The pseudo-potential method in its complete form results from a transformation of the Schroedinger equation applied to the lattice potential, $V(r)$, and is exact. In the transformation, the ordinary lattice potential, $V(r)$, is as we saw replaced by a weak effective potential part of which arises from the pseudo-potential. This in its full generality, is a non-local integral operator, containing exchange terms and terms that arise from the orthogonalization of the crystal wave function to the occupied ion core electron states. The method becomes particularly useful if:

(a) The pseudo-potential integral operator can be treated as essentially a simple potential.
(b) The Fourier expansion of the resultant effective potential requires only a few terms corresponding to small reciprocal lattice vectors for its accurate representation.

In the above description I have used the term "pseudo-potential" to refer to the repulsive part of the interaction that offsets the attractive interaction with the nucleus. The resultant interaction I have called the "effective" interaction. This seems to have been the original usage, but it is now common to refer to the *resultant* potential as the pseudo-potential and so I shall do so from now on.

The result of replacing the actual potential inside the crystal by the weak pseudo-potential is that now the problem to be solved in finding the band structure of the metal is formally equivalent to that of the nearly-free-electron model of a metal.

Let me briefly remind the reader of how a simple one-dimensional calculation of this kind is carried out (Mott and Jones, 1936, p. 61). In a periodic lattice of lattice spacing a, the solution of the Schroedinger equation:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \tag{16}$$

is a Bloch function:

$$\psi = \mathrm{e}^{\mathrm{i}kx}\, u(x)$$

where $u(x)$, like $V(x)$, is periodic with the period a. Let us expand $u(x)$ in a Fourier series: