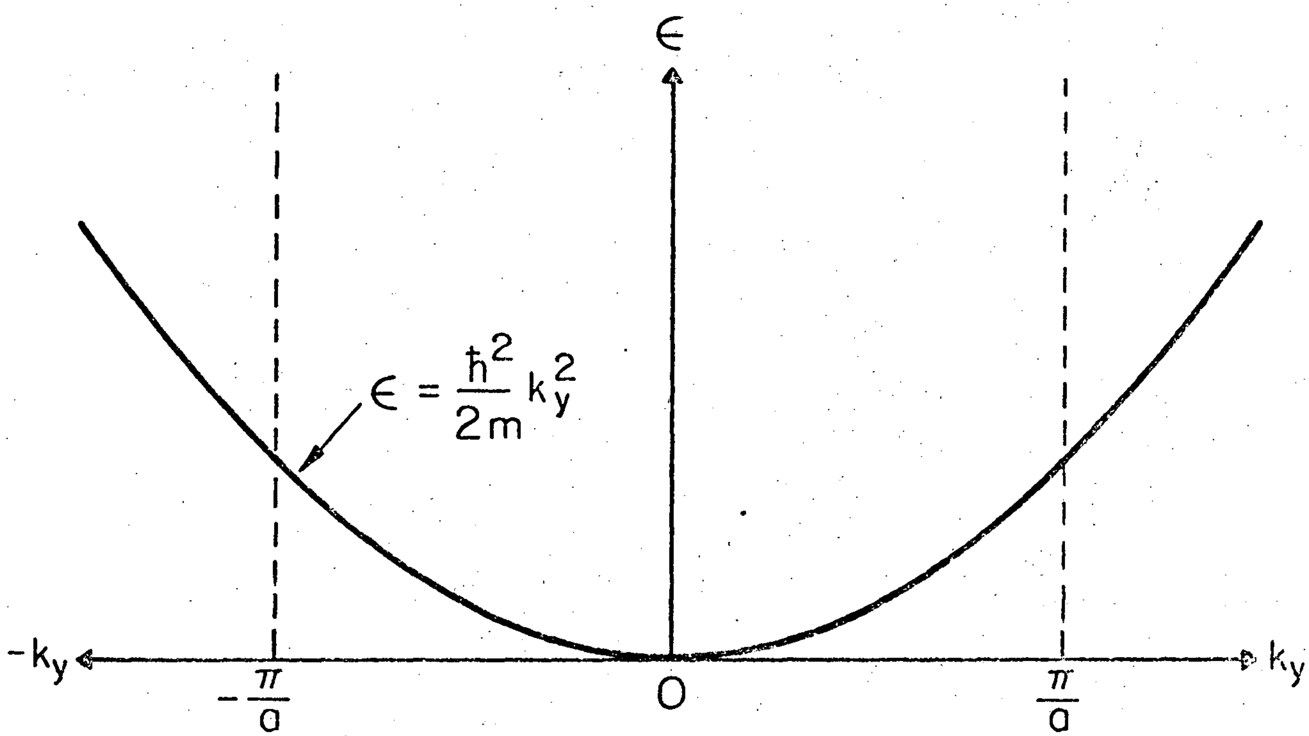

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Fig. 4

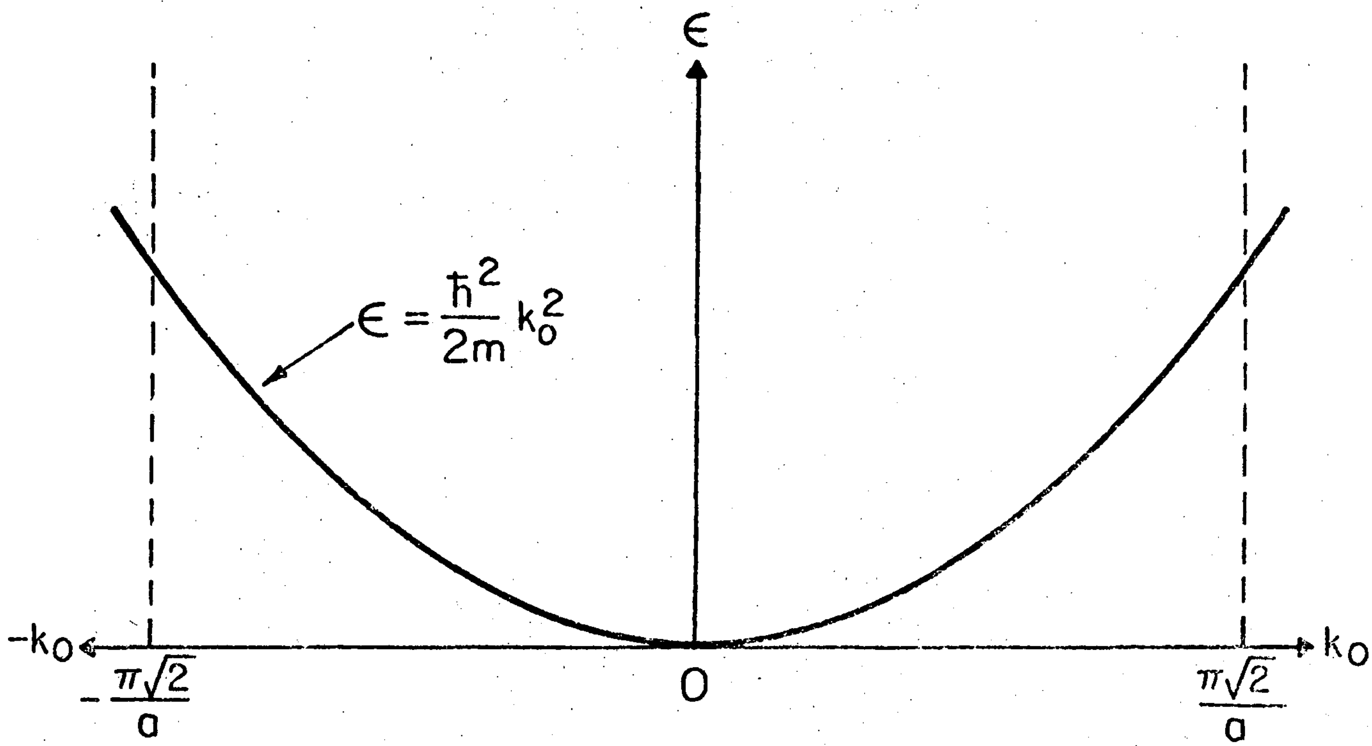

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Fig. 5

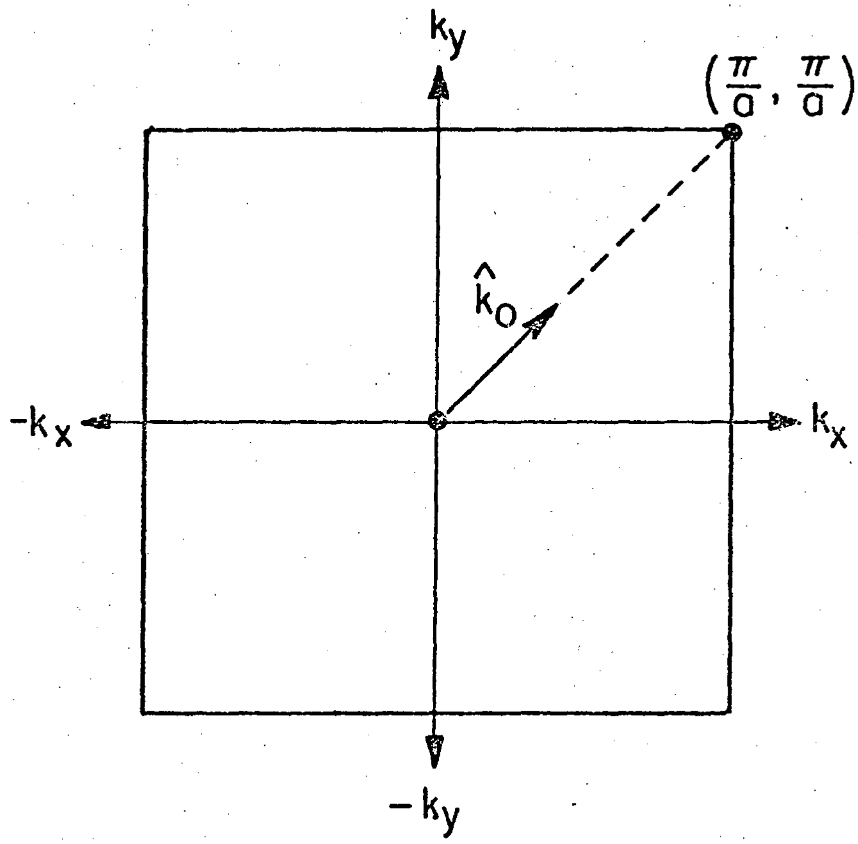

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Fig. 5