Angular Dependence of Matrix Elements for Scattering in III-V Compounds

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We have calculated the overlap integral between periodic parts of Bloch functions for two arbitrarily directed crystal momenta $\vec{k}_1$ and $\vec{k}_2$. Contrary to conjectures in the literature that there is a dependence on the direction of $\vec{k}_1$ in addition to the angle between $\vec{k}_1$ and $\vec{k}_2$, our results show only an angular dependence on $(\vec{k}_1 \cdot \vec{k}_2)/(k_1 k_2)$. The final expression obtained is identical in form with results previously deduced by aligning $\vec{k}_1$ with a principal axis of the crystal.

I. INTRODUCTION

In the recent past, a number of authors[1-3] have theoretically studied the effects of nonparabolicity of the energy bands on transport properties in III-V compounds. Of principal importance to such considerations is a prescription for the angular dependence and variation with energy of the probability of transition between states of crystal momentum $\vec{k}_1$ and $\vec{k}_2$, in addition to details of band shapes. Ehrenreich[4] has derived an expression for the transition probability for any given scattering process. His result consists of a scalar function, describing the situation for plane waves or S states, multiplied by an overlap integral $\mathcal{G}$ between periodic parts of Bloch functions at $\vec{k}_1$ and $\vec{k}_2$. He evaluated $\mathcal{G}$ for the special case in which the initial direction of $\vec{k}_1$ is parallel to a principal axis of the crystal. In doing so, however, he states that the validity of this result for all other initial directions is an *assumption*, and that, in general, $\mathcal{G}$ depends on the direction of $\vec{k}_1$ as well as the angle between $\vec{k}_1$ and $\vec{k}_2$. For polar optical modes in GaAs, the effects of the admixture of p-type valence-band functions with conduction-band functions on $\mathcal{G}$ appear to be less important for transport coefficients than its effects on band structure. In this case $\mathcal{G} \simeq 1$ is a reasonable approximation, and only the modifications in the energy-momentum relation are of major concern.[1,2] However, for InSb and InAs, where at large values of $\vec{k}_i$ there is substantial p-function admixture,[4] $\mathcal{G}$ differs significantly from 1. In calculations of hot-electron effects, Matz[3] used Ehrenreich's expression for $\mathcal{G}$, with the conjecture that any anisotropy in the scattering matrix element introduced by picking a preferred direction for $\vec{k}_1$ is small. It is the purpose of this paper to show explicitly that Ehrenreich's result is valid for arbitrary choices of the directions of $\vec{k}_1$ and $\vec{k}_2$.

In Sec. II a reformulation of the problem in terms of angular momentum states is developed for mathematical convenience. Section III contains details of the calculation of $\mathcal{G}$ by means of matrix elements of Euler rotation operators in this representation of states.

II. FORMULATION OF THE PROBLEM

According to Ehrenreich, the multiplicative factor in the transition probability is defined by

$$\mathcal{G}(\vec{k}_1, \vec{k}_2) = \frac{1}{2} \sum_{\mu_1,\mu_2} \left| \int d\vec{r}\, u^*_{\mu_2 \vec{k}_2}(\vec{r}) u_{\mu_1 \vec{k}_1}(\vec{r}) \right|^2 . \quad (1)$$

This measures the overlap between periodic parts $u_{\mu_i \vec{k}_i}(\vec{r})$ of Bloch functions summed over the doubly degenerate spin states μ_2 and averaged over initial spin states μ_1. The functions $u_{\mu \vec{k}}$ are given by Kane,[5] and may be interpreted as follows. With respect to the crystallographic axes let us write the two linear combinations of wave functions having the symmetry properties of atomic s and p orbitals under the operations of the tetrahedral group:

$$|\alpha, \vec{k}\rangle = a_k [iS \downarrow] + b_k [(X - iY) \uparrow]/\sqrt{2} + c_k [Z \downarrow], \quad (2)$$

$$|\beta, \vec{k}\rangle = a_k [iS \uparrow] + b_k [-(X + iY) \downarrow]/\sqrt{2} + c_k [Z \uparrow]. \quad (3)$$

The coefficients a_k, b_k, and c_k are real numbers, and the arrows refer to up and down spin states. Further, let (φ, θ) be the azimuthal and polar angles of $\vec{k}$ with respect to the axes of the crystal. Then, $u_{\mu,k}$ is generated from $|\mu, k\rangle$ by

$$u_{\mu, \vec{k}} = U(\varphi, \theta) |\mu, \vec{k}\rangle, \quad (4)$$

where U is defined in terms of the angular momentum components J_y and J_z by

$$U(\varphi, \theta) = \exp[-i\varphi J_z]\exp[-i\theta J_y]. \quad (5)$$

In Eq. (4) the index μ may assume values α or β. If the definitions (2) and (3) are now inserted in Eq. (1), we may rewrite

$$\mathcal{G} = \frac{1}{2} \sum_{\mu_1, \mu_2 = \alpha, \beta} \left| (\mu_1, \vec{k}_1 | R | \mu_2, k_2) \right|^2, \quad (6)$$

where the operator of rotation is

$$R = U^{-1}(\varphi_1, \theta_1) U(\varphi_2, \theta_2). \quad (7)$$

A significant interpretation of the states (2) and (3) is further obtained by adopting an angular momentum representation of states $|j_1, j_2; J, M\rangle$. These are, by definition, simultaneous eigenfunctions of $\vec{j}_1^2, \vec{j}_2^2, \vec{J}^2$, and J_z, where $\vec{J} = \vec{j}_1 + \vec{j}_2$. In terms of these product states it is straightforward to verify that[6]

$$[S\!\uparrow] = |0, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}\rangle,$$

$$[S\!\downarrow] = |0, \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle,$$

$$[Z\!\uparrow] = -(3)^{-1/2}|1, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}\rangle$$
$$+ (\tfrac{2}{3})^{1/2}|1, \tfrac{1}{2}; \tfrac{3}{2}, \tfrac{1}{2}\rangle$$

$$[Z\!\downarrow] = 3^{-1/2}|1, \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle + (\tfrac{2}{3})^{1/2}|1, \tfrac{1}{2}; \tfrac{3}{2}, -\tfrac{1}{2}\rangle, \quad (8)$$

$$[-(X+iY)/\sqrt{2}\!\uparrow] = (\tfrac{2}{3})^{1/2}|1, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}\rangle + 3^{-1/2}|1, \tfrac{1}{2}; \tfrac{3}{2}, \tfrac{1}{2}\rangle,$$

$$[(X-iY)/\sqrt{2}\!\uparrow] = -(\tfrac{2}{3})^{1/2}|1, \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}$$
$$+ 3^{-1/2}|1, \tfrac{1}{2}; \tfrac{3}{2}, -\tfrac{1}{2}\rangle.$$

In this representation the states of interest then become

$$|\alpha, \vec{k}\rangle = ia_k|0, \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle + A|1, \tfrac{1}{2}; \tfrac{1}{2}; -\tfrac{1}{2}\rangle$$
$$+ B|1, \tfrac{1}{2}; \tfrac{3}{2}, -\tfrac{1}{2}\rangle,$$

$$|\beta, \vec{k}\rangle = ia_k|0, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}\rangle - A|1, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}\rangle + B|1, \tfrac{1}{2}; \tfrac{3}{2}, \tfrac{1}{2}\rangle,$$
$$(9)$$

where the coefficients are defined by

$$A = (c_k - \sqrt{2}\, b_k)/\sqrt{3} \quad \text{and} \quad B = (\sqrt{2}\, c_k + b_k)/\sqrt{3}. \quad (10)$$

In this form it is evident that $|\alpha, \vec{k}\rangle$ and $|\beta, \vec{k}\rangle$ are eigenfunctions of J_z. This accounts in part for the significant simplification of the problem when $\vec{k}_1$ is presumed parallel to the Z axis of the crystal. For, in that instance, R represents a single Euler rotation whose J_z dependence merely introduces complex phases in φ. The angle φ immediately drops out of the calculation. A further simplification results from the fact that the four matrix elements whose norms define $\mathcal{G}$ occur, apart from phase factors, as conjugate pairs, i.e.,

$$(\beta, \vec{k}_2|R|\beta, \vec{k}_1) = (\alpha, \vec{k}_2|R|\alpha, \vec{k}_1)^*,$$
$$(\beta, \vec{k}_2|R|\alpha, \vec{k}_1) = -(\alpha, \vec{k}_2|R|\beta, \vec{k}_1)^*. \quad (11)$$

Finally, it becomes possible to take advantage of certain special properties of the matrix elements of R between angular momentum states. These follow from the well-known analogs for the unitary operator $\exp[-i\theta J_y]$.[7] Since the latter (and in consequence R) connects only states with the same

values of j_1, j_2, and J, it is sufficient to consider matrix elements of the form

$$r^J_{mm'} = \langle J, m|\exp[-i\theta J_y]|J, m'\rangle.$$

These possess the following properties:

$$r^J \text{ is real}, \quad (12a)$$

$$r^J_{mm'} = (-1)^{m-m'} r^J_{-m,-m'}, \quad (12b)$$

$$r^J_{mm'}(\theta) = r^J_{m'm}(-\theta), \quad (12c)$$

which implies that

$$[r^{-1}(\theta)]^J_{mm'} = r^J_{m'm}(\theta).$$

From these properties and the definition

$$R^J_{mm'} = \sum_{m_1=-J}^{J} e^{im_1(\varphi_1-\varphi_2)} r^J_{m_1 m}(\theta_1) r^J_{m_1 m'}(\theta_2),$$

it may be readily deduced that

$$R^J_{mm'} = (-1)^{m-m'} R^{J*}_{-m,-m'} \quad (13)$$

and that R^J is complex only by virtue of its φ dependence.

The relations (11) and (13) can be used to reduce $\mathcal{G}$ to the more transparent expression

$$\mathcal{G} = \sum_{m=\pm 1/2} \left\{ [a_{k_1}^2 a_{k_2}^2 + A_1^2 A_2^2]|R^{1/2}_{1/2,m}|^2 + B_1 B_2 \right.$$

$$\times [B_1 B_2|R^{3/2}_{1/2,m}|^2 + 2a_{k_1} a_{k_2} \text{Re}(R^{3/2}_{1/2,m} R^{1/2*}_{1/2,m})]$$

$$+ 2A_1 A_2 (-1)^{m-1/2}[a_{k_1} a_{k_2}|R^{1/2}_{1/2,m}|^2$$

$$\left. + B_1 B_2 \text{Re}(R^{3/2}_{1/2,m} R^{1/2*}_{1/2,m})]\right\}. \quad (14)$$

In Sec. III we will demonstrate explicitly that $\mathcal{G}$ is a function of $\cos\gamma = (\vec{k}_1 \cdot \vec{k}_2)/k_1 k_2)$ via the expression

$$\cos\gamma = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2).$$

III. CALCULATION OF $\mathcal{G}$

The first term of Eq. (14) can be immediately evaluated by using the unitarity of R and the completeness of the states to write

$$\sum_{m=\pm 1/2} |R^{1/2}_{1/2,m}|^2 = 1. \quad (15)$$

To calculate the remaining terms it is convenient to perform a further reduction of terms by factorization. Accordingly, consider the general expression

$$\text{Re}\{R^{J_1}_{1/2,1/2} R^{J_2*}_{1/2,1/2} \pm R^{J_1}_{1/2,-1/2} R^{J_2*}_{1/2,-1/2}\} = \sum_{m_1=-J_1}^{J_1} \sum_{m_2=-J_2}^{J_2} \cos[(m_1 - m_2)(\varphi_1 - \varphi_2)] r^{J_1}_{m_1,1/2}(\theta_2) r^{J_2}_{m_2,1/2}(\theta_2)$$

$$\times \{r^{J_1}_{m_1,1/2}(\theta_1) r^{J_2}_{m_2,1/2}(\theta_1) \pm r^{J_1}_{m_1,-1/2}(\theta_1) r^{J_2}_{m_2,-1/2}(\theta_1)\}. \quad (16)$$

By coupling in turn terms in which m_1 and m_2 are of like and unlike sign, and using properties (12b) and (12c), we deduce the factorized form

$$\sum_{m_1, m_2 > 0} \left\{ \cos((m_1 - m_2)(\varphi_1 - \varphi_2)) \prod_{i=1}^{2} (r^{J_1}_{m_1, 1/2} r^{J_2}_{m_2, 1/2} \pm r^{J_1}_{m_1, -1/2} r^{J_2}_{m_2, -1/2})_{\theta_i} + \cos[(m_1 + m_2)(\varphi_1 - \varphi_2)] \right.$$

$$\left. \times \prod_{i=1}^{2} (r^{J_1}_{m_1, 1/2} r^{J_2}_{m_2, -1/2} \mp r^{J_1}_{m_1, -1/2} r^{J_2}_{m_2, 1/2})_{\theta_i} \right\} . \tag{17}$$

This formula highlights the expected symmetry of $\mathcal{G}$ in its angular variables. It is further seen by inspection that terms with the minus sign in the second sum vanish for the case $J_1 = J_2$ and $m_1 = m_2$.

In order to complete the evaluation of Eq. (14) via Eq. (17), we need the following explicit forms for the matrix elements[8]:

$$r^{3/2}_{3/2, 1/2} = -\tfrac{1}{2}\sqrt{3} \cos\tfrac{1}{2}\theta \sin\theta ,$$

$$r^{3/2}_{3/2, -1/2} = \tfrac{1}{2}\sqrt{3} \sin\tfrac{1}{2}\theta \sin\theta ,$$

$$r^{3/2}_{1/2, 1/2} = -\tfrac{1}{2}\cos\tfrac{1}{2}\theta (1 - 3\cos\theta) , \tag{18}$$

$$r^{3/2}_{1/2, -1/2} = -\tfrac{1}{2}\sin\tfrac{1}{2}\theta (1 + 3\cos\theta) ,$$

$$r^{1/2}_{1/2, 1/2} = \cos\tfrac{1}{2}\theta , \quad r^{1/2}_{1/2, -1/2} = -\sin\tfrac{1}{2}\theta .$$

By a straightforward substitution we may obtain explicitly that

$$\left| R^{1/2}_{1/2, 1/2} \right|^2 - \left| R^{1/2}_{1/2, -1/2} \right|^2 = \cos\gamma , \tag{19}$$

$$\left| R^{3/2}_{1/2, 1/2} \right|^2 + \left| R^{3/2}_{1/2, -1/2} \right|^2 = \tfrac{1}{4}(1 + 3\cos^2\gamma) , \tag{20}$$

$$\text{Re}\{ R^{3/2}_{1/2, 1/2} R^{1/2*}_{1/2, 1/2} + R^{3/2}_{1/2, -1/2} R^{1/2*}_{1/2, -1/2} \} = \cos\gamma , \tag{21}$$

and

$$\text{Re}\{ R^{3/2}_{1/2, 1/2} R^{1/2*}_{1/2, 1/2} - R^{3/2}_{1/2, -1/2} R^{1/2*}_{1/2, -1/2} \}$$

$$= \tfrac{1}{2}(3\cos^2\gamma - 1). \tag{22}$$

With these results $\mathcal{G}$ is finally expressible in the form

$$\mathcal{G} = a^2_{k_1} a^2_{k_1} + 2a_{k_1} a_{k_2}(A_1 A_2 + B_1 B_2)\cos\gamma$$

$$+ (A_1 A_2 + B_1 B_2)^2 \cos^2\gamma + (A_1 A_2 - \tfrac{1}{2}B_1 B_2)^2$$

$$\times (1 - \cos^2\gamma) , \tag{23}$$

where in terms of the original coefficients

$$A_1 A_2 + B_1 B_2 = b_{k_1} b_{k_2} + c_{k_1} c_{k_2} ,$$

and

$$A_1 A_2 - \tfrac{1}{2}B_1 B_2 = \tfrac{1}{2} b_{k_1} b_{k_2} - 2^{-1/2}(b_{k_1} c_{k_2} + b_{k_2} c_{k_1}). \tag{24}$$

This corresponds to Matz's expression,[9] and exhibits the explicit dependence of $\mathcal{G}$ on the cosine of the angle between $\vec{k}_1$ and $\vec{k}_2$.

A qualitative physical picture of this result may be constructed as follows. The function $\mathcal{G}$ is a linear combination of terms, each of which measures the overlap between states of definite J_z. When $\vec{k}_1$ is aligned with the crystallographic Z axis, each term is invariant under rotations about the Z axis, and $\mathcal{G}$ is thus cylindrically symmetric about $\vec{k}_1$. Still further, the states of interest are direct products of spin states with s and p orbitals. Although the crystal has tetrahedral symmetry, these particular states have the same transformation properties under rotation as they would for a spherically symmetric system. It is therefore reasonable to expect that $\mathcal{G}$ will remain invariant in form when the direction of $\vec{k}_1$ is arbitrary.

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[5] E. O. Kane, J. Phys. Chem. Solids 1, 249 (1957), see Eq. (14) in particular.

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