Electron-mediated indirect interaction in narrow-band-gap semiconductors

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The effect of the hybridization of Bloch states between strongly interacting bands on the interband-transition matrix element is considered. We show that, due to the damping effect of the phase factor and the orthogonality condition between hybridized states, the interband transition between the light-hole and conduction band is restricted in the region around the Γ point, where the density of states is very small. Thus, in narrow-band-gap semiconductors, such as InSb and GaAs, the dominant indirect interaction is mediated by heavy-hole electrons with shorter exponential-decay length for the long-range interaction.

Experimental results concerning the phonon-dispersion relation of semiconductors exhibit the characteristic feature that the transverse-acoustic phonon branch has an unusually low frequency at the zone boundary and is very flat away from the zone center. This behavior has been studied by Weber¹ with the extended Philips's bond-charge model² of lattice vibration. Sokel and Harrison³ showed that Weber's bond-charge model can be described in terms of a Born-von Karman expansion and will lead to electronically mediated indirect long-range two-body interaction between atoms. From the point of view of symmetry, the local potential disturbance arising from the transversal atomic displacement associated with phonon excitations is antisymmetric with respect to the vibration center, and will induce coupling between band states with different parities, such as the s - and p -band edges located at the Γ point of a polar semiconductor. In narrow-band-gap semiconductors, there is strong hybridization of Bloch states with different parities in the energy band when the wave vector $\mathbf{k}$ is away from the zone center. Owing to the hybridization of Bloch states the interband-transition matrix element of the perturbing potential will depend on the wave vectors of the band states involved in the interband transitions. In this paper, an interband matrix element, which is consistent with the symmetry of the basic states involved in the electron-hole excitations is adopted to study the long-range indirect interaction in narrow-band-gap semiconductors such as InSb and GaAs.

Using second-order perturbation theory, the electron-mediated indirect interaction between two atoms separated by a distance $\mathbf{R}$ can be written in the form

$$H(\mathbf{R}) = -\frac{1}{\Omega^2} \sum_{nn', \mathbf{k}, \mathbf{k}'} \left[\frac{|V_{nn'}(\mathbf{k}, \mathbf{k}')|^2 e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}}}{E_{n'}(\mathbf{k}') - E_n(\mathbf{k})} + \text{c.c.} \right], \quad (1)$$

where $E_{n'}(\mathbf{k}')$ and $E_n(\mathbf{k})$ are the conduction- and valence-band energy, respectively. Here Ω is the volume of the crystal, and the wave vectors $\mathbf{k}$ and $\mathbf{k}'$ are to be summed over the first Brillouin zone (BZ). The interband matrix element $V_{nn'}(\mathbf{k}, \mathbf{k}')$ is evaluated with the involved

atom site as the origin, and the change of phase of the Bloch function over the two atom sites gives rise to the phase factor $e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}}$.

Consider now a direct-band-gap semiconductor with s - and p -band edges locate at the Γ point. Neglecting the spin-orbital interaction, the periodic part of the Bloch functions of the conduction band and light-hole band can be written as

$$|n\mathbf{k}\rangle = a_n(\mathbf{k})|s\rangle + c_n(\mathbf{k})|z\rangle \quad (2)$$

for $\mathbf{k}$ along the [001] direction, and n denoting the band index. The s state and p_z state are hybridized via the unperturbed crystal Hamiltonian, and the matrix element between them is given by Slater and Koster⁴ as

$$(s/z) = \frac{8i}{\sqrt{3}}(sp\sigma)\sin\left[\frac{ka}{4}\right] \quad (3)$$

for the nearest-neighbor interaction. Here $(sp\sigma)$ is the two-center energy integral of s and p basic orbitals, and a denotes the lattice constant. We note that the matrix element of crystal Hamiltonian in Eq. (3) will induce strong s - p_z hybridization even for small $\mathbf{k}$ value, e.g., one-tenth of $2\pi/a$, in narrow-band-gap semiconductors. The matrix element of the odd-parity perturbing potential V is represented as

$$V_{nn'}(\mathbf{k}, \mathbf{k}') = [a_n(\mathbf{k})c_{n'}^*(\mathbf{k}') + c_n(\mathbf{k})a_{n'}^*(\mathbf{k}')]V_{sp}, \quad (4)$$

where V_{sp} is the matrix element of V between s and p basic state, and is the coupling arising from the displacement of an atom, and is proportional to that displacement. The band indices n' and n denote the conduction and light-hole bands, respectively. In the intermediate range of R and beyond, due to the phase factor $e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}}$ in Eq. (1), the dominant contributions of the interband transitions come from that of the direct transition, i.e., $\mathbf{k}=\mathbf{k}'$, because the interference damping effect of the phase factor will destroy the contribution arising from the indirect transition, i.e., $\mathbf{k} \neq \mathbf{k}'$, especially for the case of large R . However, on the other hand, the orthogonality condition requires

$$a_n(\mathbf{k})a_n^*(\mathbf{k}) + c_n(\mathbf{k})c_n^*(\mathbf{k}) = \delta_{nn'}, \quad (5)$$

and, in most of the region except that around the Γ point of the BZ, the strong s - p_z hybridization will lead to

$$|a_n(\mathbf{k})| \simeq |c_n(\mathbf{k})| \quad \text{and} \quad |a_n(\mathbf{k})| \simeq |c_n(\mathbf{k})| \quad (6)$$

for the conduction and light-hole bands, respectively. The combined effects of Eqs. (5) and (6), and the very low density of states in the region around the Γ point, result in interband transitions between the light-hole band and conduction band contributing only a minor part to the indirect interaction induced by odd-parity perturbing potential in narrow-band-gap semiconductors.

For the heavy-hole bands, as their symmetry is always p_x and p_y for $\mathbf{k}$ along the $[001]$ direction, the transition matrix element between those bands and the conduction band will depend on the wave vector $\mathbf{k}'$ of the conduction-band state only. Owing to the strong s - p_z hybridization, the s state component $a_n(\mathbf{k}')$ of the conduction band will be reduced from 1 (at the Γ point) to about $\sqrt{2}/2$ (at the X point). Since reduction of the s state component results from the mixing is closely related to the crystal Hamiltonian matrix element (s/z) in Eq. (3), the interband matrix element $|V_{nn'}(\mathbf{k}, \mathbf{k}')|^2$ can be approximated to be isotropic as

$$|V_{nn'}(\mathbf{k}', \mathbf{k}')|^2 = |V_{sp}|^2 \left[1 - \frac{1}{2} \sin^2 \left[\frac{k'a}{4} \right] \right], \quad (7)$$

for polar semiconductors with zinc-blende structure. We note that the matrix element in Eq. (7) is consistent with the symmetry of the basic states involved in the interband transition and the crystal structure. The argument that the contribution arising from the transitions of light-hole electrons is not important has been numerically verified by a model with the energy band simulated by the small-gap approximation of the $\mathbf{k} \cdot \mathbf{p}$ method in the range up to $R = 15a$. It shows that in InSb the contribution to the interaction energy $H(R)$ from the light-hole electrons is about three orders of magnitude smaller than that from the heavy-hole electrons.

We assume that the energy-band structure of the semiconductor with direct energy gap E_g at Γ point is

$$E_c(\mathbf{k}') = E_g + \frac{\hbar^2 k'^2}{2m_e}, \quad E_v(\mathbf{k}) = -\frac{\hbar^2 k^2}{2m_h}, \quad (8)$$

where m_e and m_h are the effective masses of the electron and heavy holes, respectively. In evaluating the integral of $H(\mathbf{R})$ in Eq. (1), we extend the integration limit for k and k' to infinity. The spurious contribution arising from this is quite negligible. The calculated result for the interaction energy $H(R)$ is

$$H(R) = -\frac{|V_{sp}|^2 m_e E_g \sqrt{m_e m_h}}{4\pi^3 \hbar^4 R^2} \left[3(1 + \alpha^2) K_2(k_h R \sqrt{\alpha^2 + 1}) + R \left[\frac{R + a/2}{R^2 + \alpha^2(R + a/2)^2} K_2(k_h \sqrt{\alpha^2(R + a/2)^2 + R^2}) \right. \right. \\ \left. \left. + \frac{R - a/2}{R^2 + \alpha^2(R - a/2)^2} K_2(k_h \sqrt{\alpha^2(R - a/2)^2 + R^2}) \right] \right], \quad (9)$$

where

$$k_h^2 = 2m_h E_g / \hbar^2, \quad \alpha^2 = m_e / m_h. \quad (10)$$

The function K_2 in Eq. (9) is the modified Bessel function of the second order. Using the asymptotic expansion formula of the Bessel function K_2 for two limiting cases, we obtain, in the case of $k_h R \gg 1$,

$$H(R) \simeq -\frac{|V_{sp}|^2 \mu E_g}{4\pi^3 \hbar^4 R^2} \left[\frac{\pi m_e m_h}{2k_g R} \right]^{1/2} \\ \times \{ 3 + \cosh[a \sqrt{2m_e^2 E_g / (m_e + m_h) \hbar^2}] \} e^{-k_g R}, \quad (11)$$

where

$$k_g^2 = 2(m_e + m_h) E_g / \hbar^2, \quad \mu = m_e m_h / m_e + m_h. \quad (12)$$

On the other hand, when $k_h R \ll 1$, we obtain

$$H(R) \simeq -\frac{3|V_{sp}|^2 \sqrt{m_e m_h}}{4\pi^3 \hbar^2 (m_e + m_h) R^4}. \quad (13)$$

The complicated result of Eq. (9) shows an attractive interaction within the full range. In the long-range case, the form in Eq. (11) is almost similar to that of Sokel and Harrison, except that the effective mass of the heavy hole replaces that of the light hole, and the factor 1 is now replaced by the hypercosine term in Eq. (11). We note that, in the extreme limit $k_h R \gg 1$, the work of Sokel and Harrison is equivalent to include all direct transitions over the whole $\mathbf{k}$ space, and the only attenuation mechanism is the increase of the interband energy gap with k .

Now we estimate the exponential decay length in Eq. (11), where m_h is the heavy-hole mass instead of the light-hole mass. The replacement of the light-hole mass by the heavy-hole mass will reduce the ratio of the decay length to the zone-boundary wavelength k_0/k_g , calculated by Sokel and Harrison by a factor 3.63 for InSb and 2.31 for GaAs.⁵ The final results of k_0/k_g are 6.17 and 2.03, for InSb and GaAs, respectively. These values are in better agreement with that based on Weber's model, e.g., 2.9 and 2.1, than that of Sokel and Harrison, e.g., 22.4 and 4.7, for InSb and GaAs, respectively. The reduction factor for GaAs is too large. This may be due

to the fact that the s - p hybridization between interacting band states in GaAs is not as strong as that in InSb, to effectively activate the cancellation mechanism, so that the light-hole electrons involved in the interband transitions will still mediate a longer-range interaction. This implies that the cancellation mechanism stated above is valid only for semiconductors with very narrow energy gaps. We would like to stress that, for most of the semiconductors except those with narrow energy gaps, the indirect interaction mediated by the light-hole electrons

with longer decay length is still dominant as discovered by Sokel and Harrison.³ It is also interesting to compare the present result with that between local magnetic impurities, each of which generates an isotropic local disturbance on the substituted metallic sites, in polar semiconductors.⁶

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