

points. We must therefore extend the model; this has been done by Harrison and others and we now consider this extension.

So far we have seen that if there exists a weak pseudo-potential that can be treated by perturbation theory we have a valuable phenomenological method for interpolation and for correlating experimental data about the Fermi surface. Now, however, we would like to know something about this potential from a rather more fundamental point of view. In particular, we want to know how to calculate the Fourier components of the potential or, more generally, its matrix elements between plane wave states. In this outline, we follow Harrison (1965, 1966).

We begin by assuming that there exists in the crystal a weak local effective (or pseudo) potential, $W(\vec{r})$, at each point. We then assume that this total pseudo-potential can be represented as the linear superposition of the individual ionic pseudopotentials centred on the ion sites. Thus:

$$W(r) = \sum_j w(|\vec{r} - \vec{r}_j|) \quad (28)$$

where the \vec{r}_j represent the positions of the N ions in the crystal, j going from 1 to N . This is a most important assumption and we shall discuss it below when we consider in more detail the nature of W itself. For the present, however, the point is that *if* this linear superposition holds then the matrix element of $W(\vec{r})$ (between states k and $k + q$) can be expressed as a product of two factors thus:

$$W(q) = S(q) w(k, q) \quad (29)$$

where:

$$w(k, q) = \frac{1}{V_0} \int e^{-i(k+q)r} w(r) e^{ikr} d\tau$$

is the matrix element of $w(r)$ between plane wave states k and $k + q$. $w(k, q)$ is called the *form factor*; it is independent of the positions of the ions and depends only on the ionic pseudo-potential. V_0 is here the atomic volume.

If $w(r)$ is a simple potential then the k dependence in the two exponential factors in $w(k, q)$ cancels out and $w(q)$ is in this case just the Fourier transform of $w(r)$. For our present purposes this simpler form is sufficient.

The factor $S(q) = \frac{1}{N} \sum e^{-iqr_j}$ is called the *structure factor*; by contrast with $w(k, q)$, it depends only on the positions of the ions. For a