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

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

where U_1 depends on the strain components

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

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:

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

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:

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

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

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

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

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

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

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

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:

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

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:

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

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:

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

Substitution in (A.10) gives:

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

We shall show that

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

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

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

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:

$$\begin{aligned}\Sigma_P\,a(\mathbf{P})[E-E_{h0}-\Sigma_{ij}\,\alpha_{ij}P_iP_j]\exp(i\mathbf{P}\cdot\mathbf{r}/\hbar)\\ \times[u_{h0}(\mathbf{r},\epsilon)+i\mathbf{P}\cdot\mathbf{u}_{hl}(\mathbf{r},\epsilon)\cdots].\end{aligned} \qquad (A.15)$$

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.

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

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

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

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

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

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:

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

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:

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

where the energy,

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

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

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

where $\delta\psi$ is of order ϵ.

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

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

The result of the operation on ψ_h is

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