mplete form results from a
ıtion applied to the lattice
ansformation, the ordinary
ced by a weak effective po-
ıdo-potential. This in its full
·, containing exchange terms
lization of the crystal wave
states. The method becomes

tor can be treated as essen-

ıltant effective potential re-
ng to small reciprocal lattice
tion.

the term "pseudo-potential"
ction that offsets the attrac-
tant interaction I have called
have been the original usage,
ltant potential as the pseudo-
on.

ıtial inside the crystal by the
oblem to be solved in finding
ılly equivalent to that of the

ow a simple one-dimensional
Mott and Jones, 1936, p. 61).
the solution of the Schroedin-

$) \psi = 0$ (16)

)

period a. Let us expand $u(x)$

$$u(x) = \sum_{n=-\infty}^{\infty} A_n \, e^{-2\pi i nx/a} = \sum_{n=-\infty}^{\infty} A_n \, e^{-i K_n x} \tag{17}$$

where $K_n \equiv \dfrac{2\pi n}{a}$. Suppose for simplicity that apart from the constant term, A_0, only one Fourier component K_1 is important; we then have:

$$\psi = e^{ikx} (A_0 + A_1 e^{-i K_1 x}) \tag{18}$$

$$= A_0 e^{ikx} + A_1 e^{i k_1 x} \qquad \text{where } k_1 = k - K_1$$

Substituting this solution in the Schroedinger equation we find:

$$A_0 e^{ikx} \left\{ - k^2 + \frac{2m}{\hbar^2} (E - V) \right\} + A_1 e^{i k_1 x} \left\{ - k_1^2 + \frac{2m}{\hbar^2} (E - V) \right\} = 0 \tag{19}$$

If we multiply by e^{-ikx} and integrate from 0 to a, we get:

$$- A_0 k^2 a + \int_0^a \frac{2mA_0}{\hbar^2} (E - V) \, dx$$

$$- \int_0^a \frac{2mA_1}{\hbar^2} e^{-i K_1 x} V \, dx = 0 \tag{20}$$

We choose our origin of energy so that the mean value of V vanishes, i.e.:

$$\int_0^a V(x) \, dx = 0 \tag{21}$$

Thus we have:

$$A_0 (E - T_0) - A_1 V_1^* = 0 \tag{22}$$

Similarly by multiplying by $e^{-i k_1 x}$ and integrating we find:

$$- A_0 V_1 + A_1 (E - T_1) = 0 \tag{23}$$

Here:

$$T_0 = \frac{\hbar^2 k^2}{2m}$$

and:

$$T_1 = \frac{\hbar^2 k_1^2}{2m}$$

(the free-electron kinetic energies corresponding to the values k and k_1):