

odel; this has been done by this extension.

weak pseudo-potential that have a valuable phenomeno-correlating experimental data er, we would like to know er more fundamental point of ow to calculate the Fourier nerally, its matrix elements e, we follow Harrison (1965,

s in the crystal a weak local each point. We then assume presented as the linear super-potentials centred on the ion

$$|\vec{r}_j| \quad (28)$$

the N ions in the crystal, j ant assumption and we shall ore detail the nature of W t is that *if* this linear super-f $W(\vec{r})$ (between states k and two factors thus:

$$, q) \quad (29)$$

$$w(r) e^{ikr} d\tau$$

ane wave states k and $k + q$. ependent of the positions of pseudo-potential. V_0 is here

k dependence in the two ex-d $w(q)$ is in this case just the at purposes this simpler form

the *structure* factor; by con-e positions of the ions. For a

perfect lattice at the absolute zero, it vanishes everywhere except at the reciprocal lattice points where it has the value unity.

This factorization into a *structure* factor and a *form* factor, characteristic of diffraction theory, is vital here.

We turn now to the calculation of the effect of volume on the Fermi surface. One way to obtain such information is to make a calculation using the full pseudo-potential theory, essentially a full orthogonalized plane wave (OPW) calculation, at two different volumes. However, there are simpler, through of course less exact, methods; one is to use Harrison's "point ion" approximation. In this, $w(q)$ is derived by representing the effective potential as made up of three contributions:

- (1) The coulomb potential due to the valence charge on the ion.
- (2) A repulsive term (originally referred to as the pseudo-potential) arising from the core electrons. As already discussed, the conduction electrons are to some extent excluded from the core because of the Pauli principle and because these inner shells are already occupied.
- (3) The potential due to screening by the conduction electrons. Because the conduction electrons in the metal are mobile they move to regions of low potential and thus partly screen the bare potential that the electrons would otherwise see; thus a self-consistent procedure is required. Such a procedure was introduced by Bardeen (1937) in his work on electron-phonon interaction in metals. For a free, degenerate electron gas of Fermi radius, k_F , the screening can be represented by an effective dielectric constant of which the Fourier component of wave-number q is:

$$\epsilon(q) = 1 + \frac{me^2}{2\pi k_F \hbar^2 \eta^2} \left[\frac{1 - \eta^2}{2\eta} \ln \left| \frac{1 + \eta}{1 - \eta} \right| + 1 \right] \quad (30)$$

where $\eta = q/2k_F$. Here m and e are the mass and charge of the electron. Under these conditions, the ratio of $w_b(q)$, the bare potential, to $w_s(q)$, the self-consistent screened potential, is just $\epsilon(q)$. It is in part the simplicity of this self-consistent screening that makes it possible to represent the total crystal potential as the linear superposition of the individual ion potentials.

In the point ion model, the repulsive potential in (2) above is represented by a δ function (the ion core is considered as a point). If the