mplete form results from a
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ansformation, the ordinary
ced by a weak effective po-
do-potential. This in its full
, containing exchange terms
lization of the crystal wave
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tor can be treated as essen-

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the term "pseudo-potential"
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itial inside the crystal by the
oblem to be solved in finding
lly equivalent to that of the

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

$$) \psi = 0 \tag{16}$$

)

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

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

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:

$$\begin{aligned} \psi &= \mathrm{e}^{\mathrm{i}\, kx}\,(A_0 + A_1\, \mathrm{e}^{-\mathrm{i}\, K_1 x}) \\ &= A_0\, \mathrm{e}^{\mathrm{i}\, kx} + A_1\, \mathrm{e}^{\mathrm{i}\, k_1 x} \qquad \text{where } k_1 = k - K_1 \end{aligned} \tag{18}$$

Substituting this solution in the Schroedinger equation we find:

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

If we multiply by $\mathrm{e}^{-\mathrm{i}\, kx}$ and integrate from 0 to a, we get:

$$\begin{aligned} &- A_0\, k^2 a + \int_0^a \frac{2mA_0}{\hbar^2}(E - V)\, \mathrm{d}x \\ &- \int_0^a \frac{2mA_1}{\hbar^2}\, \mathrm{e}^{-\mathrm{i}\, K_1 x}\, V\, \mathrm{d}x = 0 \end{aligned} \tag{20}$$

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

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

Thus we have:

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

Similarly by multiplying by $\mathrm{e}^{-\mathrm{i}\, k_1 x}$ 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):