It is further assumed that the lattice potential in the distorted crystal depends only on the local displacement and strain. Thus if $U_0(\mathbf{r})$ is the periodic potential in the undeformed crystal and U_d is the potential in a crystal subject to the deformation δR, we take

$$U_d(\mathbf{r}) = U_0(\mathbf{r}-\delta\mathbf{R}) + U_1(\mathbf{r}, \epsilon_{ij}), \tag{A.2}$$

where U_1 depends on the strain components

$$\epsilon_{ij} = \tfrac{1}{2}[\partial(\delta R_j)/\partial x_i + \partial(\delta R_i)/\partial x_j] \tag{A.3}$$

and on position. For small strains, U_1 varies linearly with strain.

The wave equation for an electron in the deformed crystal may be written:

$$[(\hbar^2/2m)\nabla^2 + E - U_0(\mathbf{r}-\delta\mathbf{R}) - U_1(\mathbf{r}, \epsilon)]\psi_d(\mathbf{r}) = 0. \tag{A.4}$$

Both $\delta\mathbf{R}$ and ϵ are assumed to be slowly varying functions of position. We shall obtain an approximate solution for ψ_d in terms of exact wave functions for electrons in a crystal subject to a homogeneous strain.

If the strain ϵ is homogeneous so that $\delta\mathbf{R}$ is a linear function of position, the wave equation for an electron with crystal momentum $\mathbf{P}$ is:

$$[(\hbar^2/2m)\nabla^2 + E_h(\mathbf{P}, \epsilon) - U_0(\mathbf{r}-\delta\mathbf{R}) - U_1(\mathbf{r}, \epsilon)]\psi_h(\mathbf{r}, \epsilon, \mathbf{P}) = 0, \tag{A.5}$$

where E_h (h for *homogeneous*, not for *hole*) is of the form of Eq. (2.3).

$$E_h(\mathbf{P}, \epsilon) = E_{h0}(\epsilon) + \Sigma_{i,j}\, \alpha_{ij}(\epsilon) P_i P_j, \tag{A.6}$$

and where E_{h0} depends only on the dilation Δ,

$$E_{h0}(\epsilon) = E_0 + E_1\Delta. \tag{A.7}$$

The coefficients α_{ij} depend on the effective mass in the deformed crystal. The wave function ψ_h is of the form:

$$\psi_h(\mathbf{r}, \epsilon, \mathbf{P}) = \exp(i\mathbf{P}\cdot\mathbf{r}/\hbar) u_h(\mathbf{r}-\delta\mathbf{R}, \epsilon, \mathbf{P}). \tag{A.8}$$

When $\mathbf{P}$ is small compared to the size of the Brillouin zone, u_h can be expanded in a series of which the first two terms are:

$$u_h(\mathbf{r}-\delta\mathbf{R}, \epsilon, \mathbf{P}) = u_{h0}(\mathbf{r}-\delta\mathbf{R}, \epsilon) + i\mathbf{P}\cdot\mathfrak{u}_{h1}(\mathbf{r}-\delta\mathbf{R}, \epsilon) + \cdots. \tag{A.9}$$

Following the line of argument used by Peckar, we show that an approximate expression for ψ_d can be obtained by use of the effective mass concept. The wave equation to be used in the method of effective mass is:

$$[\hbar^2 \Sigma\, \alpha_{ij}\partial^2/(\partial x_i \partial x_j) + E - E_{h0}(\epsilon)]A(\mathbf{r}) = 0. \tag{A.10}$$

This equation applies to an electron with effective mass given by the tensor α_{ij} moving in an effective potential, $E_{h0}(\epsilon)$, called the deformation potential, where ϵ depends on position. Suppose that a solution of this equation is expressed in the form of a Fourier series or integral:

$$A(\mathbf{r}) = \Sigma_P\, a(\mathbf{P}) \exp(i\mathbf{P}\cdot\mathbf{r}/\hbar). \tag{A.11}$$

Substitution in (A.10) gives:

$$\Sigma\, a(\mathbf{P})[\Sigma\, \alpha_{ij}P_iP_j + E - E_{h0}(\epsilon)] \exp(i\mathbf{P}\cdot\mathbf{r}/\hbar) = 0. \tag{A.12}$$

We shall show that

$$\psi_d = \Sigma_P\, a(P)\psi(\mathbf{r}, \epsilon, \mathbf{P}), \tag{A.13}$$

with ϵ now considered to be a function of $\mathbf{r}$, is an approximate solution of (A.4) provided that ϵ varies sufficiently slowly with $\mathbf{r}$.

Substitution of (A.13) into (A.4) gives

$$\Sigma_P\, a(\mathbf{P})[E - E_{h0} - \Sigma_{i,j}\, \alpha_{ij}P_iP_j]\psi_h(\mathbf{r}, \epsilon, \mathbf{P}) = (\hbar^2/2m)\, \Sigma_P\, a(\mathbf{P}) \exp(i\mathbf{P}\cdot\mathbf{r}/\hbar) \left[\sum_{j,k,l}\left\{\frac{\partial u_h}{\partial \epsilon_{kl}}\left(\frac{2iP_j}{\hbar}\frac{\partial \epsilon_{kl}}{\partial x_j} + \frac{\partial^2 \epsilon_{kl}}{\partial x_j^2}\right) + 2\frac{\partial^2 u_h}{\partial \epsilon_{kl}\partial x_j}\frac{\partial \epsilon_{kl}}{\partial x_j}\right\} + \sum_{kl}\frac{\partial u_h}{\partial x_l}\frac{2\epsilon_{kl}}{\partial x_k}\right]. \tag{A.14}$$

Terms quadratic in ϵ have been omitted. Use has been made of the fact that ψ_h with ϵ constant satisfied (A.5.) The terms on the right-hand side arise from terms in the kinetic energy which depend on a variation of ϵ with position and are small if this variation is sufficiently gradual. The wave function on the left-hand side may be expanded in a power series in P to give:

$$\Sigma_P\, a(\mathbf{P})[E - E_{h0} - \Sigma_{ij}\, \alpha_{ij}P_iP_j] \exp(i\mathbf{P}\cdot\mathbf{r}/h) \times [u_{h0}(\mathbf{r}, \epsilon) + i\mathbf{P}\cdot\mathfrak{u}_{h1}(\mathbf{r}, \epsilon)\cdots]. \tag{A.15}$$

The dominant term vanishes because of (A.12). Thus (A.13) is an approximate solution of (A.4).

Peckar considers the limits of validity of the method as applied to a space variation of potential. Similar considerations apply when the shifts in the energy bands result from lattice deformations.

B. Calculation of the Matrix Element

A calculation of the probability that an electron be scattered from momentum state $\mathbf{P}'$ to state $\mathbf{P}$ as a result of an interaction with a lattice wave depends on an evaluation of the matrix element.

$$M(\mathbf{P}, \Delta') = \int \psi(\mathbf{P}')^* V_p \psi(\mathbf{P}) d\tau, \tag{A.16}$$

where V_p represents the perturbation produced by the lattice wave. The matrix element vanishes unless

$$\mathbf{P}' = \mathbf{P} \pm \hbar\mathbf{k} \pm \hbar\mathbf{K}, \tag{A.17}$$

where $\mathbf{k}(|k| = 2\pi/\lambda)$ is the wave vector of the lattice wave and $\mathbf{K}$ is a lattice vector of the reciprocal lattice space. Since we are concerned with transitions for which both $\mathbf{P}$ and $\mathbf{P}'$ are relatively small, we can set $\mathbf{K} = 0$.

We shall show that the matrix element may be calculated by replacing V_p by the deformation potential, $E_1\Delta(\mathbf{r})$, so that

$$M(\mathbf{P}, \mathbf{P}') = \int \psi(\mathbf{P}')^* E_1\Delta(\mathbf{r})\psi(\mathbf{P}) d\tau = (E_1/V)\int \exp(\pm i\mathbf{P}\cdot\mathbf{r}/\hbar)\Delta(\mathbf{r}) d\tau. \tag{A.18}$$

where V is the volume of the crystal. Although this result follows from the method of effective mass, we shall give a direct proof of (A.18) which shows more directly the relation between the present and previous interaction potentials. It is based on the assumption that V_p is the difference between the potential in the deformed lattice, $U_d(\mathbf{r})$, as given by (A.2) and $U_0(\mathbf{r})$, the periodic potential in the undeformed lattice:

$$V_p = U_d(\mathbf{r}) - U_0(\mathbf{r}) = U_0(\mathbf{r}-\delta\mathbf{R}) - U_0(\mathbf{r}) + U_1(\mathbf{r}, \epsilon_{ij}). \tag{A.19}$$

The first two terms on the right give the "deformable potential" used by Bloch and Bethe.[5]

We shall show that the error involved in using $E_1\Delta(\mathbf{r})$ in place of V_p is the order of $(P^2/2m) \times$ *strains*, which is generally negligible.

The unperturbed wave functions $\psi(\mathbf{P})$ satisfy the wave equation:

$$H_0\psi(\mathbf{P}) = [-(\hbar^2/2m)\nabla^2 + U_0(\mathbf{r})]\psi(\mathbf{P}) = E_0(\mathbf{P})\psi(\mathbf{P}), \tag{A.20}$$

where the energy,

$$E_0(\mathbf{P}) = E_0(0) + P^2/2m_e \tag{A.21}$$

and m_e is the effective mass. The Hamiltonian for the perturbed wave function is $H_0 + V_p$.

The proof of the desired theorem is based on use of the wave functions $\psi_h(\mathbf{r}, \epsilon, \mathbf{P})$ for electrons in homogeneously strained crystals as defined by Eq. (A.8) and the related functions obtained by assuming that the strain ϵ is a slowly varying function of $\mathbf{r}$. We shall neglect terms which are quadratic in ϵ. We may write

$$\psi_h(\mathbf{r}, \epsilon, \mathbf{P}) = \psi(\mathbf{r}, \mathbf{P}) + \delta\psi(\mathbf{r}, \epsilon, \mathbf{P}), \tag{A.22}$$

where $\delta\psi$ is of order ϵ.

To prove (A.18), first consider the integral:

$$I = \int \psi(\mathbf{r}, \mathbf{P}')[H_0 + V_p]\psi_h(\mathbf{r}, \epsilon(\mathbf{r}), \mathbf{P}) d\tau. \tag{A.23}$$

The result of the operation on ψ_h is

$$I = \int \psi(\mathbf{r}, \mathbf{P}')E_h(\mathbf{P}, \epsilon(\mathbf{r}))\psi_h(\mathbf{r}, \epsilon, \mathbf{P}) d\tau + \text{integrals involving } \partial_h/\partial\epsilon \cdot \partial\epsilon/\partial X.$$