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RESONANT AND NONRESONANT POLARONS IN NARROW GAP SEMICONDUCTORS

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Interaction of electrons with optic phonons in InSb-type semiconductors in the resonant region of $\hbar\omega_c \approx \hbar\omega_L$ is considered theoretically, taking consistently into account real band structure of narrow gap materials. Nonresonant contribution to polaron energy is also calculated as a function of magnetic field and it is shown that the "offset" effect, claimed by some authors, does not exist.

I. Introduction

Since the discovery of magneto-optical effects due to resonant interaction of electrons with optic phonons in InSb [1], resonant behavior has become subject of substantial interest [2,3,4,5,6,7].

Shortly after the discovery of the resonant polaron behavior a claim was made of an "offset" effect [8], by which the authors understood an energy shift of $\alpha\hbar\omega_L$ between lower and upper polaron branches, as ω_c passes ω_L. This was used by various authors to determine experimentally the polar coupling constant α in InSb [8], InAs [9] and HgCdTe [10].

While most experiments have been performed on narrow gap materials the existing theoretical work has used the standard one-band effective mass approximation. In this paper we describe resonant polarons in InSb-type semiconductors consistently using the real band structure of these materials (small energy gap and strong spin-orbit interaction). We apply the Green function formalism, necessary for a correct description of the upper polaron branch. In the second part we calculate the nonresonant contribution to polaron energy as a function of magnetic field and demonstrate that the "offset" effect does not exist.

II. Resonant Polarons

The initial Hamiltonian for our problem reads

$$H = P^2/2m_o + V_o(\vec{r}) + H_{so} + H_{Fr} + H_{phn} \quad , \qquad (1)$$

where m_o is the free electron mass, $\vec{P} = \vec{p} + (e/c)\vec{A}$ is the kinetic momentum, $\vec{A}$ is the vector potential of an external magnetic field, V_o is the periodic potential of the lattice, H_{so} is the spin-orbit interaction, H_{Fr} denotes the Frӧhlich polar electron-phonon interaction (assumed weak), and H_{phn} is the free phonon field.

The first three terms describe band structure of the material in the presence of a magnetic field. This electronic part is solved for the vicinity of the Γ point using a three-level model. The latter takes exactly into account the k·p interaction between Γ_6, Γ_8 and Γ_7 levels, including explicitly the small energy gap ε_g and the spin-orbit energy Δ [11,12]. The resulting electron energies (assuming $\Delta > \varepsilon_g$) are

$$\varepsilon(n,k_z,\pm) = -\varepsilon_g/2 + [(\varepsilon_g/2)^2 + \varepsilon_g D(n,k_z,\pm)]^{1/2}, \qquad (2)$$

where

$$D(n,k_z,\pm) = \hbar\omega_c(n+1/2) + \hbar^2 k_z^2/2m_o^* \mp \mu_B |g_o^*| H/2, \qquad (3)$$

with $\omega_c = eH/m_o^* c$. Here m_o^* and g_o^* denote the effective mass and the g-factor at the bottom of conduction band. Plus and minus signs refer to the two effective-spin states. The electron wavefunctions are

$$\Psi^{\pm}_{nk_z}(\vec{r}) = \Sigma\, c_l(n,k_z,\pm)\, f_l^n(\vec{r})\, u_l(\vec{r}), \qquad (4)$$

where the summation l is over the levels in question (8 states including spin). f are envelope functions of the harmonic-oscillator type and u denote the Luttinger-Kohn periodic amplitudes. The wavefunctions (4) are mixtures of s-like and p-like components, as well as spin-up and spin-down states (explicit expressions are given in [12].

In our approach the Frӧhlich interaction Hamiltonian can be used directly as a perturbation because the electron wavefunctions of eq. (4) have been obtained without the Luttinger-Kohn effective mass transformation. We consider resonant case: $\varepsilon_1^+ - \varepsilon_o^+ \approx \hbar\omega_L$, in which the upper electron state $\beta(n=1,\ k_y=0,\ k_z=0,\ s=+)$ can decay by a virtual emission of an optic phonon $\vec{q}$ to the ground state $\gamma(0,\ k_y,\ k_z,\ +)$. The resonant part of the electron selfenergy Σ of the state β is (in the lowest order of perturbation theory),

$$\Sigma(E) = \sum_{k_y k_z} \sum_{q} \frac{|(q,\gamma|H_{Fr}|0,\beta)|^2}{E+i\Gamma_o-\varepsilon_o^+-\hbar\omega_L} - i\,\Gamma_o \,. \qquad (5)$$

An additional weak scattering has been introduced by a phenomenological constant parameter $\Gamma_o > 0$. This eliminates a nonphysical divergence at $E = \varepsilon_o^+ + \hbar\omega_L$. The selfenergy is then calculated using electron energies (2),(3) and wavefunctions (4) as a function of magnetic field in the resonant region. The s-p mixing in the wavefunctions (4) results in an effective weakening of the electron-phonon interaction for a given coupling constant α (similar result is obtained in absence of a magnetic field, cf. [13]).

Next we calculate the spectral function A(E) for the state $\beta(1,0,0,+)$,

$$A(E) = \frac{1}{\pi} \frac{\Gamma}{(E-\varepsilon_1^+ - \Delta)^2 + \Gamma^2}, \qquad (6)$$

where Δ and Γ are real and imaginary parts of selfenergy, respectively: $\Sigma(E) = \Delta(E) - i\Gamma(E)$. For pure crystals, in which intraband magneto-optical transitions occur at low k_z values, maxima of spectral function correspond to maxima of the density of electron

states, i.e. to the observable polaron energies. Omitting the detailed calculations for the lack of space we note that below the resonant energy $E_c = \varepsilon_0^+ + \hbar\omega_L$ the real part of selfenergy has a strong maximum ($\Delta \sim -(E_c-E)^{-1/2}$ if $\Gamma_o \equiv 0$) and the imaginary part $\Gamma \equiv 0$ (again for $\Gamma_o \equiv 0$). Above the resonant energy the roles reverse: Δ has a finite value and Γ has a strong maximum ($\Gamma \sim (E-E_c)^{-1/2}$ if $\Gamma_o \equiv 0$). The alternating singularities of real and imaginary parts of selfenergy push away the polaron energies from the resonant value E_c, the "pinning" effect both below and above the resonance occurs.

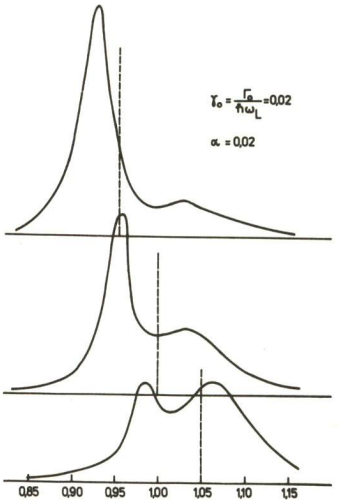

Fig.1 Spectral function (in arbitrary units) of the $|n=1, k_y=0, k_z=0, s=+)$ polaron state as a function of energy (in $\hbar\omega_L$ units) for three values of magnetic field, near the resonance with optic phonons: Upper curve is for x=0.95, middle curve for x=1.00, and lower curve for x=1.05, where $x = (\varepsilon_1^+ - \varepsilon_0^+)/\hbar\omega_L$. The dashed lines indicate respective positions of the Landau level $|1,0,0,+)$ unperturbed by the electron-phonon interaction.

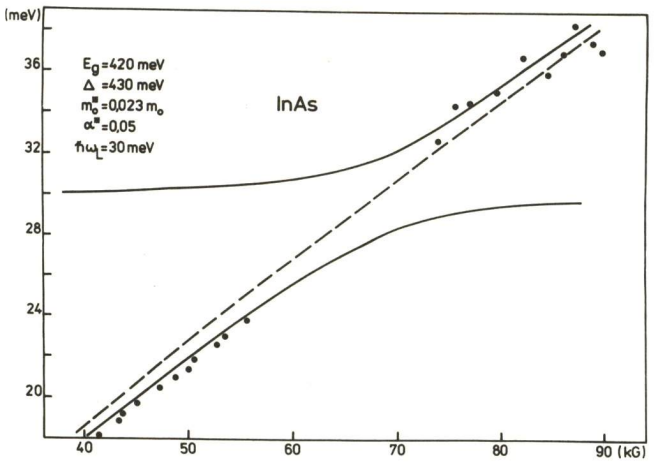

Fig. 2 Polaron energies in InAs as functions of a magnetic field in the resonant region: Experimental points are after Harper et al. [9], solid lines are theoretical (this work). Dashed line indicates the energy of the Landau level $|1,0,0,+)$ in absence of electron-phonon interaction.

Fig.1 shows the spectral function of $\beta(1,0,0,+)$ state at $k_z=0$ for three values of the magnetic field: below, at, and above the resonance. It can be seen that two maxima of the spectral function (polaron branches) appear, the upper one being broader. Far below and far above the resonance only one branch is observed. This strongly resembles the result of Vigneron et al. [7] for the optical absorption, confirming our supposition on the close relation between features of the spectral function and observables.

In Fig.2 calculated positions of the maxima are compared with experimental data of Harper et al. [9] for InAs. Equally good fit has been obtained using the same method for a two-mode polaron in the $Hg_{0.72}Cd_{0.28}Te$ mixed crystal [14].

III. Nonresonant Part of Polaron Energy

The nonresonant contribution to polaron energy is calculated by taking into account the electron-phonon coupling of a given Landau state with all other states by means of eq. (5). For n=1 state the summation excludes contribution of n=0 state, which has been calculated above. The summs can be converted into integrals (here we assume a parabolic energy band) [15]. The results are shown in Table 1. It can be seen that the nonresonant contribution is a smooth function of a magnetic field, not undergoing any dramatic change as ω_c passes ω_L.

l	s_o	s_1
0.1	1.008	0.911
0.3	1.024	0.886
0.5	1.040	0.880
0.7	1.055	0.881
0.9	1.070	0.884
1.0	1.077	0.886
1.1	1.084	0.888
1.3	1.098	0.894
1.5	1.111	0.900
1.7	1.124	0.906
1.9	1.136	0.915
2.0	1.142	0.916

Table 1 Nonresonant contribution to polaron energy for n=0 and n=1 Landau states as functions of magnetic field ($l = \hbar\omega_c/\hbar\omega_L$). The energy shifts are

$$\Sigma_o = -\alpha\hbar\omega_L s_o \qquad \Sigma_1^{nr} = -\alpha\hbar\omega_L s_1$$

Thus we conclude that the "offset" effect does not exist and that the claims of having it observed are due to incorrect calculation of the upper polaron branch (using Wigner-Brillouin perturbation theory) and to improper extrapolation of the lower polaron branch to higher magnetic fields.

References

1) E.J.Johnson and D.M.Larsen: Phys. Rev. Lett. 16 (1966) 655.
2) R.Kaplan and R.F.Wallis: Phys. Rev. Lett. 20 (1968) 1499.
3) B.D.McCombe and R.Kaplan: Phys. Rev. Lett. 21 (1968) 756.
4) C.J.Summers et al.: Solid State Commun. 5 (1967) 615.
5) P.G.Harper: Proc. Phys. Soc. London 92 (1967) 793.
6) M.Nakayama: J. Phys. Soc. Japan 27 (1969) 636.
7) J.P.Vigneron et al.: Phys. Rev. B 18 (1978) 6930.
8) D.H.Dickey et al.: Phys. Rev. Lett. 18 (1967) 599.
9) P.G.Harper et al.: Proc. Conf. Phys. Sem. Boston 1970, p.166.
10) M.A.Kinch and D.D.Buss: Proc. Conf. Phys. Semicond. and Semimet. Pergamon (1971) p.461.
11) R.Bowers and Y.Yafet: Phys. Rev. 115 (1959) 1165.
12) W.Zawadzki: in "New Developm. Semicond." Noordhoff (1973) p.441.
13) W.Zawadzki and W.Szymanska: Phys. Stat. Sol. b 45 (1971) 415.
14) L.Swierkowski et al.: Sol. St. Commun. 27 (1978) 1245.
15) D.M.Larsen: Phys. Rev. 142 (1966) 428.