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NEW SELECTION RULE FOR INTERBAND LIGHT ABSORPTION IN SEMICONDUCTOR INVERSE SUPERATOM

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Bound-bound interband transitions in semiconductor inverse superatom are analysed. The difference of dielectric permittivities is shown to induce partial breakdown of conventional selection rule for interband transitions, i.e. besides the transitions with azimuthal quantum number conserved, that are only allowed with constant dielectric permittivity, transitions with azimuthal number changed by any even number also occur.

Most semiconductor microstructures consist of several (at least two) different materials that, naturally, have different properties, such as effective mass, band gap, refractive index, etc., causing their position dependence. The position dependence of band gap (i.e. of conduction/valence band extrema) determines the fundamental quantum properties of the structure - well and barrier regions. Position dependence of the effective mass does not influence that much on the band structure, but does induce some important effects, as well-barrier inversion with increasing transversal wavevector /1/, or qualitative change in wavefunctions behaviour in quantum well in electric field, etc. Position dependence of the refractive index (i.e. high frequency dielectric permittivity) influences the band structure (when calculated self-consistently), and consequently other properties (e.g. absorption), but only through slight quantitative corrections in $GaAs$-$Al_xGa_{1-x}As$ based quantum wells and superlattices, due to a comparatively small difference of refractive indices of these materials.

The recent development of sophisticated technologies, e.g., the atomic layer epitaxy, has enabled realization of a wide variety

of quantum microstructures, the most important of these being the superatom /2/ depicted in Fig.1. Superatom is a semiconductor B sphere with radius R_o embedded in semiconductor A bulk. If the band extrema of B are bellow those of A, the structure is called the inverse superatom. Analysis of intraband transitions in this structure indicates that difference of refractive indices induces only slight quantitative corrections. In this paper we shall analyse the influence of refractive index position dependence on interband transitions in inverse superatom.

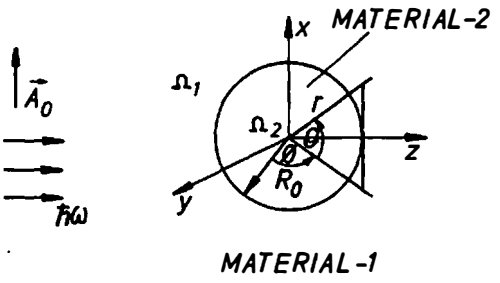

Fig.1. The inverse superatom in radiation field with magnetic vector potential $\vec{A}_o$ and frequency ω.

Due to the difference of high frequency dielectric permittivities ε_1 and ε_2, the magnetic vector potential will not be homogeneous /3/. Inside the sphere A is constant and equal to $A_2 = 3\varepsilon_1 A_o/(\varepsilon_2 + 2\varepsilon_1)$, and outside $A_1 = A_o(1+\alpha[4+4\alpha-(6+3\alpha)\sin^2\theta])^{1/2}$, where $\alpha = R_o^3(\varepsilon_2-\varepsilon_1)/(r^3(\varepsilon_2+2\varepsilon_1))$.

Specializing to the case of interband transitions between bound levels with energies E_i and E_f, corresponding to the values of radial, azimuthal and magnetic quantum numbers $n_{i,f}$, $l_{i,f}$ and $m_{i,f}$ respectively (a hole state is initial -i, and an electron one is final -f), the transition rate w_{if} is given by the Fermi "golden rule"

$$w_{if} = \frac{2\pi}{\hbar} \sum_{\substack{m_i=-l_i \\ m_i=l_i}} \sum_{\substack{m_f=-l_f \\ m_f=l_f}} |P_{if}|^2 \, \delta(E_f - E_i - \hbar\omega) \qquad (1)$$

where P_{if} is the transition matrix element. Using the conventional procedure of separate integration of rapidly varying (Bloch) and slowly varying (envelope) functions $\psi_{i,f}$ we arrive to:

$$P_{if} = A_o \frac{3\varepsilon_1}{\varepsilon_2+2\varepsilon_1} \vec{P}_{cv2}\cdot\vec{\varepsilon} \int_{\Omega_2} \psi_i^* \psi_f d^3r + \vec{P}_{cv1}\cdot\vec{\varepsilon} \int_{\Omega_1} A_1(r,\theta)\psi_i^*\psi_f d^3r \equiv J_1 + J_2 \qquad (2)$$

where $\vec{\varepsilon}\vec{P}_{cv}$ is the Kane matrix element, having different values in

the two materials. Using the well-known properties of the angular part of wavefunction the first term J_1 may be expressed as

$$J_1 = A_o \frac{3\epsilon_1}{\epsilon_2+2\epsilon_1} \vec{P}_{cv2}\cdot\vec{\epsilon}\cdot\delta_{l_i,l_f}\cdot\delta_{m_i,m_f}\cdot \int_o^{R_o} X_i X_f dr, \qquad (3)$$

and equals zero unless $l_i = l_f$ and $m_i = m_f$. Evaluation of the second term is more cumbersome. Integration over ϕ leads to

$$J_2 = \vec{P}_{cv1}\cdot\vec{\epsilon}A_o \int_{R_o}^{+\infty} X_i X_f \cdot J_3(r)dr; \quad J_3(r) = \frac{1}{2}\int_o^{\pi} P_{l_i}^m P_{l_f}^m \sqrt{1+a\sin^2\theta}\, d\theta \qquad (4)$$

where we may write approximately $a \cong 6\alpha$ in all cases of practical interest, because $\alpha<<1$. The integral J_3 is different from zero if $l_i - l_f = 2p$ $(p = 0,\pm1,\pm2,\ldots)$. Expanding $\sqrt{1+a\sin^2\theta}$ in Taylor series $\sqrt{1+a\sin^2\theta} = \sum_{k=o}^{\infty} \gamma_k a^k \sin^{2k}\theta$, and using the properties of associated Legendre polinomials /4/, we find

$$J_3 = \gamma_{\Delta l/2}\, a^{\Delta l/2}\, Q_{l\pm\Delta l} + \gamma_{1+\Delta l/2}\, a^{1+\Delta l/2}\, Q_{l-\Delta l+2} + \sigma(a), \qquad (5)$$

where signs "+" and "-" correspond to $l_f - l_i = \Delta l > 0$ and $l_i - l_f = \Delta l > 0$ $(l \equiv l_i,\ \Delta l = 0,2,4,\ldots)$, and Q depend on l, Δl and m. In further considerations we shall keep only the first term of (5), because $a<<1$ and Q_j decreases with j.

The absorption coefficient α_{if}^S of the structure due to the presence of a single superatom is defined as ω_{if} times $\hbar\omega$ devided by light intensity and structure volume V (in case $\Delta l>0$ $P_{if} = J_2$) /5/:

$$\alpha_{ij}^S = \frac{16\pi^2\hbar^2|\vec{P}_{cv1}\cdot\vec{\epsilon}|^2\beta}{Vm_o^2\hbar\omega\, n_1^{1/2}} \left[6\frac{\epsilon_2-\epsilon_1}{\epsilon_2+2\epsilon_1}\right]^{\Delta l}\cdot\gamma_{\Delta l/2}^2 \left[\int_{R_o}^{+\infty} X_{l_i} X_{l_f} \left(\frac{R_o}{r}\right)^{\frac{3\Delta l}{2}} dr\right]^2 \cdot Q_\Sigma^2 \delta(E_f - E_i - \hbar\omega) \qquad (6)$$

$$Q_\Sigma^2 = \sum_m Q_{l\pm\Delta l}^2 = \sum_{m=-l_i}^{m=l_i} \prod_{k=1}^{\Delta l} \frac{(l_i+k)^2-m^2}{4(l_i+k)^2-1} \quad \text{for} \quad l_i<l_f \text{ , and} \qquad (7)$$

$$Q_\Sigma^2 = \sum_{m=-l_f}^{m=l_f} \prod_{k=1}^{\Delta l} \frac{(l_i+1-k)^2-m^2}{4(l_i+1-k)^2-1} \quad \text{for} \quad l_i>l_f$$

where $\beta\cong 1/137$ is the fine structure constant. Obviously, with increasing V, α_{if}^S tends to zero. However, if N noninteracting atoms are present (with finite concentration $n=N/V$) the total absorption coefficient is finite and may be written as $\alpha_{if} = \alpha_{if}^S \cdot Vn \equiv \sigma_{if}\cdot n$, where σ_{if} is the absorption cross-section.

The expression (6) holds for $\Delta l>0$; for $\Delta l=0$ it represents only a slight correction to transitions which now are allowed.As one can see from (6)-(7) α_{if} rapidly decreases with Δl. Furthermore, contrary to the $\Delta l=0$ case, it is only the value of reduced matrix element in the barrier, multiplied by $(R_0/r)^{3\Delta l/2}<1$, that enters here, so the apsorption (6) will be considerably bellow that for l-conserving transitions (especially with radial quantum number conserved). However, one can expect these transitions to be experimentally observable if the involved levels are close to the barrier band edge. We are currently doing numerical evaluation of this effect.

In conclusion, the difference of refractive indices of the superatom and matrix materials leads to a partial breakdown of selection rules: along with $\Delta l=0$, interband transitions with $\Delta l=2p$ become allowed, as well.

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