Comment on Electro-optic Effect and Valence-Band Mixing in Zinc-Blende Semiconductors

Khurgin and Voisin have recently put forward the hypothesis that existing theories of the Pockels electro-optic effect and valence-band mixing in zinc-blende semiconductors are inadequate, and must be modified to account for the “permanent dipole moment” of the valence-band states [1]. It is shown here that there is no evidence to support this conjecture, and that their proposed Hamiltonian is in disagreement with basic principles of solid-state physics.

(1) They begin by stating that Aronov and Pikus’s $\mathbf{k} \cdot \mathbf{p}$ theory of the Pockels effect [2] gives “results [that are] much too small in comparison with experimental observations,” citing Ref. [3] in support of their claim. This is a gross misrepresentation of the facts. References [3] and [4] demonstrate clearly that no bulk theory can account for the Pockels effect in quantum wells; however, this has *no implications whatsoever* for the Pockels effect in bulk crystals. The theory of Aronov and Pikus is, in fact, in satisfactory agreement with both the magnitude and frequency dependence of the bulk Pockels effect [2], even though it uses only a very simple model of the band structure.

(2) They claim that $\mathbf{k} \cdot \mathbf{p}$ theory cannot be used to describe the Pockels effect, because the potential energy in this case does not satisfy periodic boundary conditions (PBCs). This is irrelevant, since nothing in $\mathbf{k} \cdot \mathbf{p}$ theory requires the use of PBCs [5]. In particular, Aronov and Pikus do not use PBCs [2].

(3) They state that the diagonal matrix elements of momentum for Bloch waves are “always zero.” This is not true; they are equal to $(m/\hbar)\nabla_{\mathbf{k}}E_n(\mathbf{k})$ [6].

(4) They claim that there is “no way to account for” effects such as piezoelectricity using PBCs, because in a periodic system, “permanent polarization must vanish.” This is false. In a periodic system, absolute polarization is ill defined, not zero [7]; also, experiments generally measure *changes* in polarization, which are well defined [7]. The quantity of interest is thus not the static dipole moment but the *current* that flows in response to a perturbation [7] (as calculated, for example, in Ref. [2]).

(5) Their valence-band Hamiltonian is given first in the Luttinger-Kohn representation [5], where they say that a uniform electric field $\mathbf{E}$ generates a dipolelike mixing of degenerate bands (i.e., mixing that is linear in E and independent of k). This is incorrect. In the Luttinger-Kohn

representation, the potential $U = e\mathbf{E} \cdot \mathbf{x}$ has matrix elements $\langle n\mathbf{k}|U|n'\mathbf{k}'\rangle = ie\mathbf{E} \cdot \nabla_{\mathbf{k}}\delta(\mathbf{k} - \mathbf{k}')\delta_{nn'}$ inside the Brillouin zone, so the lowest-order mixing between valence states X and Y is proportional to $E_x k_y - k_x E_y$ or $E_x E_y$ [see Eqs. (II.29) and (IV.7) of Ref. [5]]. There is no dipole term in the Luttinger-Kohn Hamiltonian [8].

(6) Next, they transform from the Luttinger-Kohn representation to the Bloch representation [9], and again find a k -independent mixing of degenerate bands. This too is incorrect. In the Bloch representation, the coordinate operator has the form $\mathbf{x} = i\nabla_{\mathbf{k}}\delta_{nn'} + \xi_{nn'}(\mathbf{k})$ [6,9], where

$$\xi_{nn'}(\mathbf{k}) = \int_{\text{unit cell}} u_{n\mathbf{k}}^*(\mathbf{x}) [i\nabla_{\mathbf{k}} u_{n'\mathbf{k}}(\mathbf{x})] d^3x, \quad (1)$$

and $u_{n\mathbf{k}}$ is the periodic part of a Bloch function. At a degeneracy, $u_{n\mathbf{k}}$ is always discontinuous in $\mathbf{k}$ [10,11]; consequently, the transverse components of $\xi_{nn'}(\mathbf{k})$ diverge as k^{-1} [12]. Khurgin and Voisin do not account for this non-analytic behavior; hence, their Hamiltonian is also invalid in the Bloch representation.

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