$_1{}^x dx$

tial with period $1/a$.
$A_1$ from equations (22) and

$$_1 V_1^* = 0 \qquad (24)$$

$$T_1)^2 + 4V_1 V_1^*] \qquad (25)$$

Fig. 7; it is of the familiar
wavenumber of the electron
periodicity of the reciprocal
lows from equation (25) that:

$$_1 | \qquad (26)$$



$k \longrightarrow$

rly-free-electrons.

ues of $E$ and the width of the

$$| \qquad (27)$$

ed by twice the corresponding

The above reasoning is easily generalized to three dimensions. The critical values of $k$ are then those on the walls of the Brillouin zone. If $k$ is close to a (111) face (in, say, an f.c.c. metal) then the Fourier component $V_{111}$ will be important. At the centre of this face this component may suffice to determine the energy gap. Along the edge of a zone where two faces meet (say the 111 and 200 zone faces of an f.c.c. metal) then $V_{111}$ and $V_{200}$ may become important. At a corner, three Fourier components may be required. This illustrates how the Fourier components of the potential enter into the band-structure calculations. In addition we may note for future reference that in the neighbourhood of a zone face we may expect that at least two plane waves will be needed to specify the wave function of the electron, viz.:

$$e^{-ikr} \text{ and } e^{-i(k+K_g)r}$$

where $K_g$ is the reciprocal lattice vector associated with that zone face.

All this is, of course, well known. What is new is its justification by pseudo-potential theory in relation to at least some real metals.

The method is particularly useful for constructing a Fermi surface from de Haas–van Alphen data. Where the model is most useful is, as we have seen, where only a few Fourier components of the pseudo-potential are significant. These (together with the Fermi energy) can then be taken as parameters and chosen to give the best fit with experiment in certain regions of the Fermi surface. Then the model can be used to calculate the rest of the Fermi surface and the band structure of the metal in the neighbourhood of Fermi energy. This phenomenological programme has, for example, been successfully carried out for Pb by Anderson and Gold (1965) (where, however, the situation is complicated by the strong spin-orbit coupling) and for Al by Ashcroft (1963).

The derivation of the Fermi surface, expressed in terms of a few Fourier coefficients of the effective potential, does not by itself enable us to predict what would happen to the surface under pressure. These Fourier coefficients, $V_{111}$ and $V_{200}$, say, are valid for one particular value of the Fermi energy, and hence for one particular value of the lattice parameter only (that corresponding to zero pressure). To make any predictions about pressure effects, we need to know how $V_{111}$, $V_{200}$ and $E_F$ change when the lattice parameter alters, thus changing, among other things, the relative separations of the reciprocal lattice