Pressure Dependence of the Hall Constant

of the Alkali Metals

by

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I. Introduction

A. The Fermi Surface in Metals

Considerable work has recently been done in an effort to learn more about the Fermi surface in metals, both theoretically and experimentally. In a one electron picture, the Fermi surface is a surface of constant electron energy in k space, where k is the reduced momentum; the value of the energy on this surface is the Fermi energy, E_F, defined by $f(E_F) = \frac{1}{2}$ where $f(E)$ is the Fermi-Dirac distribution function. It may also be thought of as the surface separating regions of k space where the electron states are occupied from those that are empty. Although the concept of the Fermi surface grew out of a one electron picture, recently theoretical work has been done to show that it has some justification even in a many electron picture [1]. The possible topologies of the Fermi surface in metals have been discussed by many authors. A good review of the subject has recently been given by Ziman [2].

Although band structure calculations have been performed for many metals, especially the alkalis, relatively few of these are sufficiently detailed to allow a deduction of the shape of the Fermi surface. Generally, the energy has been computed only at certain symmetry points in the Brillouin zone; to obtain the Fermi surface, curves of electron energy vs. k for several

directions in the reciprocal lattice are needed. Recent calculations on the
band structure of the alkali metals by Ham [3] are of importance for
several reasons. First, they provide curves of E vs. k for the three
principal directions and allow the deduction of an approximate shape for the
Fermi surface. Second, they are made for the entire alkali series,
(lithium, sodium, potassium, rubidium, and cesium), using the same method
in each case and should give a qualitative picture of the change in the shape
of the Fermi surface as one progresses through the series. Third, they have
been carried out for several values of lattice constant and so provide a guide as
to how the Fermi surface should change under pressure.

The work of Ham used a variational technique developed by Kohn and
Rostoker [4]. They used a potential that had only a radial dependence within
a sphere inscribed in the atomic polyhedron and was constant outside the
sphere. The wave equation is solved in the actual atomic polyhedron and gives
an $E(\vec{k})$ which is not spherically symmetric. With this form of the potential,
energy eigenvalues could be obtained using some geometrical structure con-
stants, which depend only on the type of lattice, and the values of the logarith-
mic derivative of the solution of the radial wave equation at the boundary of
the inscribed sphere. Ham [5,6] used the method of quantum defects to
obtain the logarithmic derivatives needed; this made it unnecessary to assume
a specific numerical potential. The use of the quantum defect method takes
into account the polarization of the ion cores, relativistic effects, and
exchange effects between the valence electrons and the ion cores. These
effects are important in the heavy elements and a calculation which ignored
them would probably be in error.

The accuracy of the Kohn-Rostoker technique used is limited by
the realism of the assumed potential rather than by mathematical accuracy.
Furthermore, the method is sufficiently tractable to make possible band
structure calculations elaborate enough to indicate the shape of the Fermi
surface. In the alkalis the size of the ion core is small, (about half the
nearest neighbor distance in sodium) and consequently the Kohn-Rostoker
potential may be fairly realistic.

Other band calculations have been carried out using explicit potentials;
for example Heine [7] has computed the band structure of aluminum in a
self-consistent manner using a method which takes approximate account of