PHYSICAL REVIEW VOLUME 178, NUMBER 3 15 FEBRUARY 1969

Strain Effects on Optical Critical-Point Structure in Diamond-Type Crystals

EVAN O. KANE
Bell Telephone Laboratories, Murray Hill, New Jersey 07974

(Received 24 July 1968)

The effects of strain on optical critical-point structure in the imaginary part ϵ_2 of the dielectric function are considered. The motivation is to study how the symmetry-breaking effects of strain can be used to deduce the symmetry location of the critical points $\mathbf{k}_0$. This knowledge is valuable for the empirical determination of pseudopotential parameters. The applications are to the diamond structure, but quite similar results are to be expected for any cubic material. Effective strain and kinetic energy Hamiltonians are derived in the effective-mass approximation for Γ, Δ, L, and Σ critical points with and without spin-orbit splitting. The effects of exciton binding are considered. The low-strain-induced changes of the dielectric function can be described in terms of three functions of frequency ($\mathcal{W}_1$, $\mathcal{W}_3$, and $\mathcal{W}_5$), which yield symmetry information for nondegenerate bands. For high strain, the individual critical points in the star of $\mathbf{k}_0$ [apart from the ($\mathbf{k}_0$, $-\mathbf{k}_0$) degeneracy] can be resolved, and much more symmetry information is available. Lifetime broadening limits the amount of information which can be obtained.

I. INTRODUCTION AND CONCLUSIONS

THE pseudopotential method[1] has been quite successful in describing the energy band structure of a large number of solids in terms of a small number of parameters, typically three in diamond-type structures.[2,3] One of the most widely used methods of determining these parameters in semiconductors is based on a critical-point analysis of structure in the fundamental optical reflectivity.[4]

The reflectivity may be processed, using a Kramers-Kronig transform to yield $\epsilon_2(\omega)$,[5,6] the imaginary part of the dielectric function. It is assumed that ϵ_2 may be described in terms of direct transitions with phonon interactions giving a lifetime broadening to the predicted structure. Structure in ϵ_2 results from critical points $\mathbf{k}_0$ in the optical energy function, i.e., points where $\nabla_k[E_c(\mathbf{k})-E_v(\mathbf{k})]=0$. E_c and E_v are the conduction and valence band energies. The region around these critical points yields a nonanalytic contribution to ϵ_2 of square-root form which gives rise to characteristic-structure in $\epsilon_2(\omega)$.[2] This structure may be further enhanced by exciton binding effects in the case of M_0 and M_1 singularities.[4,7]

If the location $\mathbf{k}_0$ of the critical point is known, the energy $\hbar\omega_0$ can be used to infer a pseudopotential parameter. The major uncertainty in this method is the location of the critical point $\mathbf{k}_0$. A number of arguments have been used to locate $\mathbf{k}_0$ but they have generally been rather indirect.[4]

Since the introduction of differential methods by Seraphin,[8] the sensitivity of detection of optical critical points has been greatly improved. Much work has been done using the differential electroreflectance method.[9] Differential piezoreflectance has also been studied extensively.[6,10,11] It was immediately clear[11] that the differential methods were not merely advantageous for their greater sensitivity but, because of the symmetry-breaking character of the differential perturbations, they offer the possibility of obtaining information concerning the symmetry properties of critical points which can be used to determine their location in k space.

The symmetry study of critical points is seriously complicated by lifetime broadening effects for all but minimal energy transitions. Because of this fact, a fairly detailed understanding of line shapes will be necessary to deduce the maximum amount of symmetry information. We favor the piezoreflectance method since it is somewhat easier to interpret theoretically than electroreflectance.

In this paper we concentrate on the piezoreflectance problem. If we limit ourselves to the linear response regime, it is easily shown that a cubic system can be described in terms of three constants $\mathcal{W}_1$, $\mathcal{W}_3$, and $\mathcal{W}_5$ which can be determined by polarized reflectivity measurements using stresses in the [001] and [111]

---

[1] J. C. Phillips, Phys. Rev. **112**, 685 (1958); J. C. Phillips and L. Kleinman, *ibid.* **116**, 287 (1959); M. H. Cohen and V. Heine, *ibid.* **122**, 1821 (1961); B. J. Austin, V. Heine, and L. J. Sham, *ibid.* **127**, 276 (1962).

[2] D. Brust, Phys. Rev. **134**, A1337 (1964).

[3] M. L. Cohen and T. K. Bergstresser, Phys. Rev. **141**, 789 (1966).

[4] J. C. Phillips, J. Phys. Chem. Solids **12**, 208 (1960); J. C. Phillips, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1966), Vol. 18, p. 55.

[5] F. C. Jahoda, Phys. Rev. **107**, 1261 (1957); H. R. Philipp and E. A. Taft, *ibid.* **113**, 1002 (1959).

[6] M. Garfinkel, J. J. Tiemann, and W. E. Engeler, Phys. Rev. **148**, 695 (1966).

[7] J. Hermanson, Phys. Rev. Letters **18**, 170 (1967); B. Velicky and J. Sak, Phys. Status Solidi **16**, 147 (1966); E. O. Kane (unpublished).

[8] B. O. Seraphin and R. B. Hess, Phys. Rev. Letters **14**, 138 (1965).

[9] B. O. Seraphin and N. Bottka, Phys. Rev. **139**, A560 (1965); **140**, A1716 (1965); **145**, 628 (1966); M. Cardona, K. L. Shaklee, and F. H. Pollak, *ibid.* **154**, 696 (1967).

[10] W. E. Engeler, M. Garfinkel, J. J. Tiemann, and H. Fritzsche, Phys. Rev. Letters **14**, 1069 (1965); I. Balslev, Phys. Rev. **143**, 636 (1966); Solid State Comm. **5**, 315 (1967).

[11] G. W. Gobeli and E. O. Kane, Phys. Rev. Letters **15**, 142 (1965); U. Gerhardt, D. Beaglehole and R. Sandrock, *ibid.* **19**, 309 (1967); F. H. Pollak, M. Cardona, and K. L. Shaklee, *ibid.* **16** 942 (1966).

directions. The relations are

[001] Stress

$$\delta\epsilon_{2\parallel}=\left(\frac{\mathcal{W}_1}{\sqrt{3}}(\omega)+\frac{2\mathcal{W}_3}{\sqrt{6}}(\omega)\right)\mathfrak{T}, \tag{1.1}$$

$$\delta\epsilon_{2\perp}=\left(\frac{\mathcal{W}_1}{\sqrt{3}}(\omega)-\frac{\mathcal{W}_3}{\sqrt{6}}(\omega)\right)\mathfrak{T}. \tag{1.2}$$

[111] Stress

$$\begin{aligned}\delta\epsilon_{2\parallel}&=\left(\frac{\mathcal{W}_1}{\sqrt{3}}(\omega)+2\mathcal{W}_5(\omega)\right)\mathfrak{T},\\ \delta\epsilon_{2\perp}&=\left(\frac{\mathcal{W}_1}{\sqrt{3}}(\omega)-\mathcal{W}_5(\omega)\right)\mathfrak{T}.\end{aligned} \tag{1.3}$$

These relations will be derived and discussed in more detail in Sec. III A of this paper. $\mathfrak{T}$ is the applied uniaxial stress, and the parallel and perpendicular differential dielectric constants are defined relative to the stress direction. With respect to these axes the dielectric tensor is in diagonal form.

Two types of effects contribute to $\mathcal{W}$, changes in optical matrix elements and shifts of energy bands. The latter effect is expected to dominate the former in the vicinity of a critical point by a factor $(\Delta E)/\Gamma$ where Γ is a lifetime broadening energy. For a nondegenerate band, ΔE is a typical energy gap at $\mathbf{k}_0$, generally of the order of 1 or 2 eV or more. For degenerate bands whose degeneracy is lifted by spin-orbit interaction, ΔE is the spin-orbit energy. For truly degenerate bands, ΔE may be as small as an exciton binding energy. The linear response regime is, of course, limited to strain energy shifts small compared to either Γ or ΔE.

The energy shift contributions to $\mathcal{W}$ are the most interesting because they contain the most symmetry information. For nondegenerate critical points in the [001] direction or Γ_2 symmetry in the [110] direction, $\mathcal{W}_5^{\text{shift}}=0$; for [111] critical points, $\mathcal{W}_3^{\text{shift}}=0$; and for [000] critical points $\mathcal{W}_3^{\text{shift}}=\mathcal{W}_5^{\text{shift}}=0$. A Kramers-degenerate band is effectively nondegenerate.

For degenerate critical points or for [110] critical points having Γ_1 or Γ_3 symmetry or for a general critical point there are no special relations involving the $\mathcal{W}$'s to indicate the symmetry. Actually, in the degenerate case, $\delta\epsilon_2$ is a nonanalytic function of stress direction which might serve to characterize the degenerate case.

Another way to characterize the degenerate case or the [110] case is to look at terms which are higher order in the strain. If the strain splittings are large enough compared to the lifetime broadening, the critical points which were symmetry degenerate in zero strain may be individually resolved and counted. In the intermediate case, the lines may not be individually resolved but the line shape may be altered sufficiently so that with a reasonable theory for the line shape it would be possible to infer the symmetry character of $\mathbf{k}_0$.

In this paper we study the strain splittings of critical points in the effective mass approximation. We phrase our discussion largely in terms of excitons. If by "exciton" we mean electron-hole pair with their mutual Coulomb interaction accounted for, then our discussion is completely general. It is sometimes convenient to ignore the Coulomb interactions but this will not be necessary for the type of symmetry argument we apply. It will be sufficient to assume that exciton binding energies are large or small compared to strain splitting and lifetime broadening energies. If the exciton binding energy is large compared to lifetime broadening or strain splitting one expects a set of exciton states which transform irreducibly under the group of the critical point $\mathbf{k}_0$. We call these states a symmetry multiplet and we can use group theory to deduce a considerable amount of information concerning the optical matrix elements and strain energy shifts of the multiplet states. We also derive the changes in the multiplet matrix elements which are first order in the strain and which result from strain induced changes in the exciton binding energy. This part of our analysis, which we call the low strain limit, treats strain interactions exactly within the multiplet states and treats strain interactions between multiplets to first order in the strain. We assume that the line shape of the unstrained multiplet states is given by a Lorentzian, hence the differential line shape would be the derivative of a Lorentzian for energy-shift effects and Lorentzian for matrix-element changes.

The case of a nondegenerate critical point is particularly simple. The strain shifts the energy band "as a whole" so that no change in exciton binding relative to the band edge occurs and no change in optical matrix elements results. We ignore wave function admixture effects from higher bands. In this case the differential line shape is a simple frequency derivative of the unstrained line shape. This result is true, of course, regardless of the nature or magnitude of the electron-hole interaction. It is true for the individual exciton states and it is equally true for the sum over all exciton states associated with a given critical point $\mathbf{k}_0$. If the individual exciton states are not resolved, due to lifetime broadening or because they are in the continuum, then the "effective line" is the superposition of all the Lorentzian broadened individual exciton lines. The differential "line shape" of a nondegenerate critical point is the energy derivative of the unstrained "effective line." There will be one such "effective line" for each point in the star of $\mathbf{k}_0$. The vectors $\mathbf{k}_0$ and $-\mathbf{k}_0$ are always degenerate, and other degeneracies may occur for symmetric stresses.

In the case of degenerate bands a strain which is totally symmetric under the group of $\mathbf{k}_0$ will not split the degeneracy. The results in this case are the same as for a nondegenerate band.

For strains which act to split the degeneracy, if the strain splitting is large compared to the lifetime broadening and the exciton-binding energy, we again arrive at a simple result. The bands are effectively "strain decoupled" and the description given above for the nondegenerate case applies, except that now we have a "symmetry multiplet" of bands with a complete exciton spectrum in each (both discrete and continuous).

The energy shifts of bands can be derived from group theory. Optical matrix elements depend on both the periodic part of the Bloch functions and on the exciton envelope functions. The matrix elements due to the periodic parts are related for different multiplet members. In particular, certain polarization directions give zero response. However, the envelope part of the exciton wave function depends on the effective mass parameters so that the over-all matrix element magnitudes are not simply related by group theory in the high strain case. In this respect the symmetry results are less complete than they are for the low strain limit.

For cases intermediate to the limiting cases described above the effective mass formalism can, in principle, be used to derive the line shape function, but in practice this would be quite difficult and we do not attempt it here.

The important symmetry locations for critical points in the diamond structure are the Γ and L points and the Δ and Σ directions and we treat the symmetry properties of these points in detail in Sec. III. The Λ direction and the X point are theoretically possible critical point locations, but for the bands of interest the existence of energy terms linear in $\mathbf{k}-\mathbf{k}_\Lambda$ and $\mathbf{k}-\mathbf{k}_X$ seems to preclude their importance as critical points. Spin-orbit splitting will, in fact, overcome the $\mathbf{k}-\mathbf{k}_\Lambda$ linear terms, but unless spin-orbit splitting is very large, the resulting critical point would be expected to be weak.

We study all the symmetry types which have allowed optical matrix elements. We introduce spin-orbit interaction into the orbital multiplet and treat the symmetry properties of the resulting double group. This approach involves the approximation that only the hole (electron) spin is coupled to the orbital motion and that the wave function and energy are independent of the electron (hole) spin coordinate.

Pollak and Cardona[12] have independently derived many of the symmetry results presented here although their treatment is less general and they do not consider exciton binding effects.

We have discovered the interesting fact that exciton-binding effects generally reduce the absolute magnitude of those deformation potential constants which lead to splitting of band degeneracies.

Outline of Paper

In Sec. II we develop the general formalism based on the effective mass approximation. We perform a symmetry analysis based on the group of $\mathbf{k}_0$, the critical point, following the symmetry notation used by Koster *et al.*[13] Much of our analysis is based on the unitary Clebsch-Gordan matrices γ which give the irreducibly transforming linear combinations of the outer product of two irreducibly transforming functions. These γ matrices have been extensively tabulated by Koster *et al.*[13] for all point groups. The problem of indices becomes rather formidable. We have adopted the convention of reserving the subscript position for symmetry information referring to the group of $\mathbf{k}_0$, although a few exceptions to this rule have been allowed.

In Sec. III we apply the general formalism to specific cases: the Γ point, Δ line, L point, and Σ line in that order. The discussion in the succeeding sections becomes progressively less detailed to avoid tiresome repetition. The case of [001], [111], and [110] strains is treated in most detail.

The principal results of this paper consist of the energy shifts with strain and the optical matrix element changes with strain. They are given for the $\mathbf{k}=0$ point without spin-orbit interaction in Eqs. (3.39) through (3.45) and (3.49) through (3.52). For the fourfold band at $\mathbf{k}=0$ (considering spin-orbit splitting) the results are given in Eqs. (3.77) through (3.80) with (3.83) and (3.84). For the twofold (Kramers degenerate) band at $\mathbf{k}=0$ the results are given in Eqs. (3.94) through (3.96).

For critical points in the Δ direction, the results are summarized in Tables II, III, and IV; for critical points in the Λ direction, Tables VI, VII, and VIII apply. The Σ direction is given in Table IX. The quantity $F_x{}^t$ gives the contribution to the principal axis component x of the dielectric tensor from the state t, F is defined in Eq. (2.13). The D's are "band-edge" deformation potential parameters, while the $\mathfrak{D}^t$'s are deformation parameters which take into account the change of exciton binding energy of state t with strain. η_1, η_3, and η_5 are strain components defined in Eqs. (3.10) through (3.19). The principal axes of the dielectric tensor depend on the stress direction and are defined in Eqs. (3.1) and (3.2). E^t is the unstrained exciton binding energy of state t and $\pm\lambda$ is the spin-orbit energy. f^{t0} is a matrix element parameter in the unstrained crystal while f^{t3} and f^{t5} are matrix-element changes induced by η_3 and η_5 strain components, respectively.

In Sec. IV we compare our notation to that of other authors in the current literature.

We have not treated effects such as spatial dispersion,[14] electron-hole spin-spin interactions due to exchange scattering,[15] or valley-orbit splitting[16] due to the overlap of k-space wave functions associated with dif-

---

[12] F. H. Pollak and M. Cardona Phys. Rev. **172**, 816 (1968).

[13] G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups* (MIT Press, Cambridge, Mass. 1963).

[14] J. J. Hopfield and D. G. Thomas, Phys. Rev. **132**, 563 (1963).

[15] R. S. Knox, *Solid State Physics* (Academic Press Inc., New York (1963)) Supplement 5, p. 45.

[16] W. Kohn *Solid State Physics* (Academic Press Inc., New York (1957), Vol. 5, p. 289.

ferent points in the star of $\mathbf{k}_0$. In special cases, any or all of these effects may be important. We remark that in the presence of strong valley-orbit splitting the exciton is best regarded as belonging to the group of $\Gamma(\mathbf{k}=(0,0,0))$. Our "low strain" results for Γ would be applicable to this case.

II. GENERAL FORMALISM

A. Optical Dielectric Function

We are concerned with the absorptive part $\boldsymbol{\varepsilon}_2(\omega)$ of the tensor optical dielectric function $\boldsymbol{\varepsilon}(\omega)$, where

$$\boldsymbol{\varepsilon}(\omega)=\boldsymbol{\varepsilon}_1(\omega)+i\boldsymbol{\varepsilon}_2(\omega). \tag{2.1}$$

For a cubic crystal the $\boldsymbol{\varepsilon}$ tensor is isotropic and may be replaced by a scalar. Under the action of strain the cubic symmetry is destroyed and the tensor character of $\boldsymbol{\varepsilon}$ becomes important. If we assume that the strain dependence of $\boldsymbol{\varepsilon}$ is an analytic function, we can write the linear strain dependence in the form

$$\begin{aligned}\delta\epsilon_{2,xx}(\omega)&=W_{11}(\omega)e_{xx}+W_{12}(\omega)(e_{yy}+e_{zz}),\\ \delta\epsilon_{2,xy}(\omega)&=W_{44}(\omega)e_{xy}.\end{aligned} \tag{2.2}$$

These relations have the same form as the relations connecting the strain tensor $\mathbf{e}$ and the stress tensor $\mathfrak{T}$ where $\mathbf{W}$ is the analog of the compliance tensor $\mathbf{s}$ ($\mathbf{W}$ and $\mathbf{s}$ are actually fourth rank tensors but the abbreviated notation is standard). In Sec. III A we will discuss the form that Eq. (2.2) assumes when $\mathbf{e}$ and $\boldsymbol{\varepsilon}_2$ are written in symmetry adapted notation.

We wish to obtain more information about $\boldsymbol{\varepsilon}_2$ than is available from Eq. (2.2). One approach would be to continue the expansion of $\boldsymbol{\varepsilon}_2$ to quadratic and higher terms in the strain. This has been suggested by Gerhardt in a private communication and it may be a useful procedure in some cases. Our approach in this paper is to look into the microscopic theory of the dielectric function and to study the strain dependence of optical energies and matrix elements in the effective mass approximation. In simple cases we can obtain the functional form of the ω dependence as well as stress dependences in the range where a power series expansion for ϵ_2 would not converge, namely, when energy shifts due to stress are greater than the lifetime broadening energy. We also study degenerate bands where the stress dependence of ϵ_2 is nonanalytic. We find, however, that (2.2) is still correct for stresses in the [001], [111], and [110] directions.

We will treat only direct transitions and ignore the small k vector of the light. We also ignore phonon interactions except insofar as they can be treated phenomenologically as a lifetime broadening process.

The dielectric tensor can be written[2]

$$\epsilon_{2,lm}(\omega)=\frac{4\pi^2e^2}{3m_0{}^2\omega^2V}\sum_t\langle 0|p_l|\psi^t\rangle \times\langle\psi^t|p_m|0\rangle\delta(\mathcal{E}^t-\mathcal{E}^0-\hbar\omega), \tag{2.3}$$

where p_l is the lth component of the momentum operator and $|0\rangle$ refers to the ground state of the crystal at absolute zero with energy $\mathcal{E}^0$, assumed to be totally symmetric under the crystal symmetry group. $|\psi^t\rangle$ refers to a complete set of excited states labelled by the index t, having energy $\mathcal{E}^t$. Because of time reversal, ϵ_2 is always a symmetric tensor, $\epsilon_{2,lm}=\epsilon_{2,ml}$ in the absence of external magnetic fields. (We do not treat the effect of magnetic fields.)

The excited states ψ^t consist of an electron and hole of total momentum zero (ignoring the wave vector of the light). When Coulomb interactions between the electron and hole can be ignored, ψ^t can be written as a product of Bloch functions

$$\psi^t=V^{-1/2}e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}u_{n_1}(\mathbf{k},\mathbf{r}_1)u_{n_2}{}^\dagger(\mathbf{k},\mathbf{r}_2) \tag{2.4}$$

$$\mathcal{E}^t=E_{n_1}(\mathbf{k})-E_{n_2}(\mathbf{k}), \tag{2.5}$$

where $\mathbf{r}_1$, $\mathbf{r}_2$ are the coordinates of the electron and hole in energy bands n_1 and n_2, respectively. We take the usual "one-electron" view so the hole wave function is the adjoint of the corresponding one-electron wave function.

ϵ_2 is then the energy density of the pair states (the optical density of states or "joint" density of states) weighted by the matrix elements of p. The optical density of states has analytic singularities (of square-root type) at the critical points $\mathbf{k}_0$ for which

$$\nabla_{\mathbf{k}}[E_{n_1}(\mathbf{k})-E_{n_2}(\mathbf{k})]_{\mathbf{k}_0}=0, \tag{2.6}$$

$$\hbar\omega_0\equiv E_{n_1}(\mathbf{k}_0)-E_{n_2}(\mathbf{k}_0). \tag{2.7}$$

These points provide the structure in ϵ_2 and in the reflectivity and we wish to focus our attention on these regions.

In the vicinity of a critical point, the optical energy $\mathcal{E}^t(\mathbf{k})$ can be written

$$\mathcal{E}^t(\mathbf{k})=\hbar\omega_0+\sum_{j=1}^{3}R_j\frac{\hbar^2}{2}(k_j-k_{0j})^2, \tag{2.8}$$

where the R_j are reciprocal "reduced" masses. The critical point is said to be of type $M_k(k=0, 1, 2, 3)$ when k of the masses R_j are negative.[2] The minimum $\hbar\omega_0$ is, of course, always of type M_0. The saddle point types M_1 and M_2 have often been cited as giving rise to important reflectivity structure.[4] It appears that M_1 and M_2 singularities may occur close to each other in energy ("back to back" so to speak) and thus give rise to peaks in ϵ_2. M_3 singularities are probably unimportant.

Due to crystal symmetry, all points in the "star" of $\mathbf{k}_0$ are critical points. In the absence of phonon broadening and Coulomb effects the nonanalytic character of $\epsilon_2(\omega_0)$ guarantees that the interesting structure in ϵ_2 can be "localized" in k space in the vicinity of the points $\mathbf{k}_0$. Weak Coulomb effects (without lifetime broadening) blur this simple picture somewhat by forming linear combinations of pair states $\mathbf{k}$ in the vicinity of $\mathbf{k}_0$. If $\hbar\omega_0$ is the minimum direct transition energy, Coulomb effects produce stable bound states which have well defined symmetry under the group of $\mathbf{k}_0$. Hence, even in this case much precise symmetry information is available.

If $\hbar\omega_0$ is not an absolute minimum, but $\mathbf{k}_0$ is of type M_0, one expects that weak Coulomb effects will produce metastable "bound" states which are not perfectly sharp but have some lifetime for decay into pair states of equal energy at a point $\mathbf{k}$ distant from the local minimum $\mathbf{k}_0$.

Phillips[4,7] suggested that even M_1 critical points may have metastable "saddle-point excitons" associated with them if the positive reciprocal masses R_1, R_2 are much greater than the negative mass $|R_3|$. This type of metastability is that of a particle perched on top of a rather flat Λ, and Duke and Segall[17] have objected to the use of the word metastable in such a context. However, Velicky and Sak[7] and the present author have demonstrated that Coulomb effects do lead to additional structure in this case although it is not that of a Lorentzian broadened δ function.

In the presence of strong Coulomb effects (still without phonon effects), the metastable excitons will be more seriously broadened. The minimum M_0 will still have sharp excitons but they may not be described as being associated with individual values of $\mathbf{k}_0$. The situation is analogous to the case of valley-orbit splitting due to central cell effects in impurity states.[16] The true states are linear combinations of all states in the star of $\mathbf{k}_0$ and the relevant symmetry group is the group of $\mathbf{k}=0$ rather than $\mathbf{k}_0$. Valley-orbit effects should be weaker for excitons than for impurities because the hole is more spread out than the central cell potential of an impurity. We will henceforth ignore valley-orbit effects and use the group of $\mathbf{k}_0$.

When phonon broadening is considered the information content of ϵ_2 is further degraded. Let $\hbar\Gamma/2$ be the imaginary part of the self-energy where Γ is the reciprocal lifetime due to phonon scattering. Then in the absence of Coulomb effects the analytic singularity at $\hbar\omega_0$ is pushed off the real axis by an amount $i\hbar\Gamma/2$ so that $(\hbar\omega-\hbar\omega_0)^{1/2}\rightarrow \mathrm{Re}(\hbar\omega-\hbar\omega_0+i\hbar\Gamma/2)^{1/2}$. If $\hbar\Gamma/2$ is large, the structure may no longer be regarded as coming from the immediate vicinity of the point $\mathbf{k}_0$. If several critical points with inequivalent $\mathbf{k}_0$ are separated by an energy $\sim\hbar\Gamma/2$ the information in ϵ_2 is badly degraded. This is probably the case for the main transition at $\sim$4 eV in covalent crystals (sometimes called an X transition). In silicon this is known to arise from a number of near degenerate critical points.[2,18]

When Coulomb and lifetime effects are considered, the bound state delta functions become Lorentzians of the form

$$L(\omega-\omega_b)\equiv\frac{\Gamma/(2\pi)}{(\omega-\omega_b)^2+(\Gamma/2)^2}. \tag{2.9}$$

Equation (2.9) applies to the case when M_0 is an absolute minimum so that the exciton states are perfectly sharp in the absence of phonon broadening. Otherwise the phonon broadening is additional to the metastability broadening previously discussed. Of course, if the material is "direct" the phonon broadening of the lowest M_0 exciton (which is then the bandgap) must vanish at $T=0$°K. (We ignore recombination broadening which is very small.)

Phillips[19] has emphasized that the metastability broadening due to Coulomb interactions of an M_0 singularity which is not the lowest M_0 may show interference effects with the continuum resulting in a line shape which is not Lorentzian. Phonon scattering, on the other hand, is incoherent and hence gives a more nearly Lorentzian broadening.

In the present work we will ignore many of the above complications and assume that it is useful to study the strain dependence of the wave function ψ^t and energy $\mathcal{E}^t$ of an isolated state $|t\rangle$ or a group of symmetry related states which are degenerate in energy. We will calculate the wave function and energy of these states to terms linear in the strain. On this basis we will obtain symmetry relations between the energy shifts and matrix elements of states which are related by symmetry in the unstrained crystal. The usefulness of this procedure depends on the existence of an exciton binding energy which is at least comparable to lifetime broadening effects so that a measurable fraction of the dielectric function can be ascribed to a single group of symmetry related states. Some of the results we derive will be valid independent of the strength of exciton binding. For example, strains which do not split the band degeneracies cause all states associated with a given critical point $\mathbf{k}_0$ to shift together (although other critical points in the star of $\mathbf{k}_0$ may shift differently). This result is independent of the degree of exciton binding. For strain-splitting energies large compared to exciton binding energies, the formerly degenerate bands are effectively "decoupled" and again the states associated with a given band shift by the same amount independent of exciton binding effects. However, in the high-strain or "decoupled" band limit, we have no symmetry relations between the matrix elements in different bands with or without exciton effects. This is because the matrix element in either case depends upon a suitably averaged effective mass which will not be the same for the split bands. Zero values of certain matrix elements may be predicted on the basis of symmetry in this case, however.

To be more explicit, we assume we have a set of states described by the labels

$$\psi_j^{t,\alpha}(\mathbf{k}_0), \tag{2.10}$$

$$\mathcal{E}_j^{t,\alpha}(\mathbf{k}_0). \tag{2.11}$$

---

[17] C. B. Duke and B. Segall, Phys. Rev. Letters **17**, 19 (1966).

[18] E. O. Kane, Phys. Rev. **146**, 558 (1966).

[19] J. C. Phillips, Phys. Rev. Letters **12**, 447 (1964).

The states are associated with a given critical point $\mathbf{k}_0$ and have symmetry type $j\alpha$ under the group of $\mathbf{k}_0$ where j denotes the irreducible representation and α denotes a partner function of the representation. For zero strain, $\mathcal{E}_j{}^t$ will be independent of the partner index α and also of which critical point we choose in the star of $\mathbf{k}_0$. t is a repetition index of the representation $j\alpha$. For practical purposes, t will generally refer to the exciton ground state which is much stronger in binding energy and optical matrix element than any excited state (binding energy goes like n^{-2} and optical matrix element squared goes like n^{-3} where n is the principle quantum number). We will frequently wish to indicate whether or not a result depends on t so we will retain the superscript explicitly.

Using Eqs. (2.3) and (2.9) we write $\epsilon_2{}^t$, the contribution of the states of (2.10) to the dielectric function, in the form

$$\epsilon_{2,ll}{}^t(\omega)=\frac{4\pi^2e^2}{3m_0{}^2\omega^2V}\sum_{\alpha,\mathbf{k}_0} F_l{}^{t\alpha}(\mathbf{k}_0) \times L(\mathcal{E}_j{}^{t,\alpha}(\mathbf{k}_0)-\mathcal{E}^0-\hbar\omega)\,, \quad (2.12)$$

$$F_l{}^{t\alpha}\equiv\langle 0|p_l|\psi_j{}^{t,\alpha}\rangle\langle\psi_j{}^{t,\alpha}|p_l|0\rangle. \quad (2.13)$$

L is the Lorentzian function defined in Eq. (2.9). The dielectric constant is written in diagonal form $\epsilon_{2,ll}$,[20] In the case of [001], [111], and [110] strains which we discuss in detail, the principal axes are always parallel and perpendicular to the strain. $F_l{}^{t\alpha}$ will always be summed over all α, $\mathbf{k}_0$ for which $\mathcal{E}_j{}^{t,\alpha}(\mathbf{k}_0)$ is the same. We will calculate F and $\mathcal{E}$ to terms linear in the strain. We will thus be able to calculate the differential response of ϵ_2 to strain coming from both matrix element variation and energy shifts.

If we suppress as many indices as possible $\delta\epsilon_2{}^t$, the variation with strain of $\epsilon_2{}^t$, may be written

$$\frac{\delta\epsilon_2{}^t}{\epsilon_2{}^t}=\frac{e\langle t'|D|t\rangle f^{t'}}{(\mathcal{E}^t-\mathcal{E}^{t'})F^t}+\frac{e\langle t|D|t\rangle}{L}\frac{dL}{d\hbar\omega}. \quad (2.14)$$

$f^{t'}$ is analogous to F^t but involves excited states $\psi^{t'}$. $\langle t'|D|t\rangle$ represents the matrix element of the strain operator which mixes the wave functions of states t and t'. e represents the strain. Assuming $f^{t'}\sim F^t$. $\langle t'|D|t\rangle \sim\langle t|D|t\rangle$, we see that the optical matrix element variation is proportional to $(\mathcal{E}^t-\mathcal{E}^{t'})^{-1}$ while the energy shift term is proportional to $(\hbar\Gamma)^{-1}$. Thus for sufficiently small lifetime broadening, the energy-shift terms are always dominant. This conclusion is valid if the lineshape function L is a Lorentzian or if it is assumed to be of square root form. The energy denominator $\mathcal{E}^t-\mathcal{E}^{t'}$ may vary over a wide range. For a nondegenerate band the only wave function admixture results from higher bands at $\mathbf{k}_0$ which may typically be separated in energy by 1 or 2 eV or more from the band of interest. We neglect these terms in our detailed calculations in the spirit of the "effective mass approximation" but they do actually make a finite contribution to the linear strain effect on ϵ_2. For bands whose degeneracy is lifted by spin-orbit interaction, $\mathcal{E}^t-\mathcal{E}^{t'}$ will be of the order of the spin-orbit splitting. We treat the symmetry properties of these terms in detail in Sec. III. For truly degenerate bands, $\mathcal{E}^t-\mathcal{E}^{t'}$ will be of the order of the exciton binding energy. The optical matrix element variations will clearly be of greatest importance in the case of degenerate bands for strains which act to split the degeneracy. If the lifetime broadening is of the order of the exciton binding, or greater than the exciton binding, $(\mathcal{E}^t-\mathcal{E}^{t'})\sim\hbar\Gamma$ and both types of terms are comparable. The line shape contributions from energy-shift effects and optical matrix element changes will certainly be different but probably not qualitatively different. There are sum rules effectively guaranteeing conservation of ϵ_2,[21] so that if the matrix element increases at one frequency it must decrease at a nearby frequency. Hence both terms will tend to have a "derivative" shape consisting of positive and negative peaks.

The importance of strain induced optical matrix element changes have also been emphasized by Gerhardt[22] and by Pollak and Cardona.[12]

B. Pair Wave Functions

We construct the electron-hole pair wave function out of one-electron-band functions using a Luttinger-Kohn basis[23] about the point $\mathbf{k}_0$. That is, we use as a basis the complete set of functions $e^{i\mathbf{k}\cdot\mathbf{r}}u_n(\mathbf{k}_0,\mathbf{r})$. Since all points in the star of $\mathbf{k}_0$ are equivalent we implicitly assume that the region of $\mathbf{k}$ about $\mathbf{k}_0$ which we will need to consider does not overlap an adjacent equivalent region. There will inevitably be some overlap which leads to what has been called valley-orbit splitting in the theory of impurity wave functions.[16] If the overlap is strong the $\mathbf{k}_0$ basis is unsuitable and one should use a basis with $\mathbf{k}_0=0$. The appropriate symmetry group is then that of Γ.

Of course, in a sense, the symmetry group of Γ is appropriate in any case. One can always form combinations of states belonging to different but equivalent $\mathbf{k}_0$ which transform irreducibly under Γ. However, for weak valley-orbit effects, there will be several different representations of Γ which are nearly degenerate with each

---

[20] In studying optical reflection at normal incidence for weak perturbations on a cubic system, we need only consider the change in the diagonal component of the dielectric tensor in the direction of the polarization vector of the incident light. This is because the reflected power is proportional to $|\mathbf{E}_0+\delta\mathbf{E}|^2$ where $\mathbf{E}_0$ is the unperturbed reflected electric field vector and $\delta\mathbf{E}$ is the perturbed field. The term $\delta\mathbf{E}\cdot\delta\mathbf{E}$ is negligible compared to $\mathbf{E}_0\cdot\delta\mathbf{E}$ and $\mathbf{E}_0$ is the same direction as the incident field.

[21] See for example, Eq. (10) in H. R. Philipp and H. Ehrenreich, Phys. Rev. **129**, 1550 (1963).

[22] U. Gerhardt, Phys. Rev. Letters **15**, 401 (1965).

[23] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).

other. In this case it is simpler to study the group of $\mathbf{k}_0$ first and take account of the equivalent $\mathbf{k}_0$ at the end of the calculation.

The pair state consists of an electron and hole which we describe by a two-particle wave function

$$\psi^t(\mathbf{r}_1,\mathbf{r}_2)=\sum_{n_1,n_2}\varphi_{n_1n_2}{}^t(\mathbf{r}_1-\mathbf{r}_2)e^{i\mathbf{k}_0\cdot(\mathbf{r}_1-\mathbf{r}_2)}\times u_{n_1}(\mathbf{r}_1)u_{n_2}{}^\dagger(\mathbf{r}_2)\,. \tag{2.15}$$

The coordinate $\mathbf{r}_2$ refers to the hole, hence the † (adjoint) on its wave function. The "envelope" function $\varphi(\mathbf{r}_1-\mathbf{r}_2)$ is constructed out of $\mathbf{k}$ vectors over a single Brillouin zone.

$$\varphi^t(\mathbf{r}_1-\mathbf{r}_2)\equiv\int_{\mathrm{BZ}}b^t(\mathbf{k})e^{i(\mathbf{k}-\mathbf{k}_0)\cdot(\mathbf{r}_1-\mathbf{r}_2)}d\mathbf{k}\,. \tag{2.16}$$

The superscript t indexes a complete set of φ's subject to Eq. (2.16). φ is a function of $\mathbf{r}_1-\mathbf{r}_2$ because we are considering "direct" transitions and ignoring the small wave vector of the light. Hence our exciton has zero total crystal momentum.

We will work within the effective mass approximation as developed for degenerate bands by Luttinger and Kohn.[23] The effective Hamiltonian for the envelope function φ in the absence of strain is given by

$$H_0=H_{\mathrm{KE}}+H_{\mathrm{C}}+\hbar\omega_0\,, \tag{2.17}$$

$$\hbar\omega_0\equiv E_{n_1}(\mathbf{k}_0)-E_{n_2}(\mathbf{k}_0)\,, \tag{2.18}$$

$$H_{\mathrm{C}}=-\frac{e^2}{\epsilon_0|r_1-r_2|}\,, \tag{2.19}$$

$$H_{\mathrm{KE}}=p_{\varphi l}p_{\varphi m}G_{lm}/2\equiv T_{lm}G_{lm}\,. \tag{2.20}$$

$\hbar\omega_0$ is the band energy at the critical point, $\mathbf{k}_0$, H_{C} is the mutual Coulomb interaction of electron and hole. ϵ_0 is the zero-frequency, zero-wave-number dielectric constant. A more sophisticated treatment of the dielectric function may be desirable in some cases but we will not treat these complications. We also assume that H_{C} is a diagonal operator in band indices, which again is only approximately true. We have neglected the exchange contribution to H_{C} which leads to a correlation between the electron and hole spins.[15] The kinetic energy operator H_{KE} is quadratic in p_φ, a crystal momentum operator which acts only on φ, and an effective-mass tensor G_{lm} which is also implicitly an operator on band indices. These operators can be expressed in terms of matrices whose dimension is equal to the number of degenerate bands. The matrices must transform under the group of $\mathbf{k}_0$ in the same way that $p_{\varphi l}p_{\varphi m}/2\equiv T_{lm}$ transforms.

The strain Hamiltonian can be written

$$H_{\mathrm{str}}=\sum_{l,m}e_{lm}h_{lm}\,, \tag{2.21}$$

where e_{lm} is the strain tensor. Because the strain has infinite wavelength it commutes with the envelope wave function, φ, but operates on the pair bands $u_{n_1}u_{n_2}{}^\dagger$. This operator can also be expressed in terms of matrix operators. In fact, because e and $p_\varphi{}^2$ are both symmetric second rank tensors, the structure of H_{str} and H_{KE} is formally identical.

We also wish to discuss the optical matrix element of the momentum operator between the ground state $|0\rangle$ and the exciton state $\psi^t(\mathbf{r}_1,\mathbf{r}_2)$. Following Elliott,[24] this can be written

$$\langle 0|p_i|\psi^t\rangle=\sum_{n_1,n_2}V^{1/2}\varphi_{n_1,n_2}{}^t(0)\times\int_{\mathrm{cell}}u_{n_2}{}^\dagger(\mathbf{r})p_iu_{n_1}(\mathbf{r})\frac{d\mathbf{r}}{\tau}\,. \tag{2.22}$$

The integral is over the unit cell of volume τ. V is the crystal volume, $\varphi(0)$ is the envelope function evaluated at the origin, $\mathbf{r}_1-\mathbf{r}_2=0$.

C. Symmetry Properties

Group of $\mathbf{k}_0$

We wish to use the symmetry properties of the group of $\mathbf{k}_0$ to characterize the exciton wave function and to parameterize the effective-interaction Hamiltonian.

We assume we are interested in a set of band states $u_{j_1,\alpha_1}(\mathbf{r}_1)$. $u_{j_2{}^\dagger,\alpha_2}(\mathbf{r}_2)$ for the electron and hole which have been selected to give irreducible representations j_1, j_2 of the group of $\mathbf{k}_0$. The symbols α_1, α_2 label the partner functions of the irreducible representations j_1, j_2.

Throughout this paper we use $j\alpha$ in the subscript position to indicate symmetry transformation properties under the group of $\mathbf{k}_0$. It is sometimes convenient to use $j\alpha$ as a label without implying symmetry properties. In this case we promote it to superscript position. We try as much as possible to reserve the subscript position for symmetry information pertaining to the group of $\mathbf{k}_0$. We use Koster *et al.*'s[13] notation for the representations of the point groups.

(*a*) *Irreducible pair bands,* We wish to form linear combinations of pair bands which will themselves transform irreducibly under $\mathbf{k}_0$. This is analogous to the coupling of products of angular momentum functions with Clebsch-Gordan coefficients to give total angular momentum states. We can write

$$U_{j\alpha}(\mathbf{r}_1,\mathbf{r}_2)=\sum_{\alpha_1,\alpha_2}\gamma_{j_1\alpha_1,(j_2\alpha_2)^*;j\alpha}u_{j_1\alpha_1}(\mathbf{r}_1)\times u_{j_2\alpha_2}{}^\dagger(\mathbf{r}_2)e^{i\mathbf{k}_0\cdot(\mathbf{r}_1-\mathbf{r}_2)}\,. \tag{2.23}$$

We will call the U's pair bands. The indices $(j_2\alpha_2)$ have been starred to indicate that the matrix transforming $u_{j_2\alpha_2}{}^\dagger$ is the complex conjugate of the matrix transforming $u_{j_2\alpha_2}$. γ is a unitary matrix. The analogous matrix

---

[24] R. J. Elliott, Phys. Rev. **108**, 1384 (1957).

without the * has been tabulated by Koster *et al.*[13] for all point groups. Their results are immediately applicable for real basis functions, of course.

In Sec. II C 1(g) we discuss how one can make use of Kramers time-reversal operator to adapt the Koster tables to the complex case as well.

(*b*) *Effective strain Hamiltonian.* The strain operator of Eq. (2.21) may also be written in an irreducibly transforming manner:

$$H_{\mathrm{str}}=\sum_{s,j,\alpha}(e_{j\alpha}{}^{s})^{*}h_{j\alpha}{}^{s}. \qquad (2.24)$$

s is a repetition index which is needed for some poin. groups. The transformation between $e_{j\alpha}{}^{s}$ and e_{lm} wilt be explicitly given in the detailed applications in Secl III. Since e_{lm} is real, the * in Eq. (2.24) only affects the transformation coefficients. Most single-group representations are real so the * is usually not needed. Equation (2.24) looks unsymmetrical, but the * could equally well have been chosen to operate on $h_{j\alpha}{}^{s}$ instead of $e_{j\alpha}{}^{s}$. Equations (2.21) or (2.24) can be looked on as a generalized scalar product of the quantities e and h. A unitary transformation on h must be accompanied by the conjugate transformation on e to maintain the scalar product invariant.

In studying the symmetry conditions imposed on the matrix elements between band states U of the operator $h_{j\alpha}{}^{s}$ in Eq. (2.24) we write the following linear combinations, using the unitary Clebsch-Gordan matrix γ as in Eq. (2.23):

$$\sum_{\alpha_1,\alpha_2}\gamma_{(j_1\alpha_1)^*,j_2\alpha_2;(j'\alpha')^*}\langle U_{j_1\alpha_1}|h_{j\alpha}|U_{j_2\alpha_2}\rangle = D_j\delta_{jj'}\delta_{\alpha\alpha'}\sqrt{n}. \qquad (2.25)$$

The $\sqrt{n}$ is introduced for convenience. n is the dimension of j.

By explicit construction, the left-hand side of (2.25) transforms like $(j'\alpha')$ if $h_{j\alpha}$ is not transformed. If $h_{j\alpha}$ is transformed as well, the requirement $\delta_{jj'}\delta_{\alpha\alpha'}$ is necessary and sufficient for the left-hand side of Eq. (2.25) to be invariant under symmetry transformations of the group of $\mathbf{k}_0$. Our approach is very similar to that of Pikus.[25] Our results for the Γ point are analogous to those of Luttinger[26] as generalized to the case of the strain operator by Kleiner and Roth.[27] We feel that Luttinger's approach was unsatisfactory in not emphasizing the fundamental role played by the representations generated by $U_{j_1}{}^{*}\times U_{j_2}$.

Equation (2.25) may be considered to be the definition of the quantity D_j which is a deformation potential constant connecting the pair bands U_{j_1} and U_{j_2}. We will generally be interested in the case where j_1 and j_2 refer to the same band. Using the unitary character of γ, Eq. (2.25) is easily inverted

$$\begin{aligned}\langle U_{j_1\alpha_1}|h_{j\alpha}|U_{j_2\alpha_2}\rangle &= (\gamma_{(j_1\alpha_1)^*,j_2\alpha_2;(j\alpha)^*})^{*}D_j\sqrt{n}\\ &=\gamma_{j_1\alpha_1,(j_2\alpha_2)^*;j\alpha}D_j\sqrt{n}.\end{aligned} \qquad (2.26)$$

n is the dimension of j. For real representations, the conjugations on γ are superfluous. For the complex case we can simplify the conjugations somewhat using time-reversal symmetry as discussed in Sec. II C 1(g). [See Eq. (2.51).] Equation (2.26) is the point group analog of the Wigner-Eckart[28] theorem for the rotation group. Equation (2.26) may also be regarded as defining h as an operator on band indices. In this usage we will use the abbreviation $\gamma_{j\alpha}$. Equation (2.24) can then be written

$$\begin{aligned}H_{\mathrm{str}}&=\sum_{s,j,\alpha}(e_{j\alpha}{}^{s})^{*}\tilde{\gamma}_{j\alpha}D_j{}^{s},\\ \langle j_1\alpha_1|\tilde{\gamma}_{j\alpha}|j_2\alpha_2\rangle&\equiv\sqrt{n}\gamma_{j_1\alpha_1,(j_2\alpha_2)^*;j\alpha},\end{aligned} \qquad (2.27)$$

where n is the dimension of the representation j. An entirely analogous expression may be written for the kinetic energy operator

$$H_{\mathrm{KE}}=\sum_{s,j,\alpha}(T_{j\alpha}{}^{s})^{*}\tilde{\gamma}_{j\alpha}R_j{}^{s}. \qquad (2.28)$$

The quantities $R_j{}^{s}$ which are the analogs of the $D_j{}^{s}$ are reciprocal effective mass parameters. The formal identity of Eqs. (2.27) and (2.28) stems from the fact that e and T are both symmetric second-rank tensors.

The pair band deformation parmeters $D_j{}^{s}$ and reciprocal mass parameters $R_j{}^{s}$ of Eqs. (2.27) and (2.28) can be related to the corresponding one electron parameters through the use of Eq. (2.23), using the fact that the strain and kinetic energy operators are given by the difference of two one-electron operators $\mathcal{O}(\mathbf{r}_1)-\mathcal{O}(\mathbf{r}_2)$. The minus sign refers to the hole operator. To give a simple example, assume the conduction band transforms like the identity. We then have

$$\begin{aligned}R_j{}^{s}&=r_1{}^{s}\delta_{1j}-r_j{}^{s},\\ D_j{}^{s}&=d_1{}^{s}\delta_{1j}-d_j{}^{s},\end{aligned} \qquad (2.29)$$

where the d's are the single-band analogs of the pair-band D's. Similar relations may be written for less trivial cases, but there will be different numerical coefficients.

With the strain and kinetic energy operators of Eqs. (2.27) and (2.28) and the Coulomb operator of Eq. (2.19) we are, in principal, equipped to calculate the exciton spectrum in the effective mass approximation. (The Coulomb operator should be multiplied by the identity matrix.) Calculations of this sort, involving nonspherical kinetic energy operators, have usually been performed by variational methods[16,29] although

---

[25] G. E. Pikus, Zh. Eksperim. i Teor. Fiz. **41**, 1258 (1961) [English transl.: Soviet Phys.—JETP **14**, 898 (1962)].

[26] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).

[27] W. H. Kleiner and L. M. Roth, Phys. Rev. Letters **2**, 334 (1959).

[28] See, for example, U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press Inc., New York, 1959), p. 76.

[29] D. Schechter, J. Phys. Chem. Solids **23**, 237 (1962).

more exact methods have been used.[30] We will not attempt such calculations here.

(*c*) *Optical matrix elements.* We wish to compute the matrix elements of the electron-photon interaction energy $\mathbf{A}\cdot\mathbf{p}$ where $\mathbf{A}$ is the vector potential and $\mathbf{p}$ is the momentum operator. We write the optical interaction in irreducible form

$$H_{\text{opt}}=\frac{e}{m_0c}\mathbf{A}\cdot\mathbf{p}=\frac{e}{m_0c}\sum_{j,\alpha}A_{j\alpha}{}^*p_{j\alpha}. \tag{2.30}$$

We want the matrix elements of this operator between the ground state $|0\rangle$ and the excited state $\psi_{j\alpha}{}^t$ which may be written

$$\langle 0|p_{j'\alpha'}|\psi_{j\alpha}{}^t\rangle=\mathcal{P}_j{}^t\delta_{jj'}\delta_{\alpha\alpha'}. \tag{2.31}$$

According to Eq. (2.22), $\mathcal{P}_j{}^t$ can be written in the form

$$\mathcal{P}_j{}^t=a_1{}^t\varphi_1{}^t(0)P_j\sqrt{V}, \tag{2.32}$$

$$P_j=\langle 0|p_{j\alpha}|U_{j\alpha}\rangle. \tag{2.33}$$

$a_1{}^t$ is a normalization constant so that $\varphi_1{}^t$ is orthonormal. Since Eq. (2.22) involves $\varphi(0)$, only the identity symmetry φ_1 contributes. Equations (2.31) and (2.32) are only valid for low strain where $\psi_{j\alpha}{}^t$ is the same as in the unstrained crystal. Equation (2.33) remains true for high strain and will be useful in showing that certain optical-matrix elements are zero. (We ignore the strain admixture of other band multiplets U_{j_1} into U_j).

We now turn to the problem of the strain dependence of exciton energies and wave functions. The results are very simple in the case where no band splitting of the $U_{j\alpha}$ multiplet occurs and will be described first. When band splitting occurs, the results are more complex but have simple limiting cases in the high and low strain limits.

(*d*) *No band splitting.* The strain symmetries $e_1{}^s$ which are totally symmetric under the group of $\mathbf{k}_0$ will not give rise to band splitting. In other words, $\tilde{\gamma}_1$ in Eq. (2.27) is always the identity matrix. Strains of this type will not change the exciton wave function or the exciton binding energy relative to the band edge (electron-hole continuum). The exciton spectrum then shifts "as a whole" with an energy shift given by $e_1{}^sD_1{}^s$. There are no optical matrix element changes (ignoring admixture of bands outside the $U_{j\alpha}$ multiplet) so that $\partial\epsilon_2/\partial e_1{}^s$ is proportional to an energy derivative of the unstrained ϵ_2, $\partial\epsilon_2/\partial(\hbar\omega)$. Hydrostatic stress always has this effect, of course. In the hydrostatic case, all members of the star of $\mathbf{k}_0$ respond in the same manner. Less symmetric strains may have components $e_1{}^s$ which are totally symmetric under the group of a given $\mathbf{k}_0$ but do not have the same value for all members of the star of $\mathbf{k}_0$. Nondegenerate bands only couple to strains of symmetry $e_1{}^s$ so that the above simple description always applies to the nondegenerate case. Bands which have only the Kramers degeneracy also behave in this way.

(*e*) *Low strain.* By low strain we mean that strain splittings are small compared to the exciton binding energy. In this case we consider the exciton wave function $\psi_{j\alpha}{}^t$ in the zero strain limit. We study the strain splitting of the partner functions α in the degenerate multiplet j. t is a repetition index but the ground state will usually be of most interest. If we ignore the matrix elements of the strain operator connecting one multiplet with another we can use the identical symmetry arguments as before to write an effective strain Hamiltonian for the multiplet t. Equation (2.27) becomes

$$H_{\text{str}}=\sum_{s,j,\alpha}(e_{j\alpha}{}^s)^*\tilde{\gamma}_{j\alpha}\mathfrak{D}_j{}^{s,t}. \tag{2.34}$$

The only difference is that we have different deformation potential constants $\mathfrak{D}$ and $\tilde{\gamma}_{j\alpha}$ is an operator on the $\psi_{j\alpha}{}^t$ subspace rather than on the pair bands, U. We may use the Clebsch-Gordan matrix γ to write the total exciton wave function $\psi_{j\alpha}{}^t$ in terms of envelope functions φ and pair band functions U.

$$\psi_{j\alpha}{}^t=\sum_{j_1}a_{j_1}{}^t\sum_{\alpha_1,\alpha_2}\gamma_{j_1\alpha_1,j_2\alpha_2;j\alpha}\varphi_{j_1\alpha_1}{}^tU_{j_2\alpha_2}. \tag{2.35}$$

We have introduced the normalization constants a so that the envelope functions φ can be taken to be orthonormal.

$$\langle\varphi_{j\alpha}{}^t|\varphi_{j'\alpha'}{}^t\rangle=\delta_{jj'}\delta_{\alpha\alpha'}. \tag{2.36}$$

Normalization of ψ and U then requires

$$\sum_{j_1}|a_{j_1}{}^t|^2=1. \tag{2.37}$$

The values of a and the functional form of φ, apart from what is determined by symmetry, must be found by solution of the effective mass equation, using Eq. (2.28). With the use of Eqs. (2.35) and (2.37) the constants $\mathfrak{D}_j{}^{s,t}$ in Eq. (2.34) may be related to the corresponding constants $D_j{}^s$ in Eq. (2.27). We will not attempt this in the general case, but will provide a number of examples in the specific cases which we treat in Sec. III.

Equation (2.34) is sufficient to calculate the energy dependence of the states $\psi_{j\alpha}{}^t$ to first order in the strain. We also wish to write $\psi_{j\alpha}{}^t$ to first order in the strain for the purpose of computing optical matrix elements to that order. The results could be written in terms of perturbation theory, but the details may be bypassed with the use of symmetry. We can write

$$\psi^{t,j\alpha}=\psi_{j\alpha}{}^t+\sum_{\substack{j_1,\alpha_1,s\\ j_2,\alpha_2}}\gamma_{j_1\alpha_1,j_2\alpha_2;j\alpha}e_{j_1\alpha_1}{}^s\psi_{j_2\alpha_2}{}^{t,s}. \tag{2.38}$$

The form of Eq. (2.38) is obtained by recognizing that $\psi^{t,j\alpha}$ must transform like $j\alpha$ if both e and ψ are transformed. If $e_{j_1\alpha_1}$ is considered fixed, then $\psi_{j\alpha}{}^t$ and $\psi^{t,j\alpha}$

---

[30] K. S. Mendelson and H. M. James, J. Phys. Chem. Solids **25**, 729 (1964).

transform differently, which we indicate by use of the superscript position.

(*f*) *High strain.* In the limit of strain splittings large compared to exciton-binding energies, the appropriate procedure is first to diagonalize the strain Hamiltonian of Eq. (2.27). Let us assume that $U_{j\beta}$ represent the bands which diagonalize (2.27). The elements of the kinetic energy operator, Eq. (2.28), which couple $U_{j\beta}$ and $U_{j\beta'}$ may be ignored in the high-strain limit and we can say that the bands have been "strain decoupled." The exciton-binding energies in the decoupled bands will depend on an appropriately averaged effective mass which will in general be a function of the index β. The wave function may be written

$$\psi^{t,j\beta}=a_1^{t\beta}\varphi_1^{t\beta}U_{j\beta}+\tilde{\psi}^{t,j\beta}, \tag{2.39}$$

where, by definition, $\tilde{\psi}$ does not contain the envelope symmetry φ_1 and hence does not contribute to the optical matrix element. The analogs of Eqs. (2.31) and (2.32) are

$$\langle 0|p_{j'\alpha'}|\psi^{t,j\beta}\rangle=\mathcal{P}_j^{t\beta}\delta_{jj'}\delta_{\alpha'\beta}, \tag{2.40}$$

$$\mathcal{P}_j^{t\beta}=a_1^{t\beta}\varphi_1^{t\beta}(0)P_j\sqrt{V}. \tag{2.41}$$

Equation (2.33) for P_j still holds. The only difference from the low-strain case is that φ_1 and $\mathcal{P}$ now depend on the partner index β. The occurrence of the $\delta_{jj'}\delta_{\alpha'\beta}$ factors, which strongly affect the polarization properties, are a consequence of the $U_{j\beta}$ term and are unaltered by the strain. The exciton states in a given band will all shift together with the same deformation potential constant which is given by the appropriate combination of D's rather than the $\mathfrak{D}$'s of the low-strain case. In this sense, the high-strain results are simpler. The strain decoupling has reduced the problem to the case of independent nondegenerate bands, $U_{j\beta}$. The wave function or optical matrix-element changes will depend inversely on strain and will vanish in the infinite strain limit assuming one can still ignore admixing of other multiplets, U_{j1}. The high-strain limit will be harder to reach for the wave function than for the energy, since wave functions are always more sensitive than energies. We illustrate the general remarks of this section in more detail in Sec. IIIA 1(b).

(*g*) *Time reversal and phase relations.* The symmetry implied by time reversal can be studied with the use of Kramers operator, K.[13] which may be defined by

$$K=-Ci\sigma_y, \tag{2.42}$$

where C is complex conjugation and $i\sigma_y$ reverses the spin direction in the usual representation associated with the Pauli matrices. For special points like Γ, X, and L where $\mathbf{k}_0$ and $-\mathbf{k}_0$ are equivalent, the operator K may be used directly to deduce symmetry relations. For any point $\mathbf{k}_0$ in the diamond lattice we may introduce the operator $\mathcal{K}$ defined by

$$\mathcal{K}=K(\boldsymbol{\tau}|J), \tag{2.43}$$

where $(\boldsymbol{\tau}|J)$ is inversion followed by a translation of $\boldsymbol{\tau}=(a/4,a/4,a/4)$. $\mathcal{K}$ leaves $\mathbf{k}_0$ invariant, commutes with the Hamiltonian, and possesses the property

$$\mathcal{K}^2=K^2=(-1)^n, \tag{2.44}$$

where n is the number of electrons in the state on which $\mathcal{K}$ operates. When n is odd, $\mathcal{K}$ cannot be diagonalized, since $\mathcal{K}\psi=\lambda\psi$ implies $\mathcal{K}^2\psi=|\lambda|^2\psi=-\psi$ which is a contradiction. Then ψ and $\mathcal{K}\psi$ are independent states called Kramers doublets and energy bands in the diamond lattice are doubly degenerate throughout the zone, a well-known result.

The discussion that follows uses the operator $\mathcal{K}$. However, we will actually use K whenever $\mathbf{k}_0$ and $-\mathbf{k}_0$ are equivalent, i.e., for Γ and L, in order to minimize conflict with Koster's conventions.

As discussed in Sec. II C 1(b), in order to find the symmetry relations between matrix elements of the form $\langle U_{j_1\alpha_1}|h_{j\alpha}|U_{j_2\alpha_2}\rangle$ we need to know the unitary Clebsch-Gordan matrix $(\gamma_{(j_1\alpha_1)^*,j_2\alpha_2;(j\alpha)^*})^*$. (See Eq. 2.26) Koster *et al.*[13] have tabulated the γ matrices without the complex conjugations. We can use these tables by noting that if the multiplet $\psi_{j\alpha}$ transforms by the matrix $D_{\alpha\alpha'}{}^j(\mathcal{R})$ where $\mathcal{R}$ is a group element, then $\mathcal{K}\psi_{j\alpha}$ transforms by the matrix $(D_{\alpha\alpha'}{}^j(\mathcal{R}))^*$. This result follows from the fact that $\mathcal{K}$ and $\mathcal{R}$ commute, modulo a Bravais lattice translation.[31] The lattice translation is irrelevant because, in Eq. (2.15), the nonperiodic part of the pair wave function involves $\mathbf{r}_1-\mathbf{r}_2$ which is invariant under translations.[32]

We can then use Koster's tables to reduce the outer products $\psi_{j_1\alpha_1}{}^*\times\psi_{j_2\alpha_2}$ if we know the relations between $\mathcal{K}\psi$ and ψ.

We will limit our discussion to the two cases we will need in the detailed examples, namely, for an even number of electrons, the case where we may take

$$\mathcal{K}\psi_{j\alpha}=\psi_{j\alpha};\quad n\text{ even} \tag{2.45}$$

and for an odd number of electrons where we may take[13]

$$\mathcal{K}\psi_{j\alpha}=(-1)^{q-\alpha}\psi_{j,-\alpha};\quad n\text{ odd}. \tag{2.46}$$

Here a basis has been chosen such that α takes half integral values from $-q$ to q. See Koster *et al.*[13] for a more general discussion.

The defining relation for Koster's γ matrices is

$$\Phi_{j\alpha}=\sum_{\alpha_1,\alpha_2}\gamma_{j_1\alpha_1,j_2\alpha_2;j\alpha}\psi_{j_1\alpha_1}\psi_{j_2\alpha_2}. \tag{2.47}$$

If the $\psi_{j\alpha}$ correspond to n even and Eq. (2.45) applies, the γ matrices must be real and all complex conjugation relations can be ignored. (It is sometimes convenient to use complex representations even when

---

[31] M. Lax, Group Theory Notes (to be published).

[32] Even for a one-electron state the lattice translation is irrelevant if one notes that $K\psi_{j\alpha}\times\psi_{j'\alpha'}$ is invariant under lattice translations when $\psi_{j\alpha}$ and $\psi_{j'\alpha'}$ have the same k vector.

(2.45) can be satisfied but we will not discuss this nonessential complication.)

In case (2.46) applies, we may substitute Eq. (2.46) for $\psi_{j_1\alpha_1}$ in (2.47) and obtain the relation

$$\Phi_{j\alpha}=\sum_{\alpha_1,\alpha_2}(-1)^{q_1-\alpha_1}\gamma_{j_1(-\alpha_1),j_2\alpha_2;j\alpha}\mathcal{K}\psi_{j_1\alpha_1}\psi_{j_2\alpha_2}. \tag{2.48}$$

Since $\mathcal{K}\psi_{j_1\alpha_1}$ transforms according to the conjugate of the transformation of $\psi_{j_1\alpha_1}$, we have the relation

$$\gamma_{(j_1\alpha_1)^*,j_2\alpha_2;j\alpha}=(-1)^{q_1-\alpha_1}\gamma_{j_1(-\alpha_1),j_2\alpha_2;j\alpha}. \tag{2.49}$$

We may further operate with $\mathcal{K}$ on both sides of Eq. (2.47) and use (2.46) to obtain the relation

$$(\gamma_{j_1\alpha_1,j_2\alpha_2;j\alpha})^*=(-1)^{q_1+q_2-\alpha_1-\alpha_2}\gamma_{j_1(-\alpha_1),j_2(-\alpha_2);j\alpha}. \tag{2.50}$$

We have assumed that $\psi_{j_1\alpha_1}$ and $\psi_{j_2\alpha_2}$ both satisfy Eq. (2.46) and that $\Phi_{j\alpha}$ satisfies Eq. (2.45).

Equations (2.49) and (2.50 may be used to write (2.26) in the simpler form

$$\langle U_{j_1\alpha_1}|h_{j\alpha}|U_{j_2\alpha_2}\rangle=(-1)^{q_2+\alpha_2}\gamma_{j_1\alpha_1,j_2(-\alpha_2);j\alpha}D_j\sqrt{n}. \tag{2.51}$$

We wish to determine the phase of the matrix elements, D_j, in (2.51) and in the analogous expression for the even electron case. These phases are essential when two matrix elements are to be added. Taking an arbitrary Hermitian operator $\mathcal{O}_{j\alpha}$ we use $\mathcal{K}$ to obtain

$$\langle\psi_{j_1\alpha_1}|\mathcal{O}_{j\alpha}|\psi_{j_2\alpha_2}\rangle=\langle\mathcal{K}\psi_{j_2\alpha_2}|\mathcal{O}_{j\alpha}{}^{\mathcal{K}}|\mathcal{K}\psi_{j_1\alpha_1}\rangle, \tag{2.52}$$

$$\mathcal{O}_{j\alpha}{}^{\mathcal{K}}\equiv\mathcal{K}\mathcal{O}_{j\alpha}\mathcal{K}^{-1}. \tag{2.53}$$

The self-adjoint character of $\mathcal{O}^{\mathcal{K}}$ has been used. For $\mathcal{O}$ equal the unperturbed Hamiltonian or the strain Hamiltonian $\mathcal{O}_{j\alpha}{}^{\mathcal{K}}=\mathcal{O}_{j\alpha}$. For $\mathcal{O}$ equal the spatial part of the spin-orbit Hamiltonian $\sim\nabla V\times\mathbf{p}$, $\mathcal{O}_{j\alpha}{}^{\mathcal{K}}=-\mathcal{O}_{j\alpha}$. For our purposes we will then assume $\mathcal{O}^{\mathcal{K}}=\pm\mathcal{O}$.

Using Hermiticity and Eq. (2.52) together with (2.45) we obtain

$$\langle\psi_{j_2\alpha_2}|\mathcal{O}_{j\alpha}{}^{\mathcal{K}}|\psi_{j_1\alpha_1}\rangle=\langle\psi_{j_2\alpha_2}|\mathcal{O}_{j\alpha}|\psi_{j_1\alpha_1}\rangle^*;\quad n\text{ even}. \tag{2.54}$$

Using (2.26), we have

$$D_j=\pm D_j^*;\ \mathcal{O}^{\mathcal{K}}=\pm\mathcal{O}. \tag{2.55}$$

For the case of n odd, the relation analogous to (2.54) is

$$\begin{aligned}&\langle\psi_{j_2(-\alpha_2)}|\mathcal{O}_{j\alpha}{}^{\mathcal{K}}|\psi_{j_1(-\alpha_1)}\rangle\\&\qquad=(-1)^{q_1-\alpha_1+q_2-\alpha_2}\langle\psi_{j_2\alpha_2}|\mathcal{O}_{j\alpha}|\psi_{j_1\alpha_1}\rangle^*.\end{aligned} \tag{2.56}$$

Using (2.26), (2.49), and (2.51) in (2.56) we can then show that Eq. (2.55) also holds for n odd. Hence the "reduced" matrix elements D_j as defined in Eq. (2.51) are real for operators $\mathcal{O}^{\mathcal{K}}=\mathcal{O}$ and pure imaginary for operators $\mathcal{O}^{\mathcal{K}}=-\mathcal{O}$.

It may seem irrelevant to discuss the odd electron case since we are concerned with electron-hole pairs. However, if the electron is nondegenerate and the hole is degenerate (or vice-versa) only one spin will be coupled to the orbit since we ignore spin-spin interactions. The dynamical problem can be solved using double group states where the spin of the nondegenerate particle is ignored. The ignored spin states must finally be summed over at the end of the calculation when we compute optical-matrix elements.

(*h*) *Spin-orbit interaction.* The spin-orbit interaction may be written in the form

$$\begin{aligned}H_{so}&=\mathbf{S}_1\cdot\boldsymbol{\sigma}_1-\mathbf{S}_2\cdot\boldsymbol{\sigma}_2,\\\mathbf{S}_i&=\frac{\hbar}{4m^2c^2}[\nabla V_i\times\mathbf{p}_i],\end{aligned} \tag{2.57}$$

where 1 and 2 refer to the electron and hole as usual. $\mathbf{S}_i$ operates on the orbital wave function and transforms like an axial vector. It has the time-reversal character $\mathcal{O}^{\mathcal{K}}=-\mathcal{O}$ as discussed in the preceding section. $\boldsymbol{\sigma}_i$ refers to the Pauli spin matrices. Since the main contribution to $\mathbf{S}_i$ comes from the atomic core where ∇V_i and $\mathbf{p}_i$ are large it is a good approximation to ignore the dependence of $\mathbf{S}_i$ on the envelope function φ and treat $\mathbf{S}_i$ as an operator which acts on the pair bands U and commutes with the envelope function φ just as in the case of the strain operator. The time-reversal property $\mathcal{O}^{\mathcal{K}}=-\mathcal{O}$ makes the spin-orbit interaction between the pair bands quite different from the strain and kinetic energy operators which are even under time reversal. We proceed to write an effective Hamiltonian for H_{so} in the usual manner. Write (2.57) in irreducibly transforming manner

$$H_{so}=\sum_{j,\alpha}(\sigma_{1,j\alpha})^*S_{1,j\alpha}-\sum_{j,\alpha}(\sigma_{2,j\alpha})^*S_{2,j\alpha}. \tag{2.58}$$

Writing the $\tilde{\gamma}_{j\alpha}$ matrices for $U^*\times U$ as in (2.27) and (2.51), we have

$$H_{so}=\sum_{j\alpha}\tilde{\gamma}_{j\alpha}(\lambda_{1,j}\sigma_{1,j\alpha}{}^*-\lambda_{2,j}\sigma_{2,j\alpha}{}^*), \tag{2.59}$$

where the λ_j are spin-orbit constants analogous to the D_j in (2.51) though coupling to different j because of the different time-reversal character.

When both electron and hole bands are degenerate we must consider both terms in Eq. (2.59). The relevant group is the single group since the wave function contains an even number of electrons. Because of the spin degrees of freedom the number of bands $U_{j\alpha}$ closely spaced in energy will be quite large. Usually more than one value of j will be represented so that our present approximation of considering only a single j would be inadequate. If one of the bands is nondegenerate, however, it has no diagonal spin-orbit coupling. The spin degree of freedom then does not enter into the Hamiltonian. For the solution of the dynamical problem the spin degree of freedom of the nondegenerate particle can be suppressed and the effective wave function belongs to the double group. The neglected spin degree of freedom must be summed over at the end of the calculation when optical matrix elements are computed.

(*i*) *Noncubic rotations and the Wigner-Eckart theorem.* The tables of Koster *et al*,[13] for the unitary matrices $\gamma_{j\alpha}$ are given in terms of a specific representation. It is frequently convenient to transform to an alternate representation appropriate to the symmetry of the problem. In this connection it is useful to consider "pseudorotations" which are more general than the true rotations compatible with cubic symmetry. Our approach is a generalization of the method of Luttinger who expressed the $\gamma_{j\alpha}$ matrices in terms of angular momentum operators.[26] Luttinger's method was first applied to the strain perturbation problem by Kleiner and Roth.[27]

Consider Eq. (2.26) which we write more compactly as

$$\langle j_1\alpha_1|h_{j\alpha}|j_2\alpha_2\rangle=\langle 1,2|\gamma|j\alpha\rangle\Delta_j. \tag{2.60}$$

We assume j_1 and j_2 are irreducible under both the cubic group and the full rotation group. The method of "pseudorotations" applies only to this case. On the other hand $|j_1\alpha_1\rangle\times|j_2\alpha_2\rangle$ may contain representations which are irreducible under the rotation group but are cubically reducible.

We apply the unitary transformation

$$\begin{aligned}|j_1\alpha_1\rangle&=\sum_{\alpha_1'} r_{1'1}|j_1\alpha_{1'}\rangle,\\|j_2\alpha_2\rangle&=\sum_{t_2'} r_{2'2}|j_2\alpha_{2'}\rangle.\end{aligned} \tag{2.61}$$

The r's correspond to an arbitrary pure rotation if $|j_1\alpha_1\rangle$, $|j_2\alpha_2\rangle$ are angular momentum eigenstates but correspond to "pseudorotations" of the cubic harmonics. A true noncubic rotation would, of course, take a cubic harmonic out of its degenerate subspace.

Substituting (2.61) in (2.60) gives

$$\begin{aligned}\langle j_1\alpha_1|h_{j\alpha}|j_2\alpha_2\rangle&=\langle 1,2|R^{-1}\gamma|j\alpha\rangle\Delta_j,\\\langle 1,2|R|1',2'\rangle&=r_{11'}r_{22'}^*.\end{aligned} \tag{2.62}$$

We may also write (2.62) in the form

$$\begin{aligned}\langle j_1\alpha_1|h_{j\alpha}|j_2\alpha_2\rangle&=\langle 1,2|\gamma\mathcal{R}|j\alpha\rangle\Delta_j,\\\mathcal{R}&\equiv\gamma^{-1}R^{-1}\gamma,\end{aligned} \tag{2.63}$$

where $\mathcal{R}$ transforms the $|j\alpha\rangle$. When $|j_1\alpha_1\rangle$, $|j_2\alpha_2\rangle$ are double group representations, $\mathcal{R}$ belongs to the single group and hence is more convenient to work with than R.

$|j_1\alpha_1\rangle\times|j_2\alpha_2\rangle$ may contain states $|j\alpha\rangle$ and $|j'\alpha'\rangle$ which are separately irreducible under the cubic group but which are "united" by a noncubic operation. Then $\mathcal{R}$ will couple j and j'.

We may think of γ as an operator $\gamma_{j\alpha}$ coupling the states $|j_1\alpha_1\rangle$, $|j_2\alpha_2\rangle$. Then $\mathcal{R}$ effects a transformation

$$(\gamma\mathcal{R})_{j\alpha}=\sum_{j'\alpha'}\gamma_{j'\alpha'}\mathcal{R}_{j'\alpha',j\alpha}. \tag{2.64}$$

Note that while γ is transformed, h is not. The γ's are the *same* for the rotation group as for the cubic group provided we use a basis for the rotation group which is irreducible under the cubic group. This follows because any transformation property which holds for the cubic group must also hold for the rotation group.

If the full rotation group applies, Eq. (2.60) is called the Wigner-Eckart theorem[28] and $\Delta_j=\Delta_{j'}$ when j and j' are united by noncubic rotations. The "pseudorotation" method does *not* assume $\Delta_j=\Delta_{j'}$, of course.

In applying the "pseudorotation" method it is convenient to use the tabulated values of Clebsch-Gordan coefficients. These refer to an angular momentum basis where raising and lowering operators have positive signs. This does not agree with Koster's choice of basis for the single group. In Condon and Shortley's notation[33] the γ's would be written

$$\gamma_{j_1m_1,j_2m_2;jm}=(j_1j_2m_1m_2|j_1j_2jm). \tag{2.65}$$

Luttinger's use of angular momentum matrices is restricted to the case $j_1=j_2$ which is less general than the Wigner-Eckart theorem.

(*2*) *Star of* $\mathbf{k}_0$

Let g^i be a minimal set of symmetry operators of the crystal point group which generate the star of $\mathbf{k}_0$.

$$g^i\mathbf{k}_0=\mathbf{k}_0{}^i. \tag{2.66}$$

All crystal properties are independent of whether we consider $\mathbf{k}_0$ or $\mathbf{k}_0{}^i$. However, the effect of the external forces of stress and vector potential are not independent of this choice. In fact, the effect of the vector potential $\mathbf{A}$ on the critical point $\mathbf{k}_0$ is equivalent to the effect of the vector potential $\mathbf{A}^i$ on the critical point $\mathbf{k}_0{}^i$, where

$$\mathbf{A}^i=(g^i)^{-1}\mathbf{A} \tag{2.67}$$

with a similar relation for $\mathbf{e}^i$ in terms of $\mathbf{e}$.

The simplest way to sum over the star of $\mathbf{k}_0$ is to keep $\mathbf{k}_0$ fixed and sum over a complete set of $\mathbf{A}^i$ and $\mathbf{e}^i$. (Whether we think of stress or strain is immaterial since the tensor connecting them is invariant under the point group). The complete set of operators $(g^i)^{-1}$ is identical with the set g^i to within an operation of the group of $\mathbf{k}_0$ which makes no difference. Since $\mathbf{e}$ is invariant under inversion and since the dielectric constant is bilinear in $\mathbf{A}$, $\mathbf{k}_0$ and $-\mathbf{k}_0$ are equivalent. This reduces the number of sets $\mathbf{A}^i$ which we have to sum over.

III. APPLICATION OF GENERAL FORMALISM TO SPECIFIC CASES

In this section we propose to investigate the symmetry properties of strain effects for critical points in the symmetry locations Γ, Δ, L, and Σ for the diamond structure. Our most detailed discussion will treat the effects of uniaxial stress in the [001], [111], and [110]

---

[33] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1959), p. 76.

directions. With this limitation on the stress direction more symmetry restrictions prevail and the results are simpler. We study all symmetry types for which optical transitions are allowed for the cases of large and small spin-orbit splitting. We follow the notation of Koster *et al.*[13] as much as possible.

For the case of [001], [111], or [110] stress, the principal axes of the dielectric-function tensor are oriented parallel and perpendicular to the stress. We introduce the following definitions of coordinates which will be useful in these three cases. x, y, z always refer to the cubic axes:

[111] Stress

$$\begin{aligned} x' &= (x-y)/\sqrt{2}\,, \\ y' &= (x+y-2z)/\sqrt{6}\,, \\ z' &= (x+y+z)/\sqrt{3}\,; \end{aligned} \tag{3.1}$$

[110] Stress

$$\begin{aligned} x'' &= (x-y)/\sqrt{2}\,, \\ y'' &= (x+y)/\sqrt{2}\,, \\ z'' &= z. \end{aligned} \tag{3.2}$$

A. Γ Point; $k_0=(0,0,0)$

At the Γ point, $\mathbf{k}_0=0$, the symmetry group is O_h in the diamond structure. All quantities have a unique parity, ±, under inversion-translation $(\tau|J)$. The strain tensor has positive parity and the vector potential has negative parity. Since the crystal ground state has symmetry Γ_{1+}, all allowed transitions lead to excitons of negative parity. To simplify the notation we will suppress the parity designation as much as possible.

Following the procedure described in Sec. II C1, we decompose the strain tensor into its irreducible representations under O_h according to the following definitions:

$$e_1 \equiv (e_{xx}+e_{yy}+e_{zz})/\sqrt{3}\,, \tag{3.3}$$

$$e_{3\alpha} \equiv (2e_{zz}-e_{xx}-e_{yy})/\sqrt{6}\,, \tag{3.4}$$

$$e_{3\beta} \equiv (e_{xx}-e_{yy})/\sqrt{2}\,, \tag{3.5}$$

$$e_{5yz} \equiv e_{yz}\,, \tag{3.6}$$

$$e_{5xz} \equiv e_{xz}\,, \tag{3.7}$$

$$e_{5xy} \equiv e_{xy}. \tag{3.8}$$

Similarly, the vector potential yields the representation

$$A_{4m} \equiv A_m;\ m=x,\,y,\,z. \tag{3.9}$$

The strain tensor e_{xy} is related to the stress tensor $\mathfrak{T}_{xy}$ by the complicance constants s_{11}, s_{12}, s_{44} in a cubic crystal. The relations are

$$e_{xx}=s_{11}\mathfrak{T}_{xx}+s_{12}(\mathfrak{T}_{yy}+\mathfrak{T}_{zz})\,, \tag{3.10}$$

$$e_{xy}=s_{44}\mathfrak{T}_{xy}/2. \tag{3.11}$$

The other relations follow by cyclic permutation of x, y, z, For convenience and for the sake of definition we also list the components of e for a uniaxial stress of magnitude $\mathfrak{T}$ in the [001], [111], and [110] directions:

[001] Stress

$$e_{xx}=e_{yy}=s_{12}\mathfrak{T};\ e_{zz}=s_{11}\mathfrak{T}\,, \tag{3.12}$$

$$e_1=(s_{11}+2s_{12})\mathfrak{T}/\sqrt{3}\equiv\eta_1\,, \tag{3.13}$$

$$e_{3\alpha}=(\sqrt{\tfrac{2}{3}})(s_{11}-s_{12})\mathfrak{T}\equiv\eta_3\,; \tag{3.14}$$

[111] Stress

$$e_{xx}=e_{yy}=e_{zz}=(s_{11}+2s_{12})\mathfrak{T}/3\,, \tag{3.15}$$

$$e_{xy}=e_{xz}=e_{yz}=s_{44}\mathfrak{T}/6\equiv\eta_5\,, \tag{3.16}$$

$$e_1=\eta_1; \tag{3.17}$$

[110] Stress

$$\begin{aligned} &e_{xx}=e_{yy}=(s_{11}+s_{12})\mathfrak{T}/2;\ e_{zz}=s_{12}\mathfrak{T}\,, \\ &e_{xy}=s_{44}\mathfrak{T}/4\,, \end{aligned} \tag{3.18}$$

$$e_1=\eta_1\,, \tag{3.19}$$

$$e_{3\alpha}=-\eta_3/2\,, \tag{3.20}$$

$$e_{xy}=\tfrac{3}{2}\eta_5. \tag{3.21}$$

All components not listed are zero.

Since the momentum operator transforms like Γ_{4-}, only excitons derived from pair bands U_{4-} will have nonzero optical matrix elements. Similarly for double group bands, only $\Gamma_{4-}\times\Gamma_{6+}=\Gamma_{6-}+\Gamma_{8-}$ will have nonzero optical matrix elements. (Γ_{6+} is the representation of spin $\frac{1}{2}$.) Hence we will treat only these cases.

Equations (3.3) to (3.8) serve to define irreducibly transforming components under O_h for any symmetric second rank tensor. If we use these definitions for $\boldsymbol{\epsilon}_2$ as well as $\mathbf{e}$, the linear dielectric response in Eq. (2.2) may be written

$$\begin{aligned} &\delta\epsilon_{2,1}(\omega)=W_1(\omega)e_1\,, \\ &\delta\epsilon_{2,3\sigma}(\omega)=W_3(\omega)e_{3\sigma};\ \sigma=\alpha,\,\beta\,, \\ &\delta\epsilon_{2,5\sigma}(\omega)=W_5(\omega)e_{5\sigma};\ \sigma=xy,\,xz,\,yz\,, \end{aligned} \tag{3.22}$$

$$\begin{aligned} W_1(\omega)&=W_{11}(\omega)+2W_{12}(\omega)\,, \\ W_3(\omega)&=W_{11}(\omega)-W_{12}(\omega)\,, \\ W_5(\omega)&=W_{44}(\omega). \end{aligned} \tag{3.23}$$

We regard W_1, W_3, and W_5 as the fundamental response functions which describe the response of the cubic medium to strains of symmetry e_1, e_3, and e_5. The W's can be determined from the polarization dependence of the dielectric function according to

[001] Stress

$$\begin{aligned} &\delta\epsilon_{2,zz}(\omega)=\frac{\eta_1}{\sqrt{3}}W_1(\omega)+\frac{2\eta_3}{\sqrt{6}}W_3(\omega);\ \text{parallel}, \\ &\delta\epsilon_{2,xx}(\omega)=\delta\epsilon_{2,yy}(\omega)=\frac{\eta_1}{\sqrt{3}}W_1(\omega)-\frac{\eta_3}{\sqrt{6}}W_3(\omega); \end{aligned} \tag{3.24}$$

[111] Stress

$$\delta\epsilon_{2,z'z'}(\omega)=\frac{\eta_1}{\sqrt{3}}W_1(\omega)+2\eta_5W_5(\omega);\ \text{parallel},$$
$$\delta\epsilon_{2,x'x'}=\epsilon_{2,y'y'}=\frac{\eta_1}{\sqrt{3}}W_1(\omega)-\eta_5W_5(\omega);\tag{3.25}$$

[110] Stress

$$\delta\epsilon_{2,x''x''}=\frac{\eta_1}{\sqrt{3}}W_1(\omega)+\frac{1}{2\sqrt{6}}\eta_3W_3(\omega)-\tfrac{3}{2}\eta_5W_5(\omega),$$
$$\delta\epsilon_{2,y''y''}=\frac{\eta_1}{\sqrt{3}}W_1(\omega)+\frac{1}{2\sqrt{6}}\eta_3W_3(\omega)+\tfrac{3}{2}\eta_5W_5(\omega);\ \text{parallel},\tag{3.26}$$
$$\delta\epsilon_{2,zz}=\frac{\eta_1}{\sqrt{3}}W_1(\omega)-\frac{\eta_3}{\sqrt{6}}W_3(\omega).$$

The three quantities W_1, W_3, and W_5 are conveniently determined from [001] and [111] stresses. The [110] results may be used as a check. For nondegenerate bands the energy shift contributions to W_3 and W_5 are expected to be zero for critical points in the [111] and [100] directions respectively. For a nondegenerate (0,0,0) critical point both W_3 and W_5 have zero energy-shift contributions. Kramers degenerate bands are effectively nondegenerate. Equations (3.22) are based entirely on symmetry considerations and the assumption of a linear relationship between $\delta\epsilon_2$ and e. Completely analogous relations can be written involving the stress rather than the strain, namely,

$$\delta\epsilon_{2,j\sigma}=\mathcal{W}_j\mathfrak{T}_{j\sigma}.\tag{3.27}$$

The symmetry character of the $\mathcal{W}$'s is the same as the W's. The $\mathcal{W}$'s were introduced and discussed in the introduction.

(*1*) *U_4 Bands*

According to Koster's tables,[13] the outer product $U_4\times U_4$ generates the representations Γ_{1+}, Γ_{3+}, Γ_{4+}, and Γ_{5+}. In an x, y, z basis the 3×3 $\tilde{\gamma}$ operators are ($\tilde{\gamma}=\sqrt{3}\gamma$)

$$\tilde{\gamma}_1=I,\tag{3.28}$$

$$\tilde{\gamma}_{3\alpha}=\frac{1}{\sqrt{2}}\begin{bmatrix}-1&0&0\\0&-1&0\\0&0&2\end{bmatrix},\qquad \tilde{\gamma}_{3\beta}=\frac{\sqrt{3}}{\sqrt{2}}\begin{bmatrix}1&0&0\\0&-1&0\\0&0&0\end{bmatrix},\tag{3.29}$$

$$\tilde{\gamma}_{4x}=\frac{\sqrt{3}}{\sqrt{2}}\begin{bmatrix}0&0&0\\0&0&1\\0&-1&0\end{bmatrix},\quad \tilde{\gamma}_{4y}=\frac{\sqrt{3}}{\sqrt{2}}\begin{bmatrix}0&0&-1\\0&0&0\\1&0&0\end{bmatrix},\quad \tilde{\gamma}_{4z}=\frac{\sqrt{3}}{\sqrt{2}}\begin{bmatrix}0&1&0\\-1&0&0\\0&0&0\end{bmatrix},\tag{3.30}$$

$$\tilde{\gamma}_{5yz}=\frac{\sqrt{3}}{\sqrt{2}}\begin{bmatrix}0&0&0\\0&0&1\\0&1&0\end{bmatrix},\quad \tilde{\gamma}_{5xz}=\frac{\sqrt{3}}{\sqrt{2}}\begin{bmatrix}0&0&1\\0&0&0\\1&0&0\end{bmatrix},\quad \tilde{\gamma}_{5xy}=\frac{\sqrt{3}}{\sqrt{2}}\begin{bmatrix}0&1&0\\1&0&0\\0&0&0\end{bmatrix}.\tag{3.31}$$

In terms of these matrices the effective strain and kinetic-energy Hamiltonians of Eqs. (2.27) and (2.28) may be written

$$H_{\mathrm{str}}=D_1e_1\tilde{\gamma}_1+D_3(e_{3\alpha}\tilde{\gamma}_{3\alpha}+e_{3\beta}\tilde{\gamma}_{3\beta})+D_5(e_{xy}\tilde{\gamma}_{5xy}+e_{xz}\tilde{\gamma}_{5xz}+e_{yz}\tilde{\gamma}_{5yz}),\tag{3.32}$$

$$H_{\mathrm{KE}}=R_1T_1\tilde{\gamma}_1+R_3(T_{3\alpha}\tilde{\gamma}_{3\alpha}+T_{3\beta}\tilde{\gamma}_{3\beta})+R_5(T_{xy}\tilde{\gamma}_{5xy}+T_{xz}\tilde{\gamma}_{5xz}+T_{yz}\tilde{\gamma}_{5yz}).\tag{3.33}$$

The D's are pair band deformation potential constants and the R's are reciprocal reduced masses. $T_{j\alpha}$ is an envelope kinetic-energy operator whose definition is identical to that of $e_{j\alpha}$ as given in Eqs. (3.3) to (3.8) with e_{lm} replaced by $(p_{\varphi l}p_{\varphi m})/2$ where the p_φ are momentum operators acting on the envelope function φ.

(*a*) *Low strain.* For zero strain the eigenfunctions of the kinetic-energy Hamiltonian of (3.33) plus the Coulomb Hamiltonian of Eq. (2.19) may be written as $\psi_{4x}{}^t$, $\psi_{4y}{}^t$, $\psi_{4z}{}^t$. Other symmetries are of no interest to us since they have vanishing optical-matrix elements. Using the Clebsch-Gordan matrix γ as in (2.35) ,we may write ψ in the form

$$\psi_{4x}{}^t = a_1{}^t\varphi_1{}^tU_{4x} + a_3{}^t\left(-\tfrac{1}{2}\varphi_{3\alpha}{}^tU_{4x} + \frac{\sqrt{3}}{2}\varphi_{3\beta}{}^tU_{4x}\right)$$
$$+ a_4{}^t\left(\frac{1}{\sqrt{2}}\varphi_{4y}{}^tU_{4z} - \frac{1}{\sqrt{2}}\varphi_{4z}{}^tU_{4y}\right)$$
$$+ a_5{}^t\left(\frac{1}{\sqrt{2}}\varphi_{5xz}{}^tU_{4z} + \frac{1}{\sqrt{2}}\varphi_{5xy}{}^tU_{4y}\right). \tag{3.34}$$

The φ's are orthonormal and the a's are real and satisfy

$$\sum_{i=1}^{5} (a_i{}^t)^2 = 1. \tag{3.35}$$

t labels a complete spectrum of states with symmetry Γ_4. The functional form of the φ's, apart from symmetry, must be determined by explicit solution of the Schrödinger equation.

On the basis of the same symmetry considerations that led to Eq. (3.32) we may write an effective-strain Hamiltonian operating on the multiplet $\psi_4{}^t$ in the form

$$H_{\mathrm{str}} = \mathfrak{D}_1{}^te_1I + \mathfrak{D}_3{}^t(e_{3\alpha}\tilde{\gamma}_{3\alpha} + e_{3\beta}\tilde{\gamma}_{3\beta})$$
$$+ \mathfrak{D}_5{}^t(e_{xy}\tilde{\gamma}_{5xy} + e_{xz}\tilde{\gamma}_{5xz} + e_{yz}\tilde{\gamma}_{5yz}). \tag{3.36}$$

The relation between the new deformation potential constants $\mathfrak{D}_j{}^t$ and the constants D_j in (3.32) may be calculated using (3.34) to be

$$\begin{aligned}
\mathfrak{D}_1{}^t &= D_1,\\
\mathfrak{D}_3{}^t &= D_3[(a_1{}^t)^2 + (a_3{}^t)^2 - \tfrac{1}{2}(a_4{}^t)^2 - \tfrac{1}{2}(a_5{}^t)^2],\\
\mathfrak{D}_5{}^t &= D_5[(a_1{}^t)^2 - \tfrac{1}{2}(a_3{}^t)^2 - \tfrac{1}{2}(a_4{}^t)^2 + \tfrac{1}{2}(a_5{}^t)^2].
\end{aligned} \tag{3.37}$$

To calculate $\mathfrak{D}_5{}^t$ we also need the expression analogous to (3.34) for $\psi_{4y}{}^t$. In deriving (3.37) we have used the orthonormality of the φ's and the fact that H_{str} commutes with φ. Note the interesting fact that, due to Eq. (3.35) we have the inequalities

$$|\mathfrak{D}_j{}^t| \leq |D_j|. \tag{3.38}$$

For the identity representation in any group we always have $\mathfrak{D}_1{}^t = D_1$ since all exciton states shift "rigidly" with the band. The differences between $\mathfrak{D}_j{}^t$ and D_j are associated with changes in the exciton binding energy relative to the band edge (electron-hole continuum threshold) due to a splitting of the degenerate bands.

We now wish to diagonalize the strain Hamiltonian of Eq. (3.36) for stresses in the [001], [110], and [111] directions. Using Eqs. (3.12) through (3.21) and (3.29) through (3.31), Eq. (3.36) can be diagonalized by inspection with the results

[001] Stress

$$\psi_{4z}{}^t;\ \mathcal{E}_{4z}{}^t = D_1\eta_1 + \frac{2\mathfrak{D}_3{}^t\eta_3}{\sqrt{2}} + E^t, \tag{3.39}$$

$$\psi_{4x}{}^t, \psi_{4y}{}^t;\ \mathcal{E}_{4x}{}^t = \mathcal{E}_{4y}{}^t = D_1\eta_1 - \frac{\mathfrak{D}_3{}^t\eta_3}{\sqrt{2}} + E^t; \tag{3.40}$$

[111] Stress

$$\psi_{4z'}{}^t \equiv (\psi_{4x}{}^t + \psi_{4y}{}^t + \psi_{4z}{}^t)/\sqrt{3};$$

$$\mathcal{E}_{4z'}{}^t = D_1\eta_1 + \frac{2\sqrt{3}\mathfrak{D}_5{}^t\eta_5}{\sqrt{2}} + E^t, \tag{3.41}$$

$$\psi_{4x'}{}^t \equiv (\psi_{4x}{}^t - \psi_{4y}{}^t)/\sqrt{2};$$

$$\mathcal{E}_{4x'}{}^t = \mathcal{E}_{4y'}{}^t = D_1\eta_1 - \frac{\sqrt{3}\mathfrak{D}_5{}^t\eta_5}{\sqrt{2}} + E^t, \tag{3.42}$$

$$\psi_{4y'}{}^t \equiv (\psi_{4x}{}^t + \psi_{4y}{}^t - 2\psi_{4z}{}^t)/\sqrt{6};$$

[110] Stress

$$\psi_{4z}{}^t;\ \mathcal{E}_{4z}{}^t = D_1\eta_1 - \frac{\mathfrak{D}_3{}^t\eta_3}{\sqrt{2}} + E^t, \tag{3.43}$$

$$\psi_{4x''}{}^t \equiv (\psi_{4x}{}^t - \psi_{4y}{}^t)/\sqrt{2};$$

$$\mathcal{E}_{4x''}{}^t = D_1\eta_1 + \frac{1}{2}\frac{\mathfrak{D}_3{}^t\eta_3}{\sqrt{2}} - \frac{3}{2}\frac{\sqrt{3}\mathfrak{D}_5{}^t\eta_5}{\sqrt{2}} + E^t, \tag{3.44}$$

$$\psi_{4y''}{}^t \equiv (\psi_{4x}{}^t + \psi_{4y}{}^t)/\sqrt{2};$$

$$\mathcal{E}_{4y''}{}^t = D_1\eta_1 + \frac{1}{2}\frac{\mathfrak{D}_3{}^t\eta_3}{\sqrt{2}} + \frac{3}{2}\frac{\sqrt{3}\mathfrak{D}_5{}^t\eta_5}{\sqrt{2}} + E^t. \tag{3.45}$$

In these formulas E^t is the energy of the state for zero strain.

Using (2.38) and (3.12) through (3.21) we can write the wave functions to first order in the strain as

[001] Stress

$$\begin{aligned}
\psi^{tx} &= \psi_{4x}{}^t - \eta_3\psi_{4x}{}^{t3},\\
\psi^{ty} &= \psi_{4y}{}^t - \eta_3\psi_{4y}{}^{t3},\\
\psi^{tz} &= \psi_{4z}{}^t + 2\eta_3\psi_{4z}{}^{t3};
\end{aligned} \tag{3.46}$$

[111] Stress

$$\begin{aligned}
\psi^{tx'} &= \psi_{4x'}{}^t - \eta_5\psi_{4x'}{}^{t5},\\
\psi^{ty'} &= \psi_{4y'}{}^t - \eta_5\psi_{4y'}{}^{t5},\\
\psi^{tz'} &= \psi_{4z'}{}^t + 2\eta_5\psi_{4z'}{}^{t5};
\end{aligned} \tag{3.47}$$

[110] Stress

$$\psi^{tx''}=\psi_{4x''}{}^{t}+\frac{\eta_3}{2}\psi_{4x''}{}^{t3}-\tfrac{3}{2}\eta_5\psi_{4x''}{}^{t5},$$

$$\psi^{ty''}=\psi_{4y''}{}^{t}+\frac{\eta_3}{2}\psi_{4y''}{}^{t3}+\tfrac{3}{2}\eta_5\psi_{4y''}{}^{t5}, \qquad (3.48)$$

$$\psi^{tz}=\psi_{4z}{}^{t}-\eta_3\psi_{4z}{}^{t3}.$$

We ignore the admixture of wave functions whose optical matrix elements are zero. The implicit definition of the first-order wave functions $\psi_{4x}{}^{3t}$ and $\psi_{4x}{}^{t5}$ agree with Eq. (2.38) except for a constant factor introduced for convenience. The quantities $\psi_{4x''}{}^{t3}$, $\psi_{4x'}{}^{t3}$, etc., are related to the quantities $\psi_{4x}{}^{t3}$ as indicated by Eqs. (3.41) through (3.45). x', x'', etc., also define the principle axes of the dielectric tensor as described in Eqs. (2.12) and (2.13). Using (3.46) through (3.48) the quantities $F_l{}^{t\alpha}$ in Eq. (2.13) may be written

[001] Stress

$$F_z{}^{tz}=f^{t0}+2\eta_3f^{t3},$$
$$F_y{}^{ty}=F_x{}^{tx}=f^{t0}-\eta_3f^{t3}; \qquad (3.49)$$

[111] Stress

$$F_{z'}{}^{tz'}=f^{t0}+2\eta_5f^{t5},$$
$$F_{x'}{}^{tx'}=F_{y'}{}^{ty'}=f^{t0}-\eta_5f^{t5}; \qquad (3.50)$$

[110] Stress

$$F_{x''}{}^{tx''}=f^{t0}+\frac{\eta_3}{2}f^{t3}-\tfrac{3}{2}\eta_5f^{t5},$$

$$F_{y''}{}^{ty''}=f^{t0}+\frac{\eta_3}{2}f^{t3}+\tfrac{3}{2}\eta_5f^{t5}, \qquad (3.51)$$

$$F_z{}^{tz}=f^{t0}-\eta_3f^{t3};$$

$$f^{t0}\equiv\langle0|p_x|\psi_{4x}{}^{t}\rangle^2,$$
$$f^{t3}\equiv2\langle0|p_x|\psi_{4x}{}^{t3}\rangle\langle\psi_{4x}{}^{t3}|p_x|0\rangle, \qquad (3.52)$$
$$f^{t5}\equiv2\langle0|p_x|\psi_{4x}{}^{t5}\rangle\langle\psi_{4x}{}^{t5}|p_x|0\rangle.$$

The functions ψ are assumed real, as is permitted by time reversal. The $F_l{}^{t\alpha}$ not listed, such as $F_y{}^{tx}$ are all zero.

The listing of the F's in (3.49) through (3.52) together with the $\mathcal{E}$'s in (3.39) through (3.45) constitutes a complete description of the strain effects on optical properties in the low-strain regime for U_{4-} bands at the Γ point when inserted in the expression (2.12) for the dielectric constant.

In case the strain splittings are small compared to the lifetime broadening the strain split components will not be resolved. One can then write a much simpler expression for ϵ_2 which, of course, contains much less information than if the lines are resolved. The simple results are

[001] Stress

$$\delta\epsilon_{2,zz}{}^{t}=\frac{\eta_1}{\sqrt3}W_1{}^{t}+\frac{2\eta_3}{\sqrt6}W_3{}^{t};\ \text{(parallel)},$$
$$\delta\epsilon_{2,xx}{}^{t}=\delta\epsilon_{2,yy}{}^{t}=\frac{\eta_1}{\sqrt3}W_1{}^{t}-\frac{\eta_3}{\sqrt6}W_3{}^{t}; \qquad (3.53)$$

[111] Stress

$$\delta\epsilon_{2,z'z'}{}^{t}=\frac{\eta_1}{\sqrt3}W_1{}^{t}+2\eta_5W_5{}^{t};\ \text{(parallel)},$$
$$\delta\epsilon_{2,x'x'}{}^{t}=\delta\epsilon_{2,y'y'}{}^{t}=\frac{\eta_1}{\sqrt3}W_1{}^{t}-\eta_5W_5{}^{t}; \qquad (3.54)$$

[110] Stress

$$\delta\epsilon_{2,x''x''}{}^{t}=\frac{\eta_1}{\sqrt3}W_1{}^{t}+\frac{1}{2}\frac{\eta_3}{\sqrt6}W_3{}^{t}-\tfrac{3}{2}\eta_5W_5{}^{t};\ \text{(parallel)},$$

$$\delta\epsilon_{2,y''y''}{}^{t}=\frac{\eta_1}{\sqrt3}W_1{}^{t}+\frac{1}{2}\frac{\eta_3}{\sqrt6}W_3{}^{t}+\tfrac{3}{2}\eta_5W_5{}^{t}, \qquad (3.55)$$

$$\delta\epsilon_{2,zz}{}^{t}=\frac{\eta_1}{\sqrt3}W_1{}^{t}-\frac{\eta_3}{\sqrt6}W_3{}^{t};$$

$$W_1{}^{t}=\sqrt3cf^{t0}D_1\left(\frac{dL}{dE^t}\right)_{(E^t-\ \mathcal{E}^0-\hbar\omega)},$$

$$W_3{}^{t}=\sqrt6c\left[f^{t0}\mathfrak{D}_3{}^{t}\left(\frac{dL}{dE^t}\right)_{(E^t-\ \mathcal{E}^0-\hbar\omega)},\right.$$
$$\left.+f^{t3}L(E^t-\mathcal{E}^0-\hbar\omega)\right], \qquad (3.56)$$

$$W_5{}^{t}=c\left[f^{t0}\mathfrak{D}_5{}^{t}\left(\frac{dL}{dE^t}\right)_{(E^t-\ \mathcal{E}^0-\hbar\omega)},\right.$$
$$\left.+f^{t5}L(E^t-\mathcal{E}^0-\hbar\omega)\right],$$

$$c\equiv\frac{4\pi^2e^2}{3m_0{}^2\omega^2V}.$$

L is a Lorentzian function as in Eq. (2.9). Equations (3.53) through (3.56) represent the changes $\delta\epsilon_2{}^{t}$ in the contribution to the dielectric constant from the degenerate multiplet, $\psi_4{}^{t}$. The principle axes are parallel or perpendicular to the stress direction.

Equations (3.53) through (3.55) are entirely analogous to Eqs. (3.24) through (3.26). The derivation of these latter equations was much simpler than the former but the assumption of analyticity was not justified in the case of degenerate bands. Also, the detailed description in (3.56) was not obtainable by the simpler approach

Equations (3.56) show that for the case of degenerate bands at Γ there are no special relations between W_1, W_3, and W_5 so that these quantities cannot serve as a "signature" of a degenerate Γ critical point. For more general directions of stress than we have considered, the diagonalization of Eq. (3.36) leads to energy shifts and hence W's which are nonanalytic in the stress components. The dependence on stress direction would then be different from the predictions of Eqs. (3.22) which are analytic. This would be a possible means of distinguishing the degenerate Γ point from a less symmetric nondegenerate critical point.

Of course, if the energy shifts in Eqs. (3.39) through (3.45) are resolved they can be used to characterize the degenerate Γ point. For instance, the case of a Σ critical point, treated in Sec. III D, shows that the energy shifts for a [111] stress differ from the shifts in the degenerate Γ point case. Both cases lead to finite values of W_1, W_3, and W_5.

(*b*) *High strain.* In the case of high strain we diagonalize H_{str} of Eq. (3.32) and neglect the matrix elements of H_{KE}, the kinetic energy operator, between strain split bands. The diagonal kinetic energy operator will lead to different exciton binding energies for different bands. We will write out explicitly the case of a (110) stress as an example. The diagonal components of the kinetic-energy operator H_{KE} in (3.33) are

$$H_{\text{KE}}=R_1T_1-\frac{R_3T_{3\alpha}}{\sqrt{2}}-\frac{\sqrt{3}R_5T_{xy}}{\sqrt{2}}\ ;\ U_{4x''} \qquad (3.57)$$

$$H_{\text{KE}}=R_1T_1-\frac{R_3T_{3\alpha}}{\sqrt{2}}+\frac{\sqrt{3}R_5T_{xy}}{\sqrt{2}}\ ;\ U_{4y''} \qquad (3.58)$$

$$H_{\text{KE}}=R_1T_1+\frac{2}{\sqrt{2}}R_3T_{3\alpha};\quad U_{4z}, \qquad (3.59)$$

where the definition of $U_{4x''}$, $U_{4y''}$, U_{4z} parallels that in Eqs. (3.44) and (3.45).

The wave functions which contain a φ_1 component are of the form

$$\psi^{tm}=(a_1{}^{tm}\varphi_1{}^{tm}+a_3{}^{tm}\varphi_{3\alpha}{}^{tm}+a_5{}^{tm}\varphi_{5xy}{}^{tm})U_{4m}, \qquad (3.60)$$

where $m=x''$, $y''z$. There is a spectrum of states ψ^t for each band which depend on the band index, m, by virtue of the kinetic energy operator in Eqs. (3.57) to (3.59). There are no symmetry relations between the envelope functions in different bands m. Similarly the exciton binding energies will be unrelated. The strain energy can then be written

[110] Stress

$$\mathcal{E}^{t,z}=D_1\eta_1-\frac{D_3\eta_3}{\sqrt{2}}+E^{t,z}, \qquad (3.61)$$

$$\mathcal{E}^{t,x''}=D_1\eta_1+\frac{1}{2}\frac{D_3\eta_3}{\sqrt{2}}-\frac{3}{2}\frac{\sqrt{3}D_5\eta_5}{\sqrt{2}}+E^{t,x''}, \qquad (3.62)$$

$$\mathcal{E}^{t,y''}=D_1\eta_1+\frac{1}{2}\frac{D_3\eta_3}{\sqrt{2}}+\frac{3}{2}\frac{\sqrt{3}D_5\eta_5}{\sqrt{2}}+E^{t,y''}. \qquad (3.63)$$

Comparison with the low-strain results of (3.43) through (3.45) shows that the constants $\mathfrak{D}_j{}^t$ have been replaced by D_j while the exciton binding energies E^t have been replaced by $E^{t,m}$ which now depend on the band label m. In this limit all exciton states in a given band shift together so that the sum over t with fixed m may be regarded as a single line if the individual states t are not resolved.

The momentum matrix element is

$$\begin{aligned}\langle 0|p_{m'}|\psi^{tm}\rangle &= a_1{}^{tm}\varphi_1{}^{tm}(0)\langle 0|p_m|U_{4m}\rangle\delta_{mm'},\\ &\equiv \mathcal{P}_4{}^{tm}.\end{aligned} \qquad (3.64)$$

Because of the factor $a_1{}^{tm}\varphi_1{}^{tm}(0)$, the matrix elements for different bands are no longer symmetry related. The quantities $\langle 0|p_m|U_{4m}\rangle$ are related, of course, being independent of m. We may write

$$\langle 0|p_{m'}|U_{4m}\rangle = P_4\delta_{mm'}. \qquad (3.65)$$

Equation (3.65) shows that the most striking symmetry property, that due to $\delta_{mm'}$, remains but the $\mathcal{P}_4{}^{tm}$ depend on m. These properties are generally true of the high strain limit for all symmetry types. The symmetry of ψ's is lost but that of the U's remains because we make the effective mass approximation. The ψ symmetry is lost for strain splittings of the order of the exciton binding while the validity of the effective mass approximation requires the strain splittings to be small compared to the energy interval to the nearest band U not in the degenerate multiplet under consideration. We mean, of course, the "vertical" energy interval at the same value of $\mathbf{k}_0$.

(*c*) *Spin-orbit splitting.* The spin-orbit interaction is given in Eq. (2.57). We consider the case where only one of the two Bloch bands is degenerate so that we can ignore the spin coordinate of the nondegenerate particle in solving the dynamical problem. We take the degenerate band to be that of the electron. This means we must form $U_{8-}=U_{4-}\times\Gamma_{6+}$. If we considered the hole we would form $U_{8-}=U_{4-}\times(\Gamma_{6+})^*$ and we would use (2.46) to obtain the appropriately transforming combinations, namely, $(\psi_{1/2,1/2})^*\sim\psi_{1/2,-1/2}$ and $(\psi_{1/2,-1/2})^*\sim-\psi_{1/2,1/2}$. The axial vector $\mathbf{S}$ transforms like Γ_{4+}, consequently, in an x, y, z basis, the spin-orbit energy may be written

$$H_{\mathrm{SO}}=-\frac{i\Delta\sqrt{2}}{3\sqrt{3}}(\tilde{\gamma}_{4x}\sigma_x+\tilde{\gamma}_{4y}\sigma_y+\tilde{\gamma}_{4z}\sigma_z)\,, \tag{3.66}$$

where the $\tilde{\gamma}_4$ operators are defined in Eq. (3.30). The i is chosen to make Δ real and the numerical factor is introduced so that Δ will be the energy splitting of the U_{8-} and U_{6-} multiplets which are generated by $U_{4-}\times\Gamma_{6+}$. Γ_{6+} is the representation of spin $\frac{1}{2}$ at $\mathbf{k}=0$. The sign is such that the U_{8-} energy is greater than that of the U_{6-} multiplet for Δ positive.

The spin-orbit splitting is diagonalized by transforming the bands $U_{4x}\times$spin to the $|Jm_J\rangle$ representation. Koster's Γ_8 representation corresponds to $J=\frac{3}{2}$ while Γ_6 corresponds to $J=\frac{1}{2}$. We take these up separately.

(2) U_{8-} *Bands*

Koster's choice of phases is as follows (see Table 83, p. 92 in Ref. 13):

$$\begin{aligned}U_{8,3/2}&=(-iU_{4x}+U_{4y})\uparrow/\sqrt{2}\,,\\ U_{8,1/2}&=(-iU_{4x}+U_{4y})\downarrow/\sqrt{6}+i(\sqrt{\tfrac{2}{3}})U_z\uparrow\,,\\ U_{8,-1/2}&=(iU_{4x}+U_{4y})\uparrow/\sqrt{6}+i(\sqrt{\tfrac{2}{3}})U_z\downarrow\,,\\ U_{8,-3/2}&=(iU_{4x}+U_{4y})\downarrow/\sqrt{2}.\,,\end{aligned} \tag{3.67}$$

The choice of phases in (3.67) is such that Eq. (2.46) holds with K substituted for $\mathcal{K}$. We will use K rather than $\mathcal{K}$ for time reversal at Γ to agree with Koster *et al.*[13]

Using Koster's tables together with Eq. (2.51) it is easily seen that the effective Hamiltonian $\tilde{\gamma}$ matrices are

$$\begin{aligned}&\tilde{\gamma}_1=I;\ \tilde{\gamma}_{3\alpha}=\frac{1}{\sqrt{2}}\begin{pmatrix}-\sigma_z & 0\\ 0 & \sigma_z\end{pmatrix},\\ &\tilde{\gamma}_{3\beta}=\frac{1}{\sqrt{2}}\begin{pmatrix}0 & -\sigma_x\\ -\sigma_x & 0\end{pmatrix},\\ &\tilde{\gamma}_{5yz}=\frac{1}{\sqrt{2}}\begin{pmatrix}-\sigma_y & 0\\ 0 & \sigma_y\end{pmatrix};\ \tilde{\gamma}_{5xy}=\frac{1}{\sqrt{2}}\begin{pmatrix}0 & i\mathcal{I}\\ -i\mathcal{I} & 0\end{pmatrix},\\ &\tilde{\gamma}_{5xz}=\frac{1}{\sqrt{2}}\begin{pmatrix}-\sigma_x & 0\\ 0 & \sigma_x\end{pmatrix},\end{aligned} \tag{3.68}$$

$$\mathcal{I}\equiv\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix};\ \sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix};\ \sigma_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix};\ \sigma_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{3.69}$$

The $\tilde{\gamma}$'s are 4×4 matrices expressed in terms of Pauli matrices in the conventional representation.

The precise definition of $\tilde{\gamma}$ in terms of Koster's unitary γ's is

$$\begin{aligned}\tilde{\gamma}_{j\alpha}(j_1\alpha_1;\ j_2\alpha_2)&=(-1)^{q_2+\alpha_2+1}\sqrt{2}\gamma_{j_1\alpha_1,j_2(-\alpha_2);j\alpha}\,,\\ j\alpha&=3\alpha,\ 3\beta,\ 5xy,\ 5xz,\ 5yz\,,\end{aligned} \tag{3.70}$$

$$\begin{aligned}\tilde{\gamma}_{j\alpha}(j_1\alpha_1;\ j_2\alpha_2)&=(-1)^{q_2+\alpha_2+1}2\gamma_{j_1\alpha_1,j_2(-\alpha_2);j\alpha}\,,\\ j\alpha&=1.\end{aligned} \tag{3.71}$$

We have modified our usual convention here slightly in order that Eqs. (3.32) and (3.33) should be valid for either U_{4-} or U_{8-} bands with the *same* values of D_j and R_j. This can be verified with the use of Eqs. (3.32) and (3.67).

It is noteworthy that the second Γ_5 representation which Koster calls φ_5 does not occur in (3.68) and it may be questioned whether the transition from D to $\mathfrak{D}$ interaction matrices as in (3.32) to (3.36) should include the extra representation in the U_{8-} case. The answer is "no" if we want the interaction between ψ_{8-} and itself but is "yes" if we write a phenomenological interaction between two different ψ_{8-} multiplets. This result is a consequence of time reversal as embodied in (2.55). Since $\mathcal{O}^K=\mathcal{O}$ for the strain operator, we have that the $\mathfrak{D}$'s must be real. Calling the φ_5 representation $\psi_{5'}$ and adopting (3.70) we have

$$\begin{aligned}\tilde{\gamma}_{5'xy}&=\frac{i}{\sqrt{2}}\begin{pmatrix}0 & \sigma_z\\ \sigma_z & 0\end{pmatrix},\\ \tilde{\gamma}_{5'xz}&=\frac{1}{2\sqrt{2}}\begin{pmatrix}i\sigma_y & -\sqrt{3}\sigma_x\\ \sqrt{3}\sigma_x & i\sigma_y\end{pmatrix},\\ \tilde{\gamma}_{5'yz}&=-\frac{i}{2\sqrt{2}}\begin{pmatrix}\sigma_x & i\sqrt{3}\sigma_y\\ -i\sqrt{3}\sigma_y & \sigma_x\end{pmatrix}.\end{aligned} \tag{3.72}$$

Evidently the $\tilde{\gamma}$ multiplied by a real $\mathfrak{D}_{5'}$ are not Hermitian and hence cannot occur for strain interactions between states of the same ψ_8 multiplet.

In diagonalizing the strain Hamiltonians for strains in the [110] and [111] directions it is helpful to use a set of basis functions which have been "pseudorotated" from the cubic axes to the stress axes of Eqs. (3.1) and (3.2). The "pseudorotation" method was discussed in Sec. II C 2. In using Clebsch-Gordan coefficients we also want to represent the appropriate γ operators in an angular momentum basis. It is convenient to use polynomials in x, y, z to indicate transformation properties. We then have

$$\begin{aligned}\tilde{\gamma}_{2,\pm2}&\equiv\tfrac{1}{2}(x\pm iy)^2,\\ \tilde{\gamma}_{2,0}&\equiv\frac{1}{\sqrt{6}}(2z^2-x^2-y^2)\,,\\ \tilde{\gamma}_{3,\pm3}&\equiv\frac{1}{2\sqrt{2}}(x\pm iy)^3,\\ \tilde{\gamma}_{3,\pm2}&\equiv\frac{\sqrt{3}}{2}z(x\pm iy)^2.\end{aligned} \tag{3.73}$$

We can relate these operators to the earlier ones by the equations

$$\tilde{\gamma}_{3\alpha}=\tilde{\gamma}_{2,0},$$

$$\tilde{\gamma}_{xy}=\frac{1}{i\sqrt{2}}(\tilde{\gamma}_{2,2}-\tilde{\gamma}_{2,-2}), \tag{3.74}$$

$$\tilde{\gamma}_{5',xy}=\frac{i}{\sqrt{2}}(\tilde{\gamma}_{3,2}+\tilde{\gamma}_{3,-2}).$$

Equations (3.74) can be taken to determine the scale factor of the operators defined in Eq. (3.73). Using (3.73) the transformations to the stress coordinates can be written

[110] Stress coordinates

$$\tilde{\gamma}_{3\alpha}=\tilde{\gamma}_{2'',0},$$

$$\tilde{\gamma}_{xy}=-\frac{1}{\sqrt{2}}(\tilde{\gamma}_{2'',2}+\tilde{\gamma}_{2'',-2}), \tag{3.75}$$

$$\tilde{\gamma}_{5',xy}=\frac{1}{\sqrt{2}}(\tilde{\gamma}_{3'',2}-\tilde{\gamma}_{3'',-2});$$

[111] Stress coordinates

$$\begin{aligned}\tilde{\gamma}_{xy}+\tilde{\gamma}_{xz}+\tilde{\gamma}_{yz}&=\sqrt{3}\tilde{\gamma}_{2',0},\\ \tilde{\gamma}_{5'xy}+\tilde{\gamma}_{5'xz}+\tilde{\gamma}_{5'yz}&=\frac{\sqrt{3}i}{\sqrt{2}}(\tilde{\gamma}_{3',3}+\tilde{\gamma}_{3',-3}).\end{aligned} \tag{3.76}$$

The notation 2′, 2″ signifies that the axis system is given by Eqs. (3.1) and (3.2), respectively.

Low strain. For zero strain the interesting eigenfunctions of the kinetic-energy Hamiltonian plus the Coulomb Hamiltonian may be written in terms of functions $\psi_{8\alpha}{}^t$, $\alpha=\frac{3}{2}$, $\frac{1}{2}$, $-\frac{1}{2}$, $-\frac{3}{2}$ with t a repetition index. Only these representations have allowed optical-matrix elements because of the $\varphi_1(0)$ factor in Eq. (2.32). Expressions analogous to (3.34) could be written out using Koster's tables with $\psi=\varphi\times U$. The expressions are lengthy and will not be given. As previously discussed, an effective Hamiltonian operating on the $\psi_8{}^t$ subspace can be written on the basis of symmetry in a form identical to Eq. (3.32) with $\tilde{\gamma}$ given by (3.68) exexcept that the D's are replaced by $\mathfrak{D}^t$'s. As always, $\mathfrak{D}_1{}^t=D_1$. Expressions analogous to (3.37) relating the $\mathfrak{D}^t$'s and D's could be written out but we have not computed them.

We now wish to diagonalize the strain Hamiltonian for stresses in the [001], [110], and [111] directions. Using Eqs. (3.12) through (3.21) and (3.74) through (3.76) together with Condon and Shortley's Clebsch-Gordan coefficients we can write

[001] Stress

$$\begin{aligned}&\psi_{8,3/2}{}^t;\ \mathcal{E}_{8,3/2}{}^t=D_1\eta_1-\frac{\mathfrak{D}_3{}^t\eta_3}{\sqrt{2}}+E^t,\\ &\psi_{8,1/2}{}^t;\ \mathcal{E}_{8,1/2}{}^t=D_1\eta_1+\frac{\mathfrak{D}_3{}^t\eta_3}{\sqrt{2}}+E^t;\end{aligned} \tag{3.77}$$

[110] Stress

$$\begin{aligned}&\psi_{8,+}{}^t;\ \mathcal{E}_{8,+}{}^t=D^1\eta_1+E_D+E^t,\\ &\psi_{8,-}{}^t;\ \mathcal{E}_{8,-}{}^t=D_1\eta_1-E_D+E^t,\\ &r_3\equiv\frac{\eta_3\mathfrak{D}_3{}^t}{2\sqrt{2}};\ r_5\equiv-\frac{3}{2}\frac{\eta_5}{\sqrt{2}}\mathfrak{D}_5{}^t,\\ &E_D=(r_3{}^2+r_5{}^2)^{1/2},\\ &\psi_{8,+}{}^t=\alpha\psi_{8,3/2''}{}^t+\beta\psi_{8,-1/2''}{}^t,\\ &\psi_{8,-}{}^t=\beta\psi_{8,3/2''}{}^t-\alpha\psi_{8,-1/2''}{}^t,\\ &\alpha=\frac{(E_D+r_3)^{1/2}}{(2E_D)^{1/2}};\ \beta=\frac{(E_D-r_3)^{1/2}}{(2E_D)^{1/2}}\frac{\eta_5\mathfrak{D}_5{}^t}{|\eta_5\mathfrak{D}_5{}^t|};\end{aligned} \tag{3.78}$$

[111] Stress

$$\psi_{8,3/2'}{}^t;\ \mathcal{E}_{8,3/2'}{}^t=D_1\eta_1-\frac{\sqrt{3}\mathfrak{D}_5{}^t\eta_5}{\sqrt{2}}+E^t, \tag{3.79}$$

$$\psi_{8,1/2'}{}^t;\ \mathcal{E}_{8,1/2'}{}^t=D_1\eta_1+\frac{\sqrt{3}\mathfrak{D}_5{}^t\eta_5}{\sqrt{2}}+E^t. \tag{3.80}$$

The wave functions for the states which are Kramers degenerate with the states given above are obtained by applying Kramers operator, K. Note the nonanalytic nature of the strain dependence in the [110] case. E^t is the exciton binding energy for zero strain. The notation 8, $\frac{3}{2}'$ and 8, $\frac{3}{2}''$, etc., means that we use the axis system oriented along [110] and [111] as in Eqs. (3.1) and (3.2). Results similar to these were first obtained by Kleiner and Roth.[27]

We now consider the evaluation of optical-matrix elements to first order in the strain. We must first include the spin degree of freedom we have been neglecting. We do this by forming the products $\psi_{8\alpha}{}^t(\uparrow')^*$ and $\psi_{8\alpha}{}^t(\downarrow')^*$ where $\uparrow'$ and $\downarrow'$ are spin functions of the spin degree of freedom of the hole which we have been neglecting and which is assumed to have no effect on the dynamics of the exciton wave function. The product $\Gamma_{8-}\times(\Gamma_{6+})^*$ contains Γ_{4-} and Koster's Table 83 can be used to relate all the optical matrix elements of the form $\langle 0|A\cdot p|\psi_8{}^t\times(\text{spin})^*\rangle$ for a given multiplet t.

The strain will mix other wave-function symmetries into the unperturbed symmetry $\psi_8{}^t$ but we are interested only in admixtures transforming like Γ_8 since all other symmetries are optically forbidden because of the $\varphi_1(0)$ factor.

With the use of perturbation theory we write

$$\psi^{8\alpha}=\psi_{8\alpha}{}^{t}+\sum_{t'}\langle\psi_{8\beta}{}^{t'}|H_{\mathrm{str}}|\psi_{8\alpha}{}^{t}\rangle\psi_{8\beta}{}^{t'}/(E_8{}^{t}-E_8{}^{t'})\,. \qquad (3.81)$$

The matrix elements $\langle\psi_{8\beta}{}^{t'}|H_{\mathrm{str}}|\psi_{8\alpha}{}^{t}\rangle$ can be written down using symmetry in identical form to (3.36) using (3.68). The coefficients should be written $\mathfrak{D}_j{}^{t't}$. When $t'\neq t$ the non-Hermitian $\tilde{\gamma}_{5'}$ of (3.72) may also occur. We can write

$$\langle t'|H_{\mathrm{str}}|t\rangle=\mathfrak{D}_{5'}{}^{t't}(e_{xy}\tilde{\gamma}_{5'xy}+e_{xz}\tilde{\gamma}_{5'xz}+e_{yz}\tilde{\gamma}_{5'yz}) \qquad (3.82)$$

with $\mathfrak{D}_{5'}{}^{t't}$ real. With the help of (3.76) it is easily shown that the $\Gamma_{5'}$ representation does not contribute to the first-order matrix element for stresses in the [111] direction. However, it does contribute for stress in the [110] direction. It is now straightforward to write down the optical matrix elements to first order in the strain

[001] Stress

$$\begin{gathered}F_x{}^{t3/2}=F_y{}^{t3/2}=\frac{3f^{t0}}{4}-\frac{3\eta_3}{2}f^{t3};\; F_z{}^{t3/2}=0,\\ F_x{}^{t1/2}=F_y{}^{t1/2}=\tfrac{1}{4}f^{t0}+\frac{\eta_3}{2}f^{t3},\\ F_z{}^{t1/2}=f^{t0}+2\eta_3 f^{t3}.\end{gathered} \qquad (3.83)$$

The expressions for the Kramers degenerate pairs $(\frac{3}{2},-\frac{3}{2})$ and $(\frac{1}{2},-\frac{1}{2})$ are the same.

[111] Stress

$$\begin{gathered}F_{x'}{}^{t3/2}=F_{y'}{}^{t3/2}=\frac{3f^{t0}}{4}-\tfrac{3}{2}\eta_5 f^{t5};\; F_{z'}{}^{t3/2}=0,\\ F_{x'}{}^{t1/2}=F_{y'}{}^{t1/2}=\tfrac{1}{4}f^{t0}+\frac{\eta_5}{2}f^{t5},\\ F_z{}^{t1/2}=f^{t0}+2\eta_5 f^{t5}.\end{gathered} \qquad (3.84)$$

The [110] stress results are complicated and will not be given.

(3) U_{6-} Bands

Koster's phases for the U_{6-} representation are

$$\begin{aligned}U_{6,1/2}&=\frac{1}{\sqrt{3}}\{(-iU_x+U_y)\downarrow-iU_z\uparrow\},\\ U_{6,-1/2}&=\frac{1}{\sqrt{3}}\{(-iU_x-U_y)\uparrow+iU_z\downarrow\}.\end{aligned} \qquad (3.85)$$

These levels are Kramers degenerate, hence the effective strain and kinetic-energy Hamiltonians are extremely simple.

$$\begin{aligned}H_{\mathrm{str}}&=D_1e_1I,\\ H_{\mathrm{KE}}&=R_1T_1I.\end{aligned} \qquad (3.86)$$

D_1, R_1 are the same constants as in Eqs. (3.32) and (3.33) and I is the two-dimensional identity matrix. The allowed wave functions then have the simple form

$$\psi_{6,\pm1/2}{}^{t}=\varphi_1{}^{t}U_{6,\pm1/2}\,. \qquad (3.87)$$

The optical-matrix elements can be written

$$\begin{aligned}\langle 0|A\cdot p|\psi_{6,1/2}{}^{t}\downarrow^*\rangle&=-\frac{(-iA_x+A_y)}{\sqrt{2}}\mathcal{P}^t,\\ \langle 0|A\cdot p|\psi_{6,1/2}{}^{t}\uparrow^*\rangle&=+\frac{iA_z}{\sqrt{2}}\mathcal{P}^t,\\ \langle 0|A\cdot p|\psi_{6,-1/2}{}^{t}\downarrow^*\rangle&=-\frac{iA_z}{\sqrt{2}}\mathcal{P}^t,\\ \langle 0|A\cdot p|\psi_{6,-1/2}{}^{t}\uparrow^*\rangle&=\frac{(+iA_x+A_y)}{\sqrt{2}}\mathcal{P}^t.\end{aligned} \qquad (3.88)$$

These relations lead to the simple isotropic dielectric tensor

$$F_x{}^t=F_y{}^t=F_z{}^t=f^{t0}. \qquad (3.89)$$

The strain does not change the wave function if we ignore interaction with the U_{8-} bands. This is only valid if the spin-orbit splitting is very large.

For small or intermediate spin-orbit splitting, the deviations from isotropy will be significant; hence we will calculate these deviations by considering the strain admixture of wave functions from the U_{8-} band. The outer product $\Gamma_{6-}{}^*\times\Gamma_{8-}$ generates Γ_{3+}, Γ_{4+}, Γ_{5+}. The corresponding nonsquare operators can be written in terms of operators which transform like the strain components, namely,

$$\begin{aligned}H_{\mathrm{str}}=&\,\mathfrak{D}_3{}^{3/2,1/2}(e_{3\alpha}\tilde{\gamma}_{3\alpha}+e_{3\beta}\tilde{\gamma}_{3\beta})\\ &+\mathfrak{D}_5{}^{3/2,1/2}(e_{xy}\tilde{\gamma}_{xy}+e_{xz}\tilde{\gamma}_{xz}+e_{yz}\tilde{\gamma}_{yz})\,.\end{aligned} \qquad (3.90)$$

Equation (3.90) is the analog of (3.32). The matrix elements of H_{str} are most easily found using Eqs. (3.74) through (3.76) and Condon and Shortley's Clebsch-Gordan coefficients. Treating H_{str} by perturbation theory we then have

[001] Stress

$$\psi^{6,1/2}=\psi_{6,1/2}+\eta_3\psi_{8,1/2}{}^{3}; \qquad (3.91)$$

[111] Strain

$$\psi^{6,1/2'}=\psi_{6,1/2'}+\eta_5\psi_{8,1/2'}{}^{5}; \qquad (3.92)$$

[110] Strain

$$\psi^{6,1/2''}=\psi_{6,1/2''}-\frac{\eta_3}{2}\psi_{8,1/2''}{}^{3}-\frac{\sqrt{3}}{2}\eta_5\psi_{8,-3/2''}{}^{5}. \qquad (3.93)$$

The primes and double primes refer to the coordinates in Eqs. (3.1) and (3.2).

We may now form the outer product of the above wave functions with the suppressed spin coordinate and use Koster's tables (or the Wigner-Eckart theorem) to calculate the following contributions to the dielectric tensor:

[001] Strain

$$F_x{}^t = F_y{}^t = f^{t0} - \eta_3 f^{t3}, \qquad F_z{}^t = f^{t0} + 2\eta_3 f^{t3}; \tag{3.94}$$

[111] Strain

$$F_{x'}{}^t = F_{y'}{}^t = f^{t0} - \eta_5 f^{t5}, \qquad F_{z'}{}^t = f^{t0} + 2\eta_5 f^{t5}; \tag{3.95}$$

[110] Strain

$$F_{x''}{}^t = f^{t0} + \frac{\eta_3}{2} f^{t3} - \tfrac{3}{2}\eta_5 f^{t5}, \qquad F_{y''}{}^t = f^{t0} + \frac{\eta_3}{2} f^{t3} + \tfrac{3}{2}\eta_5 f^{t5}, \qquad F_z{}^t = f^{t0} - \eta_3 f^{t3}. \tag{3.96}$$

The admixture of Γ_8 wave function has lowered the symmetry from the simple isotropic result obtaining when wave function admixture was ignored. In the limit of unresolved lines, the admixture of Γ_8 wave function yields finite values for the constants W_3 and W_5 in Eqs. (3.22) to (3.26). If the spin-orbit splitting is large compared to the lifetime broadening energy these terms should be small compared to W_1.

B. Δ Direction; $\boldsymbol{k}_0 = (0,0,\boldsymbol{k})$

The group of Δ is C_{4v}. Under this group the irreducible components of the strain tensor become

$$e_1{}^1 \equiv (e_{xx} + e_{yy} + e_{zz})/\sqrt{3} = e_1, \tag{3.97}$$

$$e_1{}^3 \equiv (2e_{zz} - e_{xx} - e_{yy})/\sqrt{6} = e_{3\alpha}, \tag{3.98}$$

$$e_3 \equiv (e_{xx} - e_{yy})/\sqrt{2} = e_{3\beta}, \tag{3.99}$$

$$e_4 \equiv e_{xy}, \tag{3.100}$$

$$e_{5x} \equiv e_{zx}, \tag{3.101}$$

$$e_{5y} \equiv e_{zy}. \tag{3.102}$$

The numerical subscript is the representation under C_{4v} in Koster's notation. For the identity representation a superscript is needed as a repetition index. We use the corresponding representation of e in the full cubic group (O_h) as a repetition index in this case; e.g.

$$e_1{}^3(C_{4v}) \equiv e_{3\alpha}(O_h). \tag{3.103}$$

The vector potential may also be decomposed into irreducibly transforming components

$$A_1 \equiv A_z, \tag{3.104}$$

$$A_{5x} \equiv A_x, \tag{3.105}$$

$$A_{5y} \equiv A_y. \tag{3.106}$$

Since we are interested only in excitons which couple strongly to light, we will only consider pair bands U with symmetry U_1 and U_5.

(1) U_1 *Bands*

This case is very simple. The exciton energy can be written

$$\mathcal{E}^t = D_1{}^1 e_1{}^1 + D_1{}^3 e_1{}^3 + E^t, \tag{3.107}$$

where E^t is the exciton binding energy in the absence of strain as determined from the effective mass Hamiltonian with the kinetic-energy operator

$$H_{\mathrm{KE}} = R_1{}^1 T_1{}^1 + R_1{}^3 T_1{}^3. \tag{3.108}$$

The "bare" band-edge deformation potentials $D_1{}^1$ and $D_1{}^3$ are not altered by the exciton wave function since the exciton binding relative to the band edge is unaffected by the energy shift of the band as a whole. In this case, ac strain produces a very simple energy derivative spectrum of the unstrained dielectric function. The optical matrix element is

$$\langle 0|\mathbf{A}\cdot\mathbf{p}|\psi_1{}^t\rangle = A_1 \mathcal{P}_1{}^t. \tag{3.109}$$

The matrix element does depend on the exciton state through the envelope part of the wave function, $\varphi_1{}^t(0)$, but is independent of strain.

(2) U_5 *Bands*

In determining the effective-strain Hamiltonian, we first inquire what representations are generated by $U_5{}^* \times U_5$. According to Koster *et al*,[13] they are Γ_1, Γ_2, Γ_3, and Γ_4. We have used a polar vector representation in (3.101), (3.102) where Koster has an axial vector. Under C_{4v} these transform differently. However, the tables where Γ_5 appears twice in $\Gamma_i \times \Gamma_j = \Gamma_k$ will still be the same. We correct a misprint in the table

$$U_3 V_{5x} \sim W_{5x}, \qquad U_3 V_{5y} \sim -W_{5y}, \tag{3.110}$$

where ~ means "transforms as."

With the use of Koster's tables the strain and kinetic-energy Hamiltonians are easily written down as

$$H_{\mathrm{str}} = D_1{}^1 e_1{}^1 I + D_1{}^3 e_1{}^3 I + D_3 e_3 \tilde{\gamma}_3 + D_4 e_4 \tilde{\gamma}_4, \tag{3.111}$$

$$H_{\mathrm{KE}} = R_1{}^1 T_1{}^1 I + R_1{}^3 T_1{}^3 I + R_3 T_3 \tilde{\gamma}_3 + R_3 T_4 \tilde{\gamma}_4, \tag{3.112}$$

$$\tilde{\gamma}_4 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \tilde{\gamma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.113}$$

Although $\tilde{\gamma}_3$ and $\tilde{\gamma}_4$ can be expressed in terms of the Pauli matrices σ_z and σ_x they do not transform like an axial vector. Equation (3.113) refers to the basis set U_{5x}, U_{5y}.

We can use the $\tilde{\gamma}$ matrices to construct irreducibly transforming exciton wave functions in the absence of strain, namely,

$$\begin{aligned}\psi_{5x}{}^t&=a_1{}^t\varphi_1{}^tU_{5x}+a_2{}^t\varphi_2{}^tU_{5y}\\&\quad+a_3{}^t\varphi_3{}^tU_{5x}+a_4{}^t\varphi_4{}^tU_{5y},\\\psi_{5y}{}^t&=a_1{}^t\varphi_1{}^tU_{5y}-a_2{}^t\varphi_2{}^tU_{5x}\\&\quad-a_3{}^t\varphi_3{}^tU_{5y}+a_4{}^t\varphi_4{}^tU_{5x}.\end{aligned}\tag{3.114}$$

The a's are constants satisfying the normalization.

$$\sum_i a_i{}^2=1.\tag{3.115}$$

Since the R_i in (3.112) are real as shown in Sec. II C 1(g), the a's and φ's can be taken to be real.

We can write down an effective strain Hamiltonian for the multiplet $\psi_{5\alpha}{}^t$ corresponding to (3.111) with the D's everywhere replaced by $\mathfrak{D}$'s. Using Eq. (3.114) the relation between the two sets of D's is given by

$$\begin{aligned}\mathfrak{D}_1{}^1&=D_1{}^1,\\\mathfrak{D}_3{}^1&=D_1{}^3,\\\mathfrak{D}_3{}^t&=\{(a_1{}^t)^2-(a_2{}^t)^2+(a_3{}^t)^3-(a_4{}^t)^2\}D_3,\\\mathfrak{D}_4{}^t&=\{(a_1{}^t)^2-(a_2{}^t)^2-(a_3{}^t)^2+(a_4{}^t)^2\}D_4.\end{aligned}\tag{3.116}$$

Note that, by Eq. (3.115) we have the inequalities $|\mathfrak{D}_j{}^t|\leq|D_j|$.

We may write the wave functions to first order in the strain in the form

$$\begin{aligned}\psi^{t5x}&=\psi_{5x}{}^t+e_3\psi_{5x}{}^{t3}+e_4\psi_{5y}{}^{t4},\\\psi^{t5y}&=\psi_{5y}{}^t-e_3\psi_{5y}{}^{t3}+e_4\psi_{5x}{}^{t4}.\end{aligned}\tag{3.117}$$

In the left-hand side of these equations the symmetry label is put in the superscript position to indicate that the symmetry designation is correct only if we transform e as well as ψ. From these equations the optical matrix elements are easily calculated using the symmetry relations

$$\langle 0|p_{5x}|\psi_{5x}{}^t\rangle=\langle 0|p_{5y}|\psi_{5y}{}^t\rangle=\mathcal{P}_5{}^t.\tag{3.118}$$

Spin-orbit splitting. We write the spin-orbit Hamiltonian in the form (ignoring the spin of the hole)

$$H_{\mathrm{so}}=\mathbf{S}\cdot\boldsymbol{\sigma},\tag{3.119}$$

where the $\boldsymbol{\sigma}$ are the Pauli spin matrices and $\mathbf{S}$ is an operator transforming like an axial vector which operates on the orbital wave functions. We can write S in irreducibly transforming form

$$\begin{aligned}S_{5x}&=S_y,\\S_{5y}&=-S_x,\\S_2&=S_z.\end{aligned}\tag{3.120}$$

According to Koster's tables, only the S_2 component couples to the U_5 bands. We can then write

$$H_{\mathrm{SO}}=\lambda\sigma_z\begin{pmatrix}0&i\\-i&0\end{pmatrix},\tag{3.121}$$

where σ_z operates on spins and the explicit matrix operates on U_{5x}, U_{5y}. The i is introduced so that λ is real in keeping with Eq. (2.55) since $S^{\mathcal{K}}=-S$. The spin-orbit matrix is easily diagonalized by the band functions

$$\begin{aligned}E_{\mathrm{SO}}&=\lambda;\ \frac{(U_{5x}+iU_{5y})\downarrow}{\sqrt{2}},\frac{(U_{5x}-iU_{5y})\uparrow}{\sqrt{2}},\\E_{\mathrm{SO}}&=-\lambda;\ \frac{(U_{5x}-iU_{5y})\downarrow}{\sqrt{2}},\frac{(U_{5x}+iU_{5y})\uparrow}{\sqrt{2}}.\end{aligned}\tag{3.122}$$

The double degeneracy is of Kramers type.

We can transform to the representation given by (3.122) where the spin-orbit energy is diagonal. The transformed Hamiltonians are

$$H_{\mathrm{SO}}=\lambda\begin{pmatrix}1&0\\0&-1\end{pmatrix},\tag{3.123}$$

$$H_{\mathrm{str}}=D_1{}^1e_1{}^1I+D_1{}^3e_1{}^3I+D_3e_3\begin{pmatrix}0&1\\1&0\end{pmatrix}-D_4e_4\begin{pmatrix}0&-i\\i&0\end{pmatrix},\tag{3.124}$$

$$H_{\mathrm{KE}}=R_1{}^1T_1{}^1I+R_1{}^1T_1{}^3I+R_3T_3\begin{pmatrix}0&1\\1&0\end{pmatrix}-R_4T_4\begin{pmatrix}0&-i\\i&0\end{pmatrix}.\tag{3.125}$$

These two by two matrices refer to a basis consisting of the functions

$$\frac{(U_{5x}-iU_{5y})\uparrow}{\sqrt{2}},\frac{(U_{5x}+iU_{5y})\uparrow}{\sqrt{2}}.$$

The basis set

$$\frac{(U_{5x}+iU_{5y})\downarrow}{\sqrt{2}},\frac{(U_{5x}-iU_{5y})\downarrow}{\sqrt{2}}$$

is uncoupled to the spin-up basis set and possesses a Hamiltonian which is the complex conjugate of H_{str} and H_{KE}. The states in the spin-down set are Kramers degenerate with states in the spin-up set. We will only discuss the spin-up states explicitly.

Assuming that the spin-orbit splitting is large compared to the exciton binding energy we neglect the off-diagonal matrix elements in (3.125) and obtain the

TABLE I. Effective irreducible components of the stress tensor and vector potential for points in the star of $\mathbf{k}_0=(0,0,k_0)$. The effective components are primed and are given in terms of the true components for $(0,0,k_0)$.

	$(0,0,k_0)$	$(0,k_0,0)$	$(k_0,0,0)$
A_x'	A_x	A_z	A_y
A_y'	A_y	A_x	A_z
A_z'	A_z	A_y	A_x
$(e_1^1)'$	(e_1^1)	(e_1^1)	(e_1^1)
$(e_1^3)'$	(e_1^3)	$-\frac{1}{2}e_1^3-\frac{\sqrt{3}}{2}e_3$	$-\frac{1}{2}e_1^3+\frac{\sqrt{3}}{2}e_3$
e_3'	e_3	$\frac{\sqrt{3}}{2}e_1^3-\frac{1}{2}e_3$	$-\frac{\sqrt{3}}{2}e_1^3-\frac{1}{2}e_3$
e_4'	e_4	e_{5x}	e_{5y}
e_{5x}'	e_{5x}	e_{5y}	e_4
e_{5y}'	e_{5y}	e_4	e_{5x}

optically allowed eigenfunctions

$$\psi_6{}^t=\varphi_1{}^t\frac{(U_{5x}-iU_{5y})\uparrow}{\sqrt{2}},\qquad \psi_7{}^t=\varphi^{1t}\frac{(U_{5x}+iU_{5y})\uparrow}{\sqrt{2}}. \tag{3.126}$$

The envelope functions and exciton binding energies of states $\psi_6{}^t$, $\psi_7{}^t$ are identical because the kinetic energy operator, Eq. (3.125) is the same for both bands when off-diagonal terms are neglected. To first order in strain the energy may be written

$$\mathcal{E}_6{}^t=\lambda+E^t+D_1{}^1e_1{}^1+D_1{}^3e_1{}^3,\qquad \mathcal{E}_7{}^t=-\lambda+E^t+D_1{}^1e_1{}^1+D_1{}^3e_1{}^3. \tag{3.127}$$

The subscripts 6 and 7 are Koster's notation for the double group of C_{4v}.

In the large spin-orbit splitting limit given by (3.126) and (3.127) the exciton states behave just like nondegenerate states with the energy spectrum shifting "as a whole" under strain. The off-diagonal strain terms connecting $\psi_6{}^t$ and $\psi_7{}^t$ give an energy shift which is second order in the strain and will be neglected. However, the wave function is changed by an amount linear in the strain which we wish to consider even though the effect vanishes in the limit $\lambda\to\infty$. In practice, this limit is seldom well approximated.

Treating (3.124) by first-order perturbation theory we may write the wave function to terms linear in the strain as

$$\psi^{t6}=\psi_6{}^t+\psi_7{}^t\frac{(e_3D_3-ie_4D_4)}{2\lambda},\qquad \psi^{t7}=\psi_7{}^t+\psi_6{}^t\frac{(-e_3D_3-ie_4D_4)}{2\lambda}. \tag{3.128}$$

The very simple form of (3.128), where $\psi_6{}^t$ is only mixed with its spin-orbit split "twin" $\psi_7{}^t$, results from $\varphi_1{}^t$ being the same in both bands. For the same reason we have the optical-matrix-element relations

$$\langle 0|A\cdot p|\psi_6{}^t\rangle=(A_x-iA_y)\mathcal{P}_5{}^t,\qquad \langle 0|A\cdot p|\psi_7{}^t\rangle=(A_x+iA_y)\mathcal{P}_5{}^t. \tag{3.129}$$

The simple form of Eqs. (3.128) and (3.129) has the consequence that matrix-element change effects can be described in terms of the "band-edge" deformation parameters D_3 and D_4. For the degenerate band without spin-orbit splitting the wave functions are given in (3.117) and there is no simple relation between $\psi_{5x}{}^t$, $\psi_{5x}{}^{t3}$, and $\psi_{5y}{}^{t4}$.

(3) *Star of* $\mathbf{k}_0=(0.0.k)$

The star of $\mathbf{k}_0$ consists of $(k,0,0)$, $(0,k,0)$ and $(0,0,k)$ together with their negatives which we need not consider since $\mathbf{k}_0$ and $-\mathbf{k}_0$ have identical strain splittings and squared optical matrix elements. We use the device discussed in Sec. II C 2 and sum over the star of $\mathbf{k}_0$ by thinking of $\mathbf{k}_0$ as fixed while $\mathbf{A}$ and $\mathbf{e}$ vary. We present the apparent components of $\mathbf{A}$ and $\mathbf{e}$ in Table I. The apparent components are primed, the actual components are unprimed. The two sets coincide for $\mathbf{k}_0=(0,0,k)$.

(*a*) *U_1 bands.* The simplest case to treat is the nondegenerate case first discussed in Sec. III B 1. With the help of Table I, Eqs. (3.12) to (3.21) and (3.97) to (3.102) we can use (3.107) and (3.109) to compute the energy shifts and matrix elements of the exciton states summed over the star of $\mathbf{k}_0$. The results are presented in Table II. States degenerate in energy are not listed separately. Their dielectric contributions have simply been added together in the table. Dielectric tensor components not listed are zero.

There are no matrix element terms linear in the strain because the band is not degenerate. Actually, linear terms would arise if we considered the strain mixing between the U_1 bands and other bands at $\mathbf{k}_0$. These terms will generally be small compared to the terms we have considered except where there is a near degeneracy of two bands. If the energy separation of the states in Table II is not resolved, the results reduce to the limits

TABLE II. Energy and diagonal dielectric tensor form factor F for the nondegenerate U_1 band in the Δ direction. States degenerate in energy have their F factors summed over. Low strain approximation. Principal axes of F are parallel and perpendicular to the stress.

Energy	F, Dielectric form factor
[001] Stress	
$E^t+D_1{}^1\eta_1+D_1{}^3\eta_3$	$F_z{}^t=f^{t0}$
$E^t+D_1{}^1\eta_1-\frac{1}{2}D_1{}^3\eta_3$	$F_x{}^t=F_y{}^t=f^{t0}$
[111] Stress	
$E^t+D_1{}^1\eta_1$	$F_x{}^t=F_y{}^t=F_z{}^t=f^{t0}$
[110] Stress	
$E^t+D_1{}^1\eta_1-\frac{1}{2}D_1{}^3\eta_3$	$F_z{}^t=f^{t0}$
$E^t+D_1{}^1\eta_1+\frac{1}{4}D_1{}^3\eta_3$	$F_x{}^t=F_y{}^t=f^{t0}$

TABLE III. Energy and diagonal dielectric tensor form factor F for the degenerate U_5 band in the Δ direction. States degenerate in energy have their F factors summed over. Low strain approximation. Principal axes of F are parallel and perpendicular to the stress.

Energy	F, Dielectric form factor
[001] Stress	
$E^t+D_1{}^1\eta_1-D_1{}^3\frac{\eta_3}{2}+\frac{\sqrt{3}}{2}\mathfrak{D}_3{}^t\eta_3$	$F_z{}^t=2f^{t0}+2f^{t3}\eta_3$
$E^t+D_1{}^1\eta_1-D_1{}^3\frac{\eta_2}{2}-\frac{\sqrt{3}}{2}\mathfrak{D}_3{}^t\eta_3$	$F_x{}^t=F_y{}^t=f^{t0}-f^{t3}\eta_3$
$E^t+D_1{}^1\eta_1+D_1{}^3\eta_3$	$F_x{}^t=F_y{}^t=f^{t0}$
[111] Stress	
$E^t+D_1{}^1\eta_1+\mathfrak{D}_4{}^t\eta_5$	$\begin{cases}F_{z'}{}^t=2f^{t0}+2f^{t5}\eta_5\\ F_{x'}{}^t=F_{y'}{}^t=\frac{1}{2}f^{t0}+\frac{1}{2}f^{t5}\eta_5\end{cases}$
$E^t+D_1{}^1\eta_1-\mathfrak{D}_4{}^t\eta_5$	$F_{x'}{}^t=F_{y'}{}^t=\frac{3}{2}f^{t0}-\frac{3}{2}f^{t5}\eta_5$
[110] Stress	
$E^t+D_1{}^1\eta_1-D_1{}^3\frac{\eta_3}{2}+\frac{3}{2}\mathfrak{D}_4{}^t\eta_5$	$F_{y''}{}^t=f^{t0}+\frac{3}{2}f^{t5}\eta_5$
$E^t+D_1{}^1\eta_1-D_1{}^3\frac{\eta_3}{2}-\frac{3}{2}\mathfrak{D}_4{}^t\eta_5$	$F_{x''}{}^t=f^{t0}-\frac{3}{2}f^{t5}\eta_5$
$E^t+D_1{}^1\eta_1+D_1{}^3\frac{\eta_3}{4}-\frac{\sqrt{3}}{4}\mathfrak{D}_3{}^t\eta_3$	$F_z{}^t=2f^{t0}-f^{t3}\eta_3$
$E^t+D_1{}^1\eta_1+D_1{}^3\frac{\eta_3}{4}+\frac{\sqrt{3}}{4}\mathfrak{D}_3{}^t\eta_3$	$F_{x''}{}^t=F_{y''}{}^t=f^{t0}+\frac{1}{2}f^{t3}\eta_3$

given in Eqs. (3.24) to (3.26) except that the term W_5 is equal to zero. This fact should be very helpful in identifying this case.

(*b*) *U_5 bands.* We sum over the star of $\mathbf{k}_0$ with the use of Table I. Equations (3.97) to (3.102) together with the strain Hamiltonian in (3.111), the wave functions in (3.117) and the optical matrix element symmetries in (3.118) can be used to compute the entries in Table III. In contrast to the nondegenerate case there is now an energy shift term proportional to η_5 which comes from splitting the double degeneracy of U_5. The splitting coefficients $\mathfrak{D}_3{}^t$ and $\mathfrak{D}_5{}^t$ are altered from the D_3 and D_4 of the band edge and depend on the exciton state t as indicated in Eq. (3.116).

When spin-orbit splitting is considered and is assumed to be large compared to exciton binding energies and strain splittings the strain dependence becomes that of a simple nondegenerate band. However, the polarization dependence is different since U_1 states and U_5 states couple to orthogonal polarization modes. For finite spin-orbit splittings the linear strain admixture of wave functions between the spin-orbit split states is usually significant. With the use of Eqs. (3.128) and (3.129) the dielectric tensor has been calculated to terms linear in the strain as given in Table IV. The strain-dependent terms have opposite signs for $\pm\lambda$ states. It will be noticed that Table II lacks the linear strain terms in Table IV. This qualitative difference depends on neglecting admixtures of other band states into the band edge function U_1. The neglected terms are first order in strain but will generally be of order $\lambda/\Delta E$ smaller than the linear strain terms in Table IV where λ is the spin-orbit splitting and ΔE is the smallest energy band separation between U_1 and another band at $\mathbf{k}_0$.

C. L Point; $k_0=(2\pi/a)(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

The L point is always a critical point in the diamond structure. The symmetry group is D_{3d}. In this group the irreducible components of the strain tensor may be written

$$e_{1+}{}^1\equiv(e_{xx}+e_{yy}+e_{zz})/\sqrt{3}=e_1(O_h)\,, \tag{3.130}$$

$$e_{1+}{}^5\equiv(e_{xy}+e_{xz}+e_{yz})/\sqrt{3}\,, \tag{3.131}$$

$$e_{3\alpha+}{}^3\equiv(-e_{xx}-e_{yy}+2e_{zz})/\sqrt{6}=e_{3\alpha}(O_h)\,, \tag{3.132}$$

$$e_{3\beta+}{}^3\equiv(e_{xx}-e_{yy})/\sqrt{2}=e_{3\beta}(O_h)\,, \tag{3.133}$$

$$e_{3\alpha+}{}^5\equiv(-e_{xz}-e_{yz}+2e_{xy})/\sqrt{6}\,, \tag{3.134}$$

$$e_{3\beta+}{}^5\equiv(-e_{xz}+e_{yz})/\sqrt{2}\,. \tag{3.135}$$

The numerical subscript is the representation under D_{3d} in Koster's notation.[13] The superscript is the corresponding representation of e in O_h which is used to identify repeated representations.

TABLE IV. Energy and diagonal dielectric tensor form factor F for the degenerate U_5 band in the Δ direction with spin-orbit splitting included. States degenerate in energy have their F factors summed over. Low strain approximation. Principal axes of F are parallel and perpendicular to the stress.

Energy	F, Dielectric form factor
[001] Stress	
$\pm\lambda+E^t+D_1{}^1\eta_1-\frac{1}{2}D_1{}^3\eta_3$	$\begin{cases}F_x{}^t=F_y{}^t=\frac{f^{t0}}{2}\mp\frac{\eta_3}{2}f^{t3}\\ F_z{}^t=f^{t0}\pm\eta_3f^{t3}\end{cases}$
$\pm\lambda+E^t+D_1{}^1\eta_1+D_1{}^3\eta_3$	$F_x{}^t=F_y{}^t=\frac{f^{t0}}{2}$
[111] Stress	
$\pm\lambda+E^t+D_1{}^1\eta_1$	$\begin{cases}F_{x'}{}^t=F_{y'}{}^t=f^{t0}\mp\frac{\eta_5}{2}f^{t5}\\ F_{z'}{}^t=f^{t0}\pm\eta_5f^{t5}\end{cases}$
[110] Stress	
$\pm\lambda+E^t+D_1{}^1\eta_1+\frac{1}{4}D_1{}^3\eta_3$	$\begin{cases}F_{x''}{}^t=F_{y''}{}^t=\frac{f^{t0}}{2}\pm\frac{1}{4}\eta_3f^{t3}\\ F_z{}^t=f^{t0}\mp\frac{\eta_3}{2}f^{t3}\end{cases}$
$\pm\lambda+E^t+D_1{}^1\eta_1-\frac{1}{2}D_1{}^3\eta_3$	$\begin{cases}F_{x''}{}^t=\frac{f^{t0}}{2}\mp\frac{3}{4}\eta_5f^{t5}\\ F_{y''}{}^t=\frac{f^{t0}}{2}\pm\frac{3}{4}\eta_5f^{t5}\end{cases}$

$$f^{t5}=f^{t0}D_4/\lambda$$

$$f^{t3}=f^{t0}\frac{\sqrt{3}D_3}{2\lambda}$$

The vector potential may also be decomposed into irreducibly transforming components

$$A_{2-}\equiv(A_x+A_y+A_z)/\sqrt{3}\equiv A_{z'}, \qquad (3.136)$$

$$A_{3\alpha-}\equiv(A_x-A_y)/\sqrt{2}\equiv A_{x'}, \qquad (3.137)$$

$$A_{3\beta-}\equiv(A_x+A_y-2A_z)/\sqrt{6}\equiv A_{y'}. \qquad (3.138)$$

These results show that we need only consider pair bands of symmetry U_{2-} and U_{3-} since they are the only symmetries which will couple strongly to light.

(*1*) U_{2-} *Bands*

Since this is a nondegenerate case it is very simply treated. The exciton energy can be written

$$\mathcal{E}^t=D_1{}^1e_1{}^1+D_1{}^5e_1{}^5+E^t, \qquad (3.139)$$

where E^t is the exciton binding energy in the absence of strain as determined from the effective-mass Hamiltonian with the kinetic-energy operator

$$H_{\mathrm{KE}}=R_1{}^1T_1{}^1+R_1{}^5T_1{}^5. \qquad (3.140)$$

The deformation potentials $D_1{}^1$ and $D_1{}^5$ are not altered by the exciton binding since the energy band shifts "as a whole" under strain. The effect of ac strain is to take an energy derivative of the unperturbed dielectric function.

The optical-matrix element is

$$\langle 0|p_2|\psi_2{}^t\rangle=\mathcal{P}_2{}^t. \qquad (3.141)$$

The matrix element depends on the exciton state but is independent of strain.

(*2*) U_{3-} Bands

The primary source of symmetry information is the reduction of the outer product $U_{3-}{}^*\times U_{3-}$ into irreducibly transforming combinations. Koster *et al*,[13] use a complex representation. A real unitary Clebsch-Gordan matrix γ may be written

$$\begin{array}{ccccc} & U_{3\alpha-}V_{3\alpha-} & U_{3\alpha-}V_{3\beta-} & U_{3\beta-}V_{3\alpha-} & U_{3\beta-}V_{3\beta-} \\ W_{1+} & 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ W_{2+} & 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ W_{3\alpha+} & -1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ W_{3\beta+} & 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0\,. \end{array} \qquad (3.142)$$

We also record the γ matrix for the product of U_{2+} with U_{3-}.

$$\begin{array}{ccc} & U_{3\alpha-}V_{2+} & U_{3\beta-}V_{2+} \\ W_{3\alpha-} & 0 & -1 \\ W_{3\beta-} & 1 & 0. \end{array} \qquad (3.143)$$

With the use of (3.142), the strain- and kinetic-energy matrices can be immediately written down

$$\begin{aligned} H_{\mathrm{str}}=&D_1{}^1e_1{}^1+D_1{}^5e_1{}^5I \\ &+D_3{}^3\left\{e_{3\alpha}{}^3\begin{pmatrix}-1&0\\0&1\end{pmatrix}+e_{3\beta}{}^3\begin{pmatrix}0&1\\1&0\end{pmatrix}\right\} \\ &+D_3{}^5\left\{e_{3\alpha}{}^5\begin{pmatrix}-1&0\\0&1\end{pmatrix}+e_{3\beta}{}^5\begin{pmatrix}0&1\\1&0\end{pmatrix}\right\}, \end{aligned} \qquad (3.144)$$

$$\begin{aligned} H_{\mathrm{KE}}=&R_1{}^1T_1{}^1I+R_1{}^5T_1{}^5I \\ &+R_3{}^3\left\{T_{3\alpha}{}^3\begin{pmatrix}-1&0\\0&1\end{pmatrix}+T_{3\beta}{}^3\begin{pmatrix}0&1\\1&0\end{pmatrix}\right\} \\ &+R_3{}^5\left\{T_{3\alpha}{}^5\begin{pmatrix}-1&0\\0&1\end{pmatrix}+T_{3\beta}{}^5\begin{pmatrix}0&1\\1&0\end{pmatrix}\right\}. \end{aligned} \qquad (3.145)$$

We can use (3.142) and (3.143) to construct irreducibly transforming exciton wave functions in the absence of strain. (We must change the parities in (3.142) but this is very easy since $(\tau|J)$ commutes with all group operations so that the parity designation may be treated as a multiplicative factor.) The wave functions are

$$\begin{aligned} \psi_{3\alpha-}{}^t=&a_1{}^t\varphi_{1+}{}^tU_{3\alpha-}-a_2{}^t\varphi_{2+}{}^tU_{3\beta-} \\ &+a_3{}^t\left(-\frac{\varphi_{3\alpha+}{}^tU_{3\alpha-}}{\sqrt{2}}+\frac{\varphi_{3\beta+}{}^tU_{3\beta-}}{\sqrt{2}}\right), \end{aligned} \qquad (3.146)$$

$$\begin{aligned} \psi_{3\beta-}{}^t=&a_1{}^t\varphi_{1+}{}^tU_{3\beta-}+a_2{}^t\varphi_{2+}{}^tU_{3\alpha-} \\ &+a_3{}^t\left(\frac{\varphi_{3\alpha+}{}^tU_{3\beta-}}{\sqrt{2}}+\frac{\varphi_{3\beta+}{}^tU_{3\alpha-}}{\sqrt{2}}\right). \end{aligned} \qquad (3.147)$$

Other symmetry types have zero optical matrix elements because they do not contain the symmetric envelope function φ_{1+}. The φ's are orthonormal. The a's are scalars with the normalization

$$\sum_{j=1}^{3}(a_j{}^t)^2=1. \qquad (3.148)$$

The functional form of the φ's is determined by solving the Coulomb problem with the kinetic-energy operator given by Eq. (3.145). The φ's and a's may be taken to be real. The superscript t is a repetition index for the representation ψ_{3-}.

We can use (3.146) and (3.147) to write down an effective-strain operator for the multiplet $\psi_{3-}{}^t$ which is the exact analog of (3.144) with $\mathfrak{D}_j$ replacing D_j. The connection between the deformation constants may be written

$$\begin{aligned} \mathfrak{D}_1{}^1&=D_1{}^1, \\ \mathfrak{D}_1{}^5&=D_1{}^5, \\ \mathfrak{D}_3{}^3&=\{(a_1{}^t)^2-(a_2{}^t)^2\}D_3{}^3, \\ \mathfrak{D}_3{}^5&=\{(a_1{}^t)^2-(a_2{}^t)^2\}D_3{}^5. \end{aligned} \qquad (3.149)$$

By (3.148) we have the inequalities

$$|\mathfrak{D}_j{}^t| \leq |D_j|\,. \tag{3.150}$$

We may write the wave functions to first order in the strain in the form

$$\psi^{3\alpha-}=\psi_{3\alpha-}+\left(\frac{-e_{3\alpha}{}^3\psi_{3\alpha-}{}^3}{\sqrt{2}}+\frac{e_{3\beta}{}^3\psi_{3\beta-}{}^3}{\sqrt{2}}\right)$$
$$+\left(\frac{-e_{3\alpha}{}^5\psi_{3\alpha-}{}^5}{\sqrt{2}}+\frac{e_{3\beta}{}^5\psi_{3\beta-}{}^5}{\sqrt{2}}\right), \tag{3.151}$$

$$\psi^{3\beta-}=\psi_{3\beta-}+\left(\frac{e_{3\alpha}{}^3\psi_{3\beta-}{}^3}{\sqrt{2}}+\frac{e_{3\beta}{}^3\psi_{3\alpha-}{}^3}{\sqrt{2}}\right)$$
$$+\left(\frac{e_{3\alpha}{}^5\psi_{3\beta-}{}^5}{\sqrt{2}}+\frac{e_{3\beta}{}^5\psi_{3\alpha-}{}^5}{\sqrt{2}}\right). \tag{3.152}$$

From these equations the optical-matrix elements are easily calculated using the symmetry relations

$$\langle 0|p_{3\alpha-}|\psi_{3\alpha-}{}^t\rangle=\langle 0|p_{3\beta-}|\psi_{3\beta-}{}^t\rangle\equiv\mathcal{P}_3{}^t. \tag{3.153}$$

Spin-orbit splitting. We refer to the spin-orbit Hamiltonian of Eq. (2.57) and neglect the spin of the hole. The irreducibly transforming components of the axial vector **S** are

$$\begin{aligned}S_{2+}&=(S_x+S_y+S_z)/\sqrt{3}\equiv S_{z'}\\ S_{3\alpha+}&=(S_x-S_y)/\sqrt{2}\equiv S_{x'}\\ S_{3\beta+}&=(S_x+S_y-2S_z)/\sqrt{6}\equiv S_{y'}\,.\end{aligned} \tag{3.154}$$

Equation (3.142) indicates a coupling to both the representations W_{2+} and W_{3+}. However, W_{3+} is incompatible with time reversal and so must be thrown out. Under time reversal $S^K=-S$, hence by Eq. (2.55) the coefficient multiplying γ must be pure imaginary which conflicts with the requirement of Hermiticity for the representation W_{3+}.

The spin-orbit matrix may be written

$$H_{\text{SO}}=\lambda\sigma_{z'}\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}. \tag{3.155}$$

The i is introduced to make λ real. $\sigma_{z'}$ is the spin component in the [111] direction as indicated by Eq. (3.154). The explicit matrix in (3.155) operates on the orbital functions. $\sigma_{z'}$ is a Pauli matrix operating on the spin functions.

If H_{so} is to be treated by perturbation theory, Eq. (3.155) is in a convenient form. However, if the spin-orbit interaction is large compared to the strain-splitting or the exciton-binding energy (which is usually the case), one wants to diagonalize the spin-orbit interaction and leave the strain- and kinetic-energy operators nondiagonal. The Kramers degeneracy permits us to write

$$H_{\text{SO}}=\lambda\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \tag{3.156}$$

$$H_{\text{str}}=D_1{}^1e_1{}^1I+D_1{}^5e_1{}^5I$$
$$+D_3{}^3\left\{-e_{3\alpha}{}^3\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}+e_{3\beta}{}^3\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}\right\}$$
$$+D_3{}^5\left\{-e_{3\alpha}{}^5\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}+e_{3\beta}{}^5\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}\right\}, \tag{3.157}$$

$$H_{\text{KE}}=R_1{}^1T_1{}^1I+R_1{}^5T_1{}^5I$$
$$+R_3{}^3\left\{-T_{3\alpha}{}^3\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}+T_{3\beta}{}^3\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}\right\}$$
$$+R_3{}^5\left\{-T_{3\alpha}{}^5\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}+T_{3\beta}{}^5\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}\right\}. \tag{3.158}$$

These matrices refer to a basis consisting of the band functions

$$\frac{(U_{3\alpha-}-iU_{3\beta-})\uparrow}{\sqrt{2}}\,;\ \frac{(U_{3\alpha-}+iU_{3\beta-})\uparrow}{\sqrt{2}}\,.$$

The basis set

$$\frac{(U_{3\alpha-}+iU_{3\beta-})\downarrow}{\sqrt{2}}\,;\ \frac{(U_{3\alpha-}-iU_{3\beta-})\downarrow}{\sqrt{2}}$$

corresponds to a Hamiltonian which is the complex conjugate of Eqs. (3.157) and (3.158). The only difference is that

$$\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}\to-\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}$$

since all other quantities are real. The states in the spin-down basis set are Kramers degenerate with the corresponding spin-up states. We will only discuss the spin-up states explicitly.

If the spin-orbit splitting is large compared to the exciton binding energy we can neglect the off-diagonal components of the kinetic energy operator. The kinetic-energy Hamiltonian then takes the simple form

$$H_{\text{KE}}=R_1{}^1T_1{}^1I+R_1{}^5T_1{}^5I\,. \tag{3.159}$$

The optically interesting eigenfunctions are then

$$\begin{aligned}\psi_+{}^t&=\frac{\varphi_1{}^t(U_{3\alpha-}-iU_{3\beta-})\uparrow}{\sqrt{2}}\\ \psi_-{}^t&=\frac{\varphi_1{}^t(U_{3\alpha-}+iU_{3\beta-})\uparrow}{\sqrt{2}}\,.\end{aligned} \tag{3.160}$$

Because of the simple form of the kinetic-energy operator in Eq. (3.159), the envelope functions for both bands are identical for corresponding states t. The en-

TABLE V. Effective irreducible components of the stress tensor and vector potential for points in the star of $\mathbf{k}_0=(2\pi/a)(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. The effective components are primed and are given in terms of the true components for $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$.

	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$(\frac{1}{2},-\frac{1}{2},-\frac{1}{2})$	$(-\frac{1}{2},\frac{1}{2},-\frac{1}{2})$	$(-\frac{1}{2},-\frac{1}{2},\frac{1}{2})$
$A_{x'}$	A_x	A_x	$-A_x$	$-A_x$
$A_{y'}$	A_y	$-A_y$	A_y	$-A_y$
$A_{z'}$	A_z	$-A_z$	$-A_z$	A_z
$(e_1^1)'$	e_1^1	e_1^1	e_1^1	e_1^1
$(e_1^5)'$	e_1^5	$-\frac{\sqrt{2}}{3}e_{3\alpha}^5+\frac{\sqrt{2}}{\sqrt{3}}e_{3\beta}^5-\frac{e_1^5}{3}$	$-\frac{\sqrt{2}}{3}e_{3\alpha}^5-\frac{\sqrt{2}}{\sqrt{3}}e_{3\beta}^5-\frac{1}{3}e_1^5$	$\frac{2\sqrt{2}}{\sqrt{3}}e_{3\alpha}^5-\frac{1}{3}e_1^5$
$(e_{3\alpha}^3)'$	$e_{3\alpha}^3$	$e_{3\alpha}^3$	$e_{3\alpha}^3$	$e_{3\alpha}^3$
$(e_{3\beta}^3)'$	$e_{3\beta}^3$	$e_{3\beta}^3$	$e_{3\beta}^3$	$e_{3\beta}^3$
$(e_{3\alpha}^5)'$	$e_{3\alpha}^5$	$-\frac{2}{3}e_{3\alpha}^5-\frac{1}{\sqrt{3}}e_{3\beta}^5-\frac{\sqrt{2}}{3}e_1^5$	$-\frac{2}{3}e_{3\alpha}^5+\frac{1}{\sqrt{3}}e_{3\beta}^5-\frac{\sqrt{2}}{3}e_1^5$	$\frac{1}{3}e_{3\alpha}^5+\frac{2\sqrt{2}}{3}e_1^5$
$(e_{3\beta}^5)'$	$e_{3\beta}^5$	$-\frac{1}{\sqrt{3}}e_{3\alpha}^5+\frac{\sqrt{2}}{\sqrt{3}}e_1^5$	$\frac{1}{\sqrt{3}}e_{3\alpha}^5-\frac{\sqrt{2}}{\sqrt{3}}e_1^5$	$-e_{3\beta}^5$
$A_{2'}$	A_2	$-\frac{1}{3}A_2+\frac{\sqrt{2}}{\sqrt{3}}A_{3\alpha}+\frac{\sqrt{2}}{3}A_{3\beta}$	$-\frac{1}{3}A_2-\frac{\sqrt{2}}{\sqrt{3}}A_{3\alpha}+\frac{\sqrt{2}}{3}A_{3\beta}$	$-\frac{1}{3}A_2-\frac{2\sqrt{2}}{3}A_{3\beta}$
$A_{3\alpha'}$	$A_{3\alpha}$	$\sqrt{\frac{2}{3}}A_2+\frac{1}{\sqrt{3}}A_{3\beta}$	$-\sqrt{\frac{2}{3}}A_2-\frac{1}{\sqrt{3}}A_{3\beta}$	$-A_{3\alpha}$
$A_{3\beta}'$	$A_{3\beta}$	$\frac{\sqrt{2}}{3}A_2+\frac{1}{\sqrt{3}}A_{3\alpha}-\frac{2}{3}A_{3\beta}$	$\frac{\sqrt{2}}{3}A_2-\frac{1}{\sqrt{3}}A_{3\alpha}-\frac{2}{3}A_{3\beta}$	$-\frac{2\sqrt{2}}{3}A_2+\frac{1}{3}A_{3\beta}$

ergies are also identical apart from the spin-orbit shift

$$\begin{aligned}\mathcal{E}_+{}^t&=\lambda+E^t+D_1{}^1e_1{}^1+D_1{}^5e_1{}^5\,,\\ \mathcal{E}_-{}^t&=-\lambda+E^t+D_1{}^1e_1{}^1+D_1{}^5e_1{}^5\,.\end{aligned}\tag{3.161}$$

We have used the simple designations plus and minus rather than the double group notation. Minus corresponds to the double group symmetry Γ_{4-} while plus is a mixture of the Kramers degenerate symmetries Γ_{5-} and Γ_{6-}.

TABLE VI. Energy and diagonal dielectric tensor form factor F for the nondegenerate U_{2-} band at the L point. States degenerate in energy have their F factors summed over. Low strain approximation. Principal axes of F are parallel and perpendicular to the stress.

Energy	F, Dielectric form factor
	[001] Stress
$D_1\ \eta_1$	$F_x{}^t=F_y{}^t=F_z{}^t=\frac{4}{3}f^{t0}$
	[111] Stress
$D_1{}^1\eta_1+\sqrt{3}D_1{}^5\eta_5$	$F_{z'}{}^t=f^{t0}$
$D_1{}^1\eta_1-\frac{D_1{}^5\eta_5}{\sqrt{3}}$	$F_{x'}{}^t=F_{y'}{}^t=\frac{4}{3}f^{t0};\ F_{z'}{}^t=\frac{f^{t0}}{3}$
	[110] Stress
$D_1{}^1\eta_1+\frac{\sqrt{3}}{2}D_1{}^5\eta_5$	$F_{y''}{}^t=\frac{4}{3}f^{t0};\ F_z{}^t=\frac{2}{3}f^{t0}$
$D_1{}^1\eta_1-\frac{\sqrt{3}}{2}D_1{}^5\eta_5$	$F_{x''}{}^t=\frac{4}{3}f^{t0};\ F_z{}^t=\frac{2}{3}f^{t0}$

In the large spin-orbit splitting approximation of Eqs. (3.159) through (3.161) the exciton states behave just like nondegenerate states with the energy spectrum shifting "as a whole" under strain. The off-diagonal strain terms connecting $\psi_+{}^t$ and $\psi_-{}^t$ give a contribution to the energy which is second order in the strain but they contribute a term in the wave function which is linear in the strain. We wish to include these terms even though they vanish in the limit $\lambda\rightarrow\infty$ because they represent the dominant effect of the strain components $e_{3\alpha}$, $e_{3\beta}$ which otherwise have no effect on the spectrum. We use (3.157) in lowest order perturbation theory for the wave function. We take advantage of the orthogonality of the $\varphi_1{}^t$ in (3.160) for different t. We may then write

$$\psi^{t+}=\psi_+{}^t+\psi_-{}^t\left\{-\frac{D_3{}^3}{2\lambda}(e_{3\alpha}{}^3+ie_{3\beta}{}^3)\right.\\ \left.-\frac{D_3{}^5}{2\lambda}(e_{3\alpha}{}^5+ie_{3\beta}{}^5)\right\}\tag{3.162}$$

$$\psi^{t-}=\psi_-{}^t+\psi_+{}^t\left\{\frac{D_3{}^3}{2\lambda}(e_{3\alpha}{}^3-ie_{3\beta}{}^3)\right.\\ \left.+\frac{D_3{}^5}{2\lambda}(e_{3\alpha}{}^5-ie_{3\beta}{}^5)\right\}.\tag{3.163}$$

In using these equations to determine optical-matrix elements we note the symmetry relations

$$\langle 0|\mathbf{A}\cdot\mathbf{p}|\psi_\pm{}^t\rangle=\frac{(A_{3\alpha}\mp iA_{3\beta})}{\sqrt{2}}\mathcal{P}_3{}^t.\tag{3.164}$$

Equations (3.162) through (3.164) permit the matrix-element changes to be expressed in terms of the "band-edge" deformation parameters $D_3{}^3$ and $D_3{}^5$. This result is much simpler than Eq. (3.151) for the zero spin-orbit splitting case. We remark that $\mathcal{P}_3{}^t$ in Eq. (3.164) will not be equal to the $\mathcal{P}_3{}^t$ in Eq. (3.153) because the envelope functions φ_1 will not be the same.

(3) Star of $\mathbf{k}_0=(2\pi/a)(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

The star of $\mathbf{k}_0$ consists of $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},-\frac{1}{2},-\frac{1}{2})$, $(-\frac{1}{2},\frac{1}{2},-\frac{1}{2})$ and $(-\frac{1}{2},-\frac{1}{2},\frac{1}{2})$. We sum over the star of $\mathbf{k}_0$ by summing over the effective components of $\mathbf{A}$ and $\mathbf{e}$ as given in Table V.

The results for the nondegenerate U_{2-} bands are given in Table VI. States degenerate in energy have been summed over. Components not listed are zero. The linear-strain terms in the matrix elements have been neglected since the band is nondegenerate. The strain component η_3 does not appear in the table. This characteristic feature serves to identify a nondegenerate critical point in the (k_0,k_0,k_0) direction.

The results for the degenerate U_{3-} case are given in Table VII. Because of the degeneracy, the η_3 strain component appears both in the energy-shift and the matrix-element terms. Furthermore, if the strain splittings are not resolved one obtains formulas identical with (3.24) through (3.26) with finite values of W_3 which arise from both energy-shift and matrix-element change contributions.

Table VII. Energy and diagonal dielectric tensor form factor F for the degenerate U_{3-} band at the L point. States degenerate in energy have their F factors summed over. Low strain approximation. Principal axes of F are parallel and perpendicular to the stress.

Energy	F, Dielectric form factor
[001] Stress	
$D_1{}^1\eta_1+\mathfrak{D}_3{}^{t3}\eta_3$	$F_x{}^t=F_y{}^t=\frac{2}{3}f^{t0}+\frac{2}{3}\eta_3f^{t3}$ $F_z{}^t=\frac{8}{3}f^{t0}+\frac{8}{3}\eta_3f^{t3}$
$D_1{}^1\eta_1-\mathfrak{D}_3{}^{t3}\eta_3$	$F_x{}^t=F_y{}^t=2f^{t0}-2\eta_2f^{t3}$
[111] Stress	
$D_1{}^1\eta_1+\sqrt{3}D_1{}^5\eta_5$	$F_{x'}{}^t=F_{y'}{}^t=f^{t0}$
$D_1{}^1\eta_1-\frac{1}{\sqrt{3}}D_1{}^5\eta_5+\frac{2\sqrt{2}}{\sqrt{3}}\mathfrak{D}_3{}^{t5}\eta_5$	$F_{x'}{}^t=F_{y'}{}^t=\frac{f^{t0}}{6}+\frac{\eta_5}{6}f^{t3}$ $F_{z'}{}^t=\frac{8}{3}f^{t0}+\frac{8}{3}\eta_5f^{t3}$
$D_1{}^1\eta_1-\frac{1}{\sqrt{3}}D_1{}^5\eta_5-\frac{2\sqrt{2}}{\sqrt{3}}\mathfrak{D}_3{}^{t5}\eta_5$	$F_{x'}{}^t=F_{y'}{}^t=\frac{3}{2}f^{t0}-\frac{3}{2}\eta_5f^{t3}$
[110] Stress	
$D_1{}^1\eta_1+\frac{\sqrt{3}}{2}D_1{}^5\eta_5+\frac{1}{2}\mathfrak{D}_3{}^{t3}\eta_3-\sqrt{\frac{3}{2}}\mathfrak{D}_3{}^{t5}\eta_5$	$F_{x''}{}^t=2f^{t0}+\eta_3f^{t3}-\frac{3}{2}\eta_5f^{t5}$
$D_1{}^1\eta_1-\frac{\sqrt{3}}{2}D_1{}^5\eta_5+\frac{1}{2}\mathfrak{D}_3{}^{t3}\eta_3+\sqrt{\frac{3}{2}}\mathfrak{D}_3{}^{t5}\eta_5$	$F_{y''}{}^t=2f^{t0}+\eta_3f^{t3}+\frac{3}{2}\eta_5f^{t5}$
$D_1{}^1\eta_1+\frac{\sqrt{3}}{2}D_1{}^5\eta_5-\frac{1}{2}\mathfrak{D}_3{}^{t3}\eta_3+\sqrt{\frac{3}{2}}\mathfrak{D}_3{}^{t5}\eta_5$	$F_{y''}{}^t=\frac{2}{3}f^{t0}-\frac{1}{3}\eta_3f^{t3}+\frac{1}{2}\eta_5f^{t5}$ $F_z{}^t=\frac{4}{3}f^{t0}-\frac{2}{3}\eta_3f^{t3}+\eta_5f^{t5}$
$D_1{}^1\eta_1-\frac{\sqrt{3}}{2}D_1{}^5\eta_5-\frac{1}{2}\mathfrak{D}_3{}^{t3}\eta_3-\sqrt{\frac{3}{2}}\mathfrak{D}_3{}^{t5}\eta_5$	$F_{x''}{}^t=\frac{2}{3}f^{t0}-\frac{1}{3}\eta_3f^{t3}-\frac{1}{2}\eta_5f^{t5}$ $F_z{}^t=\frac{4}{3}f^{t0}-\frac{2}{3}\eta_3f^{t3}-\eta_5f^{t5}$

Table VIII. Energy and diagonal dielectric tensor form factor F for the degenerate U_{3-} band at the L point with spin-orbit splitting included. States degenerate in energy have their F factors summed over. Low strain approximation. Principal axes of F are parallel and perpendicular to the stress.

Energy	F, Dielectric form factor
[001] Stress	
$E^t\pm\lambda+D_1{}^1\eta_1$	$F_x{}^t=F_y{}^t=\frac{8}{3}f^{t0}\mp\frac{4}{3}\eta_3f^{t3}$ $F_z{}^t=\frac{8}{3}f^{t0}\pm\frac{8}{3}\eta_3f^{t3}$
[111] Stress	
$E^t\pm\lambda+D_1{}^1\eta_1+\sqrt{3}D_1{}^5\eta_5$	$F_{x'}{}^t=F_{y'}{}^t=f^{t0}$
$E^t\pm\lambda+D_1{}^1\eta_1-\frac{1}{\sqrt{3}}D_1{}^5\eta_5$	$F_{x'}{}^t=F_{y'}{}^t=\frac{5}{3}f^{t0}\mp\frac{4}{3}\eta_5f^{t5}$ $F_{z'}{}^t=\frac{8}{3}f^{t0}\pm\frac{8}{3}f\eta_5{}^{t5}$
[110] Stress	
$E^t\pm\lambda+D_1{}^1\eta_1-\frac{\sqrt{3}}{2}D_1{}^5\eta_5$	$F_{x''}{}^t=\frac{2}{3}f^{t0}\mp\frac{\eta_5f^{t5}}{2}\pm\frac{\eta_3}{6}f^{t3}$ $F_{y''}{}^t=2f^{t0}\pm\frac{3}{2}\eta_5f^{t5}\pm\frac{\eta_3}{2}f^{t3}$ $F_z{}^t=\frac{4}{3}f^{t0}\mp\eta_5f^{t5}\mp\frac{2}{3}\eta_3f^{t3}$
$E^t\pm\lambda+D_1{}^1\eta_1+\frac{\sqrt{3}}{2}D_1{}^5\eta_5$	$F_{x''}{}^t=2f^{t0}\mp\frac{3}{2}\eta_5f^{t5}\pm\frac{\eta_3}{2}f^{t3}$ $F_{y''}{}^t=\frac{2}{3}f^{t0}\pm\frac{\eta_5f^{t5}}{2}\pm\frac{\eta_3}{6}f^{t3}$ $F_z{}^t=\frac{4}{3}f^{t0}\pm\eta_5f^{t5}\mp\frac{2}{3}\eta_3f^{t3}$

$$f^{t3}=\frac{D_3{}^3}{\lambda}f^{t0};\quad f^{t5}=\frac{2\sqrt{2}}{\sqrt{3}}\frac{D_3{}^5}{\lambda}f^{t0}$$

When spin-orbit splitting is included, the strain dependence is indicated in Table VIII. The results for the two spin-orbit split bands are identical except for the strain dependence of the optical matrix element which is equal and opposite for the two bands. This simple result is a consequence of assuming that the spin-orbit splitting is large compared to the exciton binding energy so that the nondiagonal kinetic energy terms in Eq. (3.158) can be neglected.

The energy shift terms have the same form as for the nondegenerate U_{2-} case in Table VI. The effect of an η_3 strain component on the energy shift terms is zero. However, the η_3 strain does affect the matrix elements and hence will contribute a finite value to the W_3 com-

TABLE IX. Energy and diagonal dielectric tensor form factor F for the nondegenerate U_1, U_2, and U_3 bands in the Σ direction. States degenerate in energy have their F factors summed over. Low strain approximation. Principal axes of F are parallel and perpendicular to the stress.

	F, Dielectric form factor		
Energy	U_1	U_2	U_3
	[001] Stress		
$E^t+\eta_1D_1^1+\eta_3D_1^3$	$F_x{}^t=F_y{}^t=f^{t0}$	$F_z{}^t=2f^{t0}$	$F_x{}^t=F_y{}^t=f^{t0}$
$E^t+\eta_1D_1^1-\frac{\eta_3}{2}D_1^3$	$F_x{}^t=F_y{}^t=f^{t0}$; $F_z{}^t=2f^{t0}$	$F_x{}^t=F_y{}^t=2f^{t0}$	$F_x{}^t=F_y{}^t=f^{t0}$; $F_z{}^t=2f^{t0}$
	[111] Stress		
$E^t+\eta_1D_1^1+\eta_5D_1^5$	$F_{x'}{}^t=F_{y'}{}^t=\frac{1}{2}f^{t0}$; $F_{z'}{}^t=2f^{t0}$	$F_{x'}{}^t=F_{y'}{}^t=F_{z'}{}^t=f^{t0}$	$F_{x'}{}^t=F_{y'}{}^t=\frac{3}{2}f^{t0}$
$E^t+\eta_1D_1^1-\eta_5D_1^5$	$F_{x'}{}^t=F_{y'}{}^t=\frac{3}{2}f^{t0}$	$F_{x'}{}^t=F_{y'}{}^t=F_{z'}{}^t=f^{t0}$	$F_{x'}{}^t=F_{y'}{}^t=\frac{1}{2}f^{t0}$; $F_{z'}{}^t=2f^{t0}$
	[110] Stress		
$E^t+\eta_1D_1^1-\frac{\eta_3}{2}D_1^3+\frac{3}{2}\eta_5D_1^5$	$F_{y''}{}^t=f^{t0}$	$F_z{}^t=f^{t0}$	$F_{x''}{}^t=f^{t0}$
$E^t+\eta_1D_1^1-\frac{\eta_3}{2}D_1^3-\frac{3}{2}\eta_5D_1^5$	$F_{x''}{}^t=f^{t0}$	$F_z{}^t=f^{t0}$	$F_{y''}{}^t=f^{t0}$
$E^t+\eta_1D_1^1+\frac{\eta_3}{4}D_1^3$	$\begin{cases} F_{x''}{}^t=F_{y''}{}^t=f^{t0} \\ F_z{}^t=2f^{t0} \end{cases}$	$F_{x''}{}^t=F_{y''}{}^t=f^{t0}$	$\begin{cases} F_{x''}{}^t=F_{y''}{}^t=f^{t0} \\ F_z{}^t=2f^{t0} \end{cases}$

ponent of the dielectric function. The contrast of this result to that of the nondegenerate U_{2-} case is more quantitative than qualitative. There should be linear-strain terms in the U_{2-} case also if we had considered mixing effects from higher bands. Mixing with a U_{3-} band would lead to matrix element changes proportional to η_3. In general, the $U_{2-}(\mathbf{k}_0)-U_{3-}(\mathbf{k}_0)$ separation is likely to be a good deal larger than the spin-orbit splitting of the U_{3-} bands. The coefficient f^{t3} is inversely proportional to this separation which justifies the approximation we have made except for unusual cases of accidental near degeneracy.

D. Σ Direction; $\mathbf{k}_0=(k_0,k_0,0)$

The symmetry group of the Σ direction is C_{2v}. We follow the Γ notation of Koster *et al.* but we label our axes according to the cubic notation so that our choice of x, y, z disagrees with his. In our notation, the symmetry operations are $\sigma_v\equiv(xy\bar{z})$, $\sigma_{v'}\equiv(yxz)$, $C_2\equiv(yx\bar{z})$. The irreducible components of the strain tensor and the vector potential may then be written

$$e_1{}^1\equiv(e_{xx}+e_{yy}+e_{zz})/\sqrt{3}=e_1(O_h)\,, \tag{3.165}$$

$$e_1{}^3\equiv(-e_{xx}-e_{yy}+2e_{zz})/\sqrt{6}=e_{3\alpha}(O_h)\,, \tag{3.166}$$

$$e_1{}^5\equiv e_{xy}=e_{5xy}(O_h)\,, \tag{3.167}$$

$$e_2=(e_{xz}+e_{yz})/\sqrt{2}\,, \tag{3.168}$$

$$e_3=(e_{xx}-e_{yy})/\sqrt{2}=e_{3\beta}(O_h)\,, \tag{3.169}$$

$$e_4=(e_{xz}-e_{yz})/\sqrt{2}\,, \tag{3.170}$$

$$A_1=(A_x+A_y)/\sqrt{2}\equiv A_{y''}\,, \tag{3.171}$$

$$A_2=A_z\,, \tag{3.172}$$

$$A_3=(A_x-A_y)/\sqrt{2}\equiv A_{x''}\,. \tag{3.173}$$

All Σ bands are nondegenerate. According to (3.171) through (3.173) only U_1, U_2, U_3 bands couple to light in lowest order. Since the bands are nondegenerate $U_j\times U_j=\Gamma_1$, hence only the symmetric strain terms shift the bands. The strain- and kinetic-energy Hamiltonians are easily written

$$\begin{aligned} H_{\mathrm{str}}&=e_1{}^1D_1{}^1+e_1{}^3D_1{}^3+e_1{}^5D_1{}^5\,,\\ H_{\mathrm{KE}}&=T_1{}^1D_1{}^1+T_1{}^3D_1{}^3+T_1{}^5D_1{}^5\,, \end{aligned} \tag{3.174}$$

where the definition of the irreducibly transforming T components is the same as for e.

The effects of spin-orbit interaction can be ignored since the bands are nondegenerate and we ignore mixing

TABLE X. Comparison of the notation of this paper (Koster's) with that of Bouckaert, Smoluchowski, and Wigner and also Elliott.

$\mathbf{k}=0$		$\mathbf{k}=L$	
Koster	BSW	Koster	BSW
Γ_{1+}	Γ_1	Γ_{1+}	L_1
Γ_{2+}	Γ_2	Γ_{2+}	L_2
Γ_{3+}	Γ_{12}	Γ_{3+}	L_3
Γ_{4+}	$\Gamma_{15'}$	Γ_{1-}	$L_{1'}$
Γ_{5+}	$\Gamma_{25'}$	Γ_{2-}	$L_{2'}$
Γ_{1-}	$\Gamma_{1'}$	Γ_{3-}	$L_{3'}$
Γ_{2-}	$\Gamma_{2'}$		Elliott
Γ_{3-}	$\Gamma_{12'}$	$\Gamma_{4\pm}$	$L_{6\pm}$
Γ_{4-}	Γ_{15}	$\Gamma_{5\pm}$	$L_{4\pm}$
Γ_{5-}	$\Gamma_{25'}$	$\Gamma_{6\pm}$	$L_{5\pm}$
	Elliott	$\mathbf{k}=\Delta$	
$\Gamma_{6\pm}$	$\Gamma_{6\pm}$	Koster	BSW
$\Gamma_{7\pm}$	$\Gamma_{7\pm}$	Γ_1	Δ_1
$\Gamma_{8\pm}$	$\Gamma_{8\pm}$	Γ_2	$\Delta_{1'}$
$\mathbf{k}=\Sigma$		Γ_3	Δ_2
Koster	BSW	Γ_4	$\Delta_{2'}$
Γ_1	Σ_1	Γ_5	Δ_5
Γ_2	Σ_4		Elliott
Γ_3	Σ_2	Γ_6	Δ_6
Γ_4	Σ_3	Γ_7	Δ_7

between different bands. The Hamiltonian (3.174) is valid for any symmetry type U_j. The optical matrix elements are different for different symmetry types, however.

$$\langle 0|\mathbf{A}\cdot\mathbf{p}|\psi_j{}^t\rangle = A_j\mathcal{P}_j{}^t;\quad j=1,\,2,\,3. \tag{3.175}$$

The star of $\mathbf{k}_0$ consists of the six points $(k_0, \pm k_0, 0)$, $(k_0, 0, \pm k_0)$, $(0, k_0, \pm k_0)$ together with their six negatives which need not be considered separately. We sum over this star in the manner of Secs. III B and III C to obtain the results listed in Table IX. Only energy shift terms appear since we neglect mixing of different bands U. The different symmetries U_1, U_2, U_3 have different polarization dependences. The constants f^{t0} naturally depend upon U_j but we have not indicated this explicitly to simplify the notation.

If the individual states are unresolved the dielectric function has the general form given in Eqs. (3.24) through (3.26). Note that the term in W_5 would be zero for a band of U_2 symmetry. This is similar to a nondegenerate band in the Δ direction. The symmetry types U_1 and U_3 give finite values for W_1, W_3, and W_5 and could not be distinguished from a general point in the zone.

TABLE XI. Comparison of the notation of this paper for the deformation potential parameters, d_j, with that of Kleiner and Roth, Pikus and Bir, Herring and Vogt, and Brooks.

$\mathbf{k}=0$

This paper	Kleiner and Roth	Pikus and Bir	Pikus and Bir
d_1	$=\sqrt{3}D_d{}^v$	$=+\sqrt{3}a$	$=\dfrac{(l+2m)}{\sqrt{3}}$
d_3	$=-\dfrac{2}{\sqrt{3}}D_u$	$=\sqrt{3}b$	$=\dfrac{1}{\sqrt{3}}(l-m)$
d_5	$=-\dfrac{2\sqrt{2}}{\sqrt{3}}D_{u'}$	$=\sqrt{2}d$	$=\dfrac{\sqrt{2}}{\sqrt{3}}n$

$\Delta;\quad \mathbf{k}_0=(0,0,k_0)$

This paper	Herring and Vogt	Brooks
$d_1{}^1$	$=\sqrt{3}(\Xi_d+\frac{1}{3}\Xi_u)$	$=\sqrt{3}E_1$
$d_1{}^3$	$=\dfrac{\sqrt{2}}{\sqrt{3}}\Xi_u$	$=\dfrac{\sqrt{2}}{\sqrt{3}}E_2$

$L;\ \mathbf{k}_0=\dfrac{2\pi}{a}(\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2})$

This paper	Herring and Vogt	Brooks
$d_1{}^1$	$=\sqrt{3}(\Xi_d+\frac{1}{3}\Xi_u)$	$=\sqrt{3}E_1$
$d_1{}^5$	$=\dfrac{\Xi_u}{\sqrt{3}}$	$=\dfrac{2}{\sqrt{3}}E_2$

$\Sigma;\ \mathbf{k}_0=(k_0,k_0,0)$

This paper	Herring and Vogt	Brooks
$d_1{}^1$	$=\sqrt{3}(\Xi_d+\frac{1}{3}\Xi_u)$	$=\sqrt{3}E_1$
$d_1{}^3$	$=\dfrac{2\sqrt{2}}{\sqrt{3}}(-\Xi_u+\frac{3}{4}\Xi_p)$	$=-E_2/\sqrt{6}$
$d_1{}^5$	$=\dfrac{\Xi_p}{2}$	$=E_2$

TABLE XII. Comparison of the notation of this paper for the reciprocal mass parameters r_j with that of Dresselhaus, Kip, and Kittel and that of Luttinger.

$\mathbf{k}_0=0$

This paper	Dresselhaus, Kip, and Kittel	Luttinger
r_1	$=\dfrac{1}{\sqrt{3}}(L+2M)(2/\hbar^2)$	$=-\dfrac{\sqrt{3}\gamma_1}{m\hbar^2}$
r_3	$=\dfrac{1}{\sqrt{3}}\ (L-M)(2/\hbar^2)$	$=-\dfrac{2\sqrt{3}\gamma_2}{m\hbar^2}$
r_5	$=\dfrac{\sqrt{2}}{\sqrt{3}}N(2/\hbar^2)$	$=-\dfrac{2\sqrt{6}\gamma_3}{m\hbar^2}$

$\Delta;\ \mathbf{k}_0=(0,0,k_0)$

$$r_1{}^1=\frac{1}{\sqrt{3}}\left(\frac{1}{m_{\parallel}}+\frac{2}{m_{\perp}}\right)$$

$$r_1{}^3=\frac{\sqrt{2}}{\sqrt{3}}\left(\frac{1}{m_{\parallel}}-\frac{1}{m_{\perp}}\right)$$

$L;\ \mathbf{k}_0=\dfrac{2\pi}{a}(\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2})$

$$r_1{}^1=\frac{1}{\sqrt{3}}\left(\frac{1}{m_{\parallel}}+\frac{2}{m_{\perp}}\right)$$

$$r_1{}^5=\frac{2}{\sqrt{3}}\left(\frac{1}{m_{\parallel}}-\frac{1}{m_{\perp}}\right)$$

$\Sigma;\quad \mathbf{k}_0=(k_0,k_0,0)$

$$r_1{}^1=\frac{1}{\sqrt{3}}\left(\frac{1}{m_{\parallel}}+\frac{1}{m_{\perp z}}+\frac{1}{m_{\perp x''}}\right)$$

$$r_1{}^3=\frac{1}{\sqrt{6}}\left(\frac{2}{m_{\perp z}}-\frac{1}{m_{\parallel}}-\frac{1}{m_{\perp x''}}\right)$$

$$r_1{}^5=\frac{1}{m_{\parallel}}-\frac{1}{m_{\perp x''}}$$

IV. NOTATION

We have adopted the group-theoretic notation used by Koster *et al.*[13] rather than the notation of Bouckaert, Smoluchowski, and Wigner and also Elliott[34] which is more standard in energy-band theory. In Table X we indicate the correspondence between the two notations. We reserve x, y, z exclusively for the cubic axes. We also use axis systems oriented along the [111] and

---

[34] L. P. Bouckaert, R. Smoluchowski and E. Wigner, Phys. Rev. **50**, 58 (1936); R. J. Elliott, *ibid.* **96**, 280 (1954).

[110] directions as defined in Eqs. (3.1) and (3.2). Note that for the group of Σ, Koster uses x, y, z to refer to the [110] axis system. We have reserved the subscript position as much as possible for group theoretic information pertaining to the group of $\mathbf{k}_0$ but we have permitted a few exceptions to conform to standard notation. For the strain tensor and the associated deformation potential parameters the subscript position denotes the representation in the group of $\mathbf{k}_0$. When a repetition index is required the representation in the group of $k=0$ is used as a superscript.

A number of authors have introduced notation for the deformation potential parameters and the exactly analogous effective mass parameters. The definitions have been more or less arbitrary and no two agree. We have adopted a unique procedure based on Eqs. (2.24) and (2.26) together with Koster's tables.[13] The $e_{j\alpha}$ in Eq. (2.24) transform irreducibly under the group of $\mathbf{k}_0$ and are related to the standard stress tensor components e_{xy}, etc., by Koster's unitary Clebsch-Gordan matrix γ. Similarly, the reduced matrix elements of the operator $h_{j\alpha}$ in Eq. (2.26) are given by the Clebsch-Gordan matrix γ. Equation (2.26) is the crystal analog of the Wigner-Eckart theorem.[28]

The deformation parameters D_j and the reciprocal masses R_j so defined are strictly two-band parameters and so do not correspond to any standard notation which all relates to single-band properties. We introduce exactly analogous definitions for single-band parameters which we call d_j and r_j. Table XI relates these quantities to the notation introduced by Herring and Vogt, by Kleiner and Roth, by Brooks, and by Pikus and Bir.[35] In Table XII we give the analogous relations for the reciprocal mass parameters compared to those used by Dresselhaus, Kip, and Kittel and by Luttinger.[36]

The relations between the single-band d's and the two-band D's can be worked out with the use of Eq. (2.23). When one of the bands transforms like the identity we have the simple relations given in Eq. (2.29). In general, the relations are more complex.

ACKNOWLEDGMENTS

The author has benefited from conversations with G. Gobeli and A. U. MacRae which stimulated this work. Useful discussions with U. Gerhardt, D. Brust, F. Pollak and M. Cardona are also appreciated. He is grateful for a preprint of Pollak and Cardona's recent work. Discussions with E. I. Blount and M. Lax are acknowledged. M. Lax's unpublished notes on group theory have been particularly helpful.

The author also wishes to acknowledge the hospitality of the Aspen Center for Physics during the early stages of this work.

---

[35] C. Herring and E Vogt, Phys. Rev. **101**, 944 (1956); W. H. Kleiner and L. M. Roth, Phys. Rev. Letters **2**, 334 (1959); H. Brooks *Advances in Electronics and Electron Physics*, edited by L. Marton (Academic Press Inc., New York, 1955), Vol. 7, p. 85; G. E. Pikus and G. L. Bir, Fiz. Tverd. Tela **1**, 1642 (1959) [English transl.: Soviet Phys.—Solid State **1**, 1502 (1959)].

[36] G. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev. **98**, 368 (1955); J. M. Luttinger, *ibid.* **102**, 1030 (1956).