Effective masses and curvature of the Fermi surface or energy bands

Autor(en): **Jan, J.-P.**

Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **41 (1968)**

Heft 6-7

PDF erstellt am: **22.07.2024**

Persistenter Link: https://doi.org/10.5169/seals-113954

tion des parois pouvant être aléatoires dans une large mesure. Ceci pourrait permettre un jour une application à l'étude de corps organiques non cristallins, formés par juxtaposition de chaînes de polymères.

Toutefois, les méthodes relativement nouvelles de canalisation et de blocage ont été appliquées jusqu'à présent surtout à certains métaux (Au, Cu, W, Fe) et à quelques semi-conducteurs (Ge, Si, GaAs, GaSb) et il semble bien qu'une extension aux autres substances inorganiques intéressant actuellement le physicien du solide promette de livrer des renseigements nouveaux et précieux sur la constitution de la matière.

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Effective Masses and Curvature of the Fermi Surface or Energy Bands

by **J.-P. Jan**
Division of Pure Physics, National Research Council of Canada, Ottawa, Canada

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Abstract. The curvature of the energy function on one hand, and of the Fermi surface on the other hand, is examined in relation to the effective mass tensor.

1. Introduction

This paper is of a didactic nature. It proposes to examine the components of the effective mass tensor of electrons in a crystal lattice. They involve second derivatives of the energy function and are therefore somehow related to curvatures, but what curvatures are involved is not always clear. We shall examine both the Fermi surface, and the curves representing the energy in function of the magnitude of the wave-vector in a given direction (energy bands), and the relationships we shall establish will show that in both cases the effective mass tensor is involved in a rather complicated way.

2. Effective Mass and Curvature of the Fermi Surface

If $E(\boldsymbol{k})$ is the energy function, and E_F the Fermi energy, the equation of the Fermi surface is

$$E(\boldsymbol{k}) = E_F \,. \tag{1}$$

This is an implicit equation which does not lend itself easily to a local study of curvatures. Indeed, textbooks on differential geometry of surfaces prefer to adopt either an explicit form such as $z = z(x, y)$ (in coordinates x, y, z), or a parametric form $x = x(u, v)$, $y = y(u, v)$, $z = z(u, v)$ involving two parameters u and v. The various curvatures can be easily derived in terms of these last equations. However, the inverse effective mass energy tensor

$$m_{ij}^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \, \partial k_j} \tag{2}$$

is defined in terms of the implicit Equation (1), and its relation to the curvatures is not immediately obvious.

It should be noted also that the principal axes of the tensor (2) bear no simple relation to the local geometry of the Fermi surface. This is quite evident, for instance, in the case of the ellipsoidal surfaces

$$E(\boldsymbol{k}) = \frac{\hbar^2 k_1^2}{2 m_{11}} + \frac{\hbar^2 k_2^2}{2 m_{22}} + \frac{\hbar^2 k_3^2}{2 m_{33}} \tag{3}$$

for which the principal axes are at any point parallel to the coordinate axes.

A local study based on Equation (1) would make use of an expansion of the energy function to second order terms around a given point $\boldsymbol{k}^0$:

$$E(\boldsymbol{k}) = E(\boldsymbol{k}^0) + (k_i - k_i^0)\, \hbar\, v_i + \frac{1}{2} (k_i - k_i^0)\, (k_j - k_j^0)\, \hbar^2\, m_{ij}^{-1} \tag{4}$$

where we have introduced the electron velocity

$$\boldsymbol{v} = \frac{1}{\hbar} \boldsymbol{\nabla}_{\boldsymbol{k}} E \tag{5}$$

and adopted the standard summation convention over repeated indexes. When $E(\boldsymbol{k})$ has the form (4), (1) represents a quadric (ellipsoid, hyperboloid or paraboloid). We now change our coordinate system to a new set $(k_1' \, k_2' \, k_3')$, with the origin at point $\boldsymbol{k}^0$, the k_3' axis perpendicular to the Fermi surface in the direction of increasing energy, and the axes k_1' and k_2' chosen in the tangent plane to make $(m_{12}^{-1})' = (m_{21}^{-1})' = 0$ (cf. PIPPARD [1]), and (4) becomes a new function

$$\begin{aligned} E'(\boldsymbol{k}') = E'(0) + k_3' \, \hbar \, v + \frac{1}{2} k_1'^2 \, \hbar^2 (m_{11}^{-1})' + \frac{1}{2} k_2'^2 \, \hbar^2 (m_{22}^{-1})' + \frac{1}{2} k_3'^2 \, \hbar^2 (m_{33}^{-1})' \\ + k_1' \, k_3' \, \hbar^2 (m_{13}^{-1})' + k_2' \, k_3' \, \hbar^2 (m_{23}^{-1})' \,. \end{aligned} \tag{6}$$

The principal radii of curvature of the Fermi surface at $\boldsymbol{k}^0$ are therefore those of the paraboloid

$$k_3' = - \frac{\hbar}{2 \, v \, m_{11}'} k_1'^2 - \frac{\hbar}{2 \, v \, m_{22}'} k_2'^2 \tag{7}$$

where $m_{11}' = 1/(m_{11}^{-1})'$ and $m_{22}' = 1/(m_{22}^{-1})'$, namely

$$\varrho_1 = v \, m_{11}'/\hbar \,, \qquad \varrho_2 = v \, m_{22}'/\hbar \,. \tag{8}$$

A sign convention is implicit in (8). The choice of k'_3 makes $v = v'_3$ positive. A positive m'_{11} or m'_{22} corresponds to a positive radius and to the center of curvature «inside» the Fermi surface, meaning that, if we move from $\boldsymbol{k}^0$ towards the center of curvature, the energy decreases. This corresponds to a convex curve on the Fermi surface. The opposite holds for negative masses; m'_{11} and m'_{22} may of course have opposite signs, for instance at the necks of the Fermi surface of the noble metals.

The simple Equations (8) require the change of axes described above, and the components of the original inverse effective mass tensor (2) are not simply related to any curvature of the Fermi surface. It should also be noted that the components of the transformed tensor, which do not appear in (7) and (8), have nothing to do with the curvature of the Fermi surface; as PIPPARD [1] points out, the essential quantities are ϱ_1, ϱ_2 and v.

The preceding remarks apply not only to the Fermi surface, but to any energy surface.

3. Effective Mass and Curvature of the Energy Bands

In the one-dimensional case, the effective mass is

$$\frac{1}{m} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}. \tag{9}$$

By energy band, we mean here the curve obtained by plotting E vs. k. Its curvature is given by

$$\frac{1}{\varrho} = \frac{E''}{(1+E'^2)^{3/2}} = \frac{\hbar^2/m}{(1+\hbar^2 v^2)^{3/2}} \tag{10}$$

where $E' = \hbar v$ and $E'' = \hbar^2/m$ are the first and second derivatives of $E(k)$ respectively, and ϱ the radius of curvature. This curvature is seen to involve m directly, but also v. For instance, in a parabolic band, m is independent of k, but the curvature is not.

We generalize now these elementary remarks to three dimensions. Here, we consider how E changes in $\boldsymbol{k}$-space along a straight line whose direction is defined by a unit vector $\boldsymbol{n}$, such that $\boldsymbol{k} = \boldsymbol{k}^0 + \boldsymbol{n}\, k$. Such straight lines join points of high symmetry in the Brillouin zone in the popular energy band diagrams. It is easily shown that the curvature of $E(k)$ is

$$\frac{1}{\varrho} = \frac{\hbar^2/m_{av}}{(1+\hbar^2 v^2 \cos^2\alpha)} \tag{11}$$

where the average effective mass in the direction n is defined by

$$\frac{1}{m_{av}} = n_i\, n_j\, m_{ij}^{-1} \tag{12}$$

and α is the angle between $\boldsymbol{v}$ and $\boldsymbol{n}$. It is seen that the effective mass tensor, through the average (12), comes directly into the curvature of the energy bands. For instance, in the [100] direction, only the m_{11}^{-1} component is involved; several components come into play in more complicated crystallographic directions.

The author is grateful to Dr. W.B. PEARSON for reading the manuscript.

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