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Properties of excitons bound to neutral donors

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The binding energy of excitons to neutral donors in the approximation of spherical, nondegenerate energy bands, is calculated by a variational method for relevant range of electron-to-hole mass ratio. Estimated relative intensities of LO-phonon replicas of radiative recombination of the exciton–neutral-donor complex are in fair agreement with measured intensities of fluorescent lines.

I. INTRODUCTION

Shallow excitons bound to impurities or defects in semiconductors give rise to sharp absorption and fluorescence lines observed in good crystals at low temperatures at photon energies lower by a few millielectron volts than the intrinsic free exciton lines.[1-7] Recombination of shallow excitons bound to neutral donors and acceptors can be described in the effective-mass approximation.[8-10]

Here we will report a calculation of the exciton—neutral-donor complex ground state by a variational method. The minimization of the ground-state energy of the complex determines the optimized bound-exciton envelope which is used to compute the interparticle distances in the neutral complex, the electric dipole moment for radiative recombination, and the intensities of the LO-phonon replicas.

II. EXCITONS BOUND TO A NEUTRAL DONOR

Starting from the Hartree-Fock approximation for the many-electron system in the crystal and adopting the effective-mass approximation, Ungier[11,12] derived equations for the envelope function of the shallow bound exciton. In the calculation, the spin-orbit interaction is neglected. The conduction and the valence bands are assumed nondegenerate except for spin. The fundamental energy gap is assumed direct at the zone center where the effective masses of the electron and holes are taken to be spherically symmetric.

For the exciton bound to a neutral donor the unit of energy is the effective donor Rydberg $E_D = e^4 m_e / 2\hbar^2 \epsilon_0^2$, the unit of length the effective donor Bohr radius $a_D = \hbar^2 \epsilon_0 / e^2 m_e$, where m_e is the effective mass of the electron and ϵ_0 is the static dielectric constant of the crystal.

In these units the effective-mass Hamiltonian for the exciton bound by Coulomb potential to a neutral donor is

$$\begin{aligned} &H = T + V\,, \\ &T = -(\nabla_1^2 + \nabla_2^2 + \sigma \nabla_h^2)\,, \\ &V = 2\left(\frac{1}{r_{12}} + \frac{1}{r_h} - \frac{1}{r_1} - \frac{1}{r_2} - \frac{1}{r_{1h}} - \frac{1}{r_{2h}}\right). \end{aligned} \tag{1}$$

The subscripts 1,2 refer to two electrons; h to the hole. Thus r_{12} is the electron-electron, r_h the donor-hole, $r_{1,2}$ are the donor-electron, and $r_{1h,2h}$ the hole-electron distances, respectively. $\sigma = m_e/m_h$ is the electron-to-hole effective-mass ratio. The electron-hole exchange energy terms[11] have been neglected in (1).

Adamowski[13] computed the ground-state energy of an exciton bound to a neutral donor using the envelope function[14-16]

$$\begin{aligned} &F = \Phi_0 + c\Phi_2\,, \\ &\Phi_0 = N_0(1 + P_{12}) \exp(-\alpha r_1 - \beta r_2 - \gamma r_{1h} - \delta r_{2h})\,, \\ &\Phi_2 = N_2 r_h^2 (1 + P_{12}) \exp(-\alpha' r_1 - \beta' r_2 - \gamma' r_{1h} - \delta' r_{2h})\,. \end{aligned} \tag{2}$$

The constants N_0 and N_2 normalize respective functions to unity, P_{12} interchanges the electrons 1 and 2, and c is a linear variational parameter. The nonlinear parameters $\alpha, \beta, \gamma, \delta, \alpha', \beta', \gamma', \delta'$ have been optimized for each value of σ by minimization of the expectation value $E = (F, HF)/(F,F)$ of the Hamiltonian (1) with the help of the MINUIT program of the CERN library. The optimized values of the variational parameters and of the binding energy

$$W = E + E_X + E_D = E + E_D[1 + (1+\sigma)^{-1}]$$

for few selected values of σ are given in Table I.

III. EXCITON BOUND TO A NEUTRAL ACCEPTOR

In the approximation of nondegenerate spherical band extrema the study of an exciton bound to a neutral donor and of an exciton bound to a neutral acceptor are equivalent, if the electrons are interchanged with the holes. The energy $E(A^0, X)(\sigma^{-1})$ of the exciton-acceptor complex (A^0, X) with the

TABLE I. Binding energy $-W$, linear parameter c, and nonlinear parameters α, β, γ, δ, α', β', γ', δ' of the exciton envelope function, as functions of the electron-to-hole mass ratio $\sigma = m_e/m_h$.

σ	$-W$	$-c$	α	β	γ	δ	α'	β'	γ'	δ'
0.2	0.048 91	0.460 12	1.041 04	0.209 90	0.103 10	0.830 71	1.079 90	0.298 42	0.186 97	0.867 50
0.3	0.042 65	0.439 26	1.047 51	0.219 90	0.080 85	0.759 05	1.090 73	0.305 22	0.156 38	0.795 55
0.4	0.038 33	0.421 27	1.050 21	0.227 27	0.065 63	0.697 24	1.094 68	0.308 67	0.135 50	0.732 73
0.5	0.035 26	0.405 82	1.053 33	0.233 63	0.053 77	0.645 07	1.100 81	0.312 58	0.118 52	0.680 63
1.0	0.028 70	0.358 37	1.061 21	0.255 42	0.022 96	0.466 97	1.117 22	0.323 03	0.073 00	0.505 37
5.0	0.028 46	0.329 67	1.059 41	0.284 11	0.000 00	0.138 54	1.093 06	0.317 95	0.010 28	0.192 57
10.0	0.028 12	0.362 08	1.045 49	0.285 38	0.000 12	0.070 66	1.057 76	0.297 85	0.005 85	0.101 96

acceptor Rydberg $E_A = e^4 m_h / 2\hbar^2 \epsilon_0^2$ is related to the energy $E(D^0,X)(\sigma)$ of the exciton-donor complex (D^0,X) by

$$E(A^0,X)(\sigma^{-1})/E_A = E(D^0,X)(\sigma)/E_D\,. \tag{3}$$

For the exciton bound to a neutral acceptor Stébé and Munschy[17] have calculated the ground-state energy with the trial function of Page and Fraser[18] which for the positronium hydride PsH corresponding to $\sigma = 1$, has given the best-known results.[19] The binding energies obtained by Stébé[17] with a 35-term variational function are plotted in Fig. 1 as a function of the mass ratio σ and of the inverse σ^{-1}.

The extensive calculation of Stébé and Munschy[17] confirms the result of Adamowski *et al.*[13] about the stable Coulombic binding of excitons to a neutral donor and acceptor whatever the value of the mass ratio σ. In the important range of $\sigma \approx 1$, the binding energy depends weakly on the mass ratio. The weak dependence in this region is obtained by other methods of calculation, like the calculation in the local density approximation,[20] and calculation with a model Hamiltonian.[21] This weak dependence is consistent with the rigorous upper and lower bounds to dissociation energy of an exciton-neutral-donor complex[22] originating from the accurate calculations of the H_2 molecule.[23-25]

TABLE II. Experimental input data. In the case of anisotropic effective mass the harmonic mean, and in the case of the dielectric constant a geometric mean have been used (Ref. 12).

Compound	m_e	m_h	ϵ_0	ϵ_∞	$\hbar\omega_L$ (meV)
CdS	0.205 [a]	0.986 [a]	8.46 [b]	5.27 [c]	38 [b]
CdSe	0.13 [d]	0.56 [d]	10.2 [e]	5.88 [d]	27 [f]
CdTe	0.091 [g]	0.36 [g]	9.65 [g]	7.2 [g]	21.3 [g]
ZnSe	0.16 [h]	0.75 [h]	8.7 [d]	5.6 [d]	31.4 [f]
ZnTe	0.09 [i]	0.6 [i]	10.7 [i]	7.3 [j]	25.9 [f]

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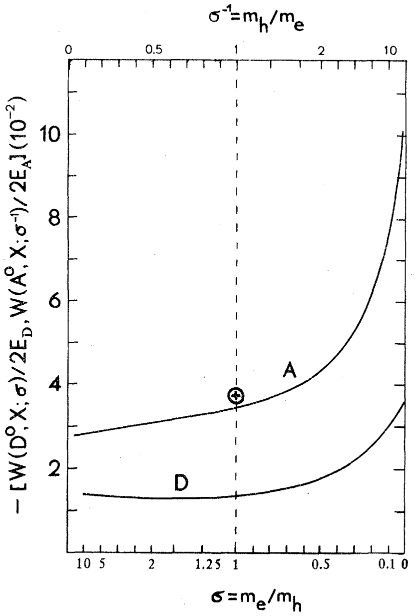

FIG. 1. Plot of the binding energy $-W$ of the (D^0, X) complex, in units of twice the donor Rydberg, versus the mass ratio $\sigma = m_e/m_h$, obtained with Adamowski (Ref. 13) wave function (curve D) and plot of the binding energy of the (A^0,X) complex, in units of twice the acceptor Rydberg, obtained by Stébé and Munschy (Ref. 17) wave function (curve A). The circled point represents the best known result achieved by Ho (Ref. 19) for $\sigma = 1$.

IV. SIZE OF THE BOUND EXCITON COMPLEX

The interparticle distances in the exciton–neutral-donor complex computed with the optimized envelope of Adamowski are shown dependent upon σ in Fig. 2. The Coulomb potential keeps the electrons at a distance from the donor smaller than the donor-hole distance which increases when the hole mass decreases. At $\sigma = 10$ the average $(r_h) = 16$, and $(r_1) = 3$ Bohr radii. This compares will with the best computed[26] average $(r_1 + r_2) = 5.42$ Bohr radii in the hydrogen ion H^-.

The envelope function of Adamowski *et al.*[13] is not sufficiently flexible: At about $\sigma \approx 1$ it yields the binding energy about one-half of that obtained by Stébé and Munschy,[17] and gives too large interparticle distances, but it is simpler for computation of the expectation values.

V. RADIATIVE RECOMBINATION

The rate of radiative recombination is proportional to the squared modulus of the electric dipole matrix element of the electronic system between the excited Ψ_b and the ground state Ψ_0 as

$$\vec{M}_{0b} = e\left(\Psi_0, \sum_i \vec{r}_i \Psi_b\right) . \tag{4}$$

Since the electronic transitions are fast in comparison with the time required to change the position of the lattice atoms we calculate the transition rate between the electronic states assuming that electrons adiabatically follow the lattice. Thus we adopt the Condon approximation[27-32]: The electronic matrix element is taken independent of lattice coordinates. In the configuration diagram of the lattice vibration the electron optic transition goes vertically, i.e., at the same value of the configurational coordinate for the initial and the final state.

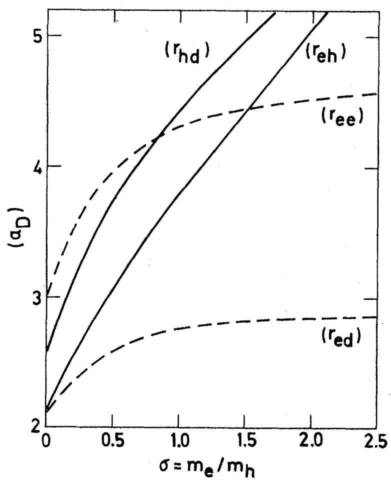

FIG. 2. Computed interparticle distances in units of the donor radius a_D, versus the mass ratio $\sigma = m_e/m_h$. Here r_{hd}: hole-donor, r_{eh}: electron-hole, r_{ee}: electron-electron, r_{ed}: electron-donor distance.

VI. PHONON REPLICAS

Radiative recombination of excitons is accompanied, particularly in polar semiconductors, by the phonon replicas. The longitudinal-optical (LO) phonons in polar semiconductors give rise to replicas (equidistant on the frequency scale) which can be unambiguously identified.[1]

Multiphonon processes are possible if the equilibrium position of the lattice atoms is different for the different electronic states between which the transition takes place.[28-37] Among the more recent papers on multiphonon processes, Ridley reported a quantum-mechanical calculation of the multiphonon nonradiative transition rate for electrons in semiconductors without assuming the Condon approximation. Ridley at first[38] made no attempt to calculate the electronic matrix elements since that would involve invoking special models for the electronic states at the impurity center or defect and for the electron-phonon interaction. Next[39] he has made a calculation with simple quantum-defect wave functions.

Ungier,[11,12,40] extending the theory of multiphonon transitions developed by Gummel and Lax,[31] described the LO-phonon replicas of the shallow bound-exciton recombination, assuming the polar coupling of the electron and the hole to the LO phonon. The interaction potential energy is linear in the normal coordinate $Q(\vec{q})$ of the longitudinal mode with wave vector $\vec{q}$,

$$V_{\text{e-ph}}(\vec{r}) = \sum_{\vec{q}} \gamma_{\vec{q}} Q(\vec{q}) e^{i\vec{q}\cdot\vec{r}} . \tag{5}$$

For optic-mode phonons $\gamma_{\vec{q}} = -i\gamma/|\vec{q}|$ with

$$\gamma = e\omega_L\left(\frac{4\pi}{\Omega}(\epsilon_\infty^{-1} - \epsilon_0^{-1})\right)^{1/2}$$
$$= \hbar\omega_L\left(\frac{2\omega_L}{\hbar m}\right)^{1/4}\left(\frac{4\pi\alpha}{\Omega}\right)^{1/2} , \tag{6}$$

and

$$\alpha = (e^2/\hbar)(m/2\hbar\omega_L)^{1/2}(\epsilon_\infty^{-1} - \epsilon_0^{-1}) \tag{7}$$

is the dimensionless Fröhlich coupling constant. (See Table II.) $\epsilon_\infty = n_\infty^2$ is the high-frequency dielectric constant of the crystal of volume Ω. For the hole $\gamma_h = -\gamma$. The LO-phonon frequency ω_L is assumed independent of $\vec{q}$.

The lattice relaxation energy[30] due to the electron-phonon interaction in the crystal ground state with energy E_0 is ΔE_0 and in the bound-exciton ground state E_b is ΔE_b. The zero-phonon line due to purely radiative recombination gives the photon of energy

$$\hbar\omega_0 = E_b - \Delta E_b - (E_0 - \Delta E_0). \tag{8}$$

At temperatures $k_B T \ll \hbar\omega_L$, recombination with emission of the LO phonon is more probable than that with absorption. The intensity of the optical line at frequency $\omega_0 - n\omega_L$ with emission of n LO phonons can be approximated by the Poisson-type distribution[11,12,26-38]

$$I(n) = \frac{4n_\infty}{3c^3} |\vec{M}_{0b}|^2 (\omega_0 - n\omega_L)^4 \frac{S^n}{n!} e^{-S}. \tag{9}$$

For the bound exciton slowly varying in space envelope, the electric dipole moment of the transition can be approximated by the product

$$\vec{M}_{0b} = \vec{M}_{vc} \cdot M_0 \tag{10}$$

of the electric dipole matrix element between the conduction and valence Bloch functions $u_{c,v}(\vec{x})$, i.e., integral over the unit cell Ω_0:

$$\vec{M}_{vc} = e \int_{\Omega_0} u_v^*(\vec{x}) \vec{x} u_c(\vec{x}) d^3x , \tag{11}$$

and the overlap integral of the bound-exciton ground-state envelope F and neutral-donor ground-state envelope $f_D(\vec{r}) = (\pi a_D^3)^{-1/2} \exp(-r/a_D)$,

$$M_0 = \int\int d^3r_1 d^3r_2 F(\vec{r}_1, \vec{r}_2, \vec{r}_h = \vec{r}_1) f_D^*(\vec{r}_1) . \tag{12}$$

In the computation of the Huang-Rhys factor S we approximate the Bloch functions by their value at $\vec{q} = 0$. Then S can be approximately computed as

$$\begin{aligned} S &= (2\hbar\omega_L^3)^{-1} \sum_{\vec{q}} |D_{\vec{q}}|^2 \\ &= \frac{e^2}{a_D \hbar\omega_L} (\epsilon_\infty^{-1} - \epsilon_0^{-1}) X(\sigma) , \end{aligned} \tag{13}$$

where

$$X(\sigma) = \frac{a_D}{(2\pi\gamma)^2} \int d^3q \, |D_{\vec{q}}|^2 \tag{14}$$

is the sum over phonon wave vectors of the squared modulus of the Fourier transform

$$\begin{aligned} D_{\vec{q}} = \gamma_{\vec{q}} \Big(\int\int\int d^3r_1 d^3r_2 d^3r_h |F(\vec{r}_1, \vec{r}_2, \vec{r}_h)|^2 \\ \times (e^{i\vec{q}\cdot\vec{r}_1} + e^{i\vec{q}\cdot\vec{r}_2} - e^{i\vec{q}\cdot\vec{r}_h}) \\ - \int d^3r \, |f_D(\vec{r})|^2 e^{i\vec{q}\cdot\vec{r}} \Big). \end{aligned} \tag{15}$$

Since the variational parameters of the envelope F have been optimized for each mass ratio σ, the functionals M_0 and X of the envelope F are functions of σ. The values of the functionals $M_0^2(\sigma)$ and $X(\sigma)$ computed with the envelope (2) of Adamowski[13] are plotted as functions of σ in Fig. 3. As the variational function (2) is not sufficiently flexible, it gives too small a value for the binding energy, too large interparticle distances and values for $M_0(\sigma)$, and too small values for the functional $X(\sigma)$. Nevertheless the computed functionals $M_0(\sigma)$ and $X(\sigma)$ are smooth monotonic functions of σ. The weak Coulomb binding of exciton to neutral donor makes the $X(\sigma)$ functional of a small absolute value and this reduces the Huang-Rhys factor by 3 orders of magnitude with respect to more common values of the order of unity.[41]

Thomas and Hopfield[1] measured the absorption and fluorescent spectra of good CdS platelets at helium temperatures and plotted in a semilogarithmic plot the intensities of the fluorescent lines measured at 1.6 K derived from no-phonon lines of exciton bound to neutral acceptors and donors. For the exciton bound to neutral donor the intensity ratio of the first LO-phonon replica, $I_2 - \mathrm{LO}$, to the no-phonon line I_2 can be read off from the plot[1] as 0.1 to 300, i.e., 3.3×10^{-4}. This compares well with our computed value $I(n=1)/I(n=0) = 2.15 \times 10^{-4}$ in Table III, where we present factors S computed for semiconductors in which excitons bound to donors and acceptors have been observed. However, for CdS the higher phonon replicas do not obey the Poisson-type distribution.

Henry and Hopfield[42] analyzed in CdS and CdSe the first LO-phonon replica of the recombination line I_2 of the exciton bound to a neutral donor and attributed its complicated shape to coupling between the LO phonons and the donor electron.

We consider here only the position of the LO-phonon replica with respect to the no-phonon line and estimate its intensity by using the optimized envelope function for the bound exciton complex.

In the crystal with the forbidden gap ω_g the oscillator strength ratio of bound exciton to the con-

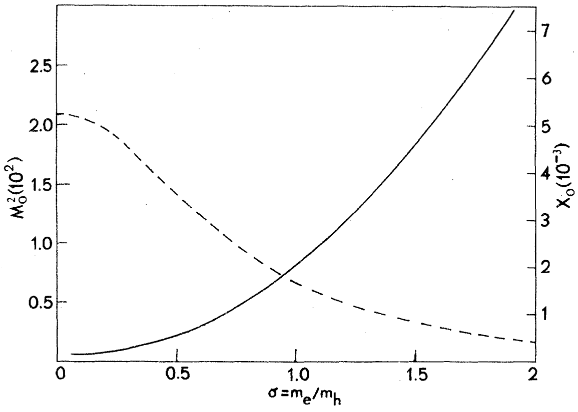

FIG. 3. Calculated oscillator strength ratio M_0^2 of the bound exciton to the conduction-band–to–valence-band transition, and the functional X, versus the mass ratio $\sigma = m_e/m_h$.

TABLE III. The electron-to-hole mass ratio σ, the effective Rydberg $\mathcal{R} = E_D$, the dimensionless electron-phonon coupling constant $\alpha_e = \alpha (m_e/m)^{1/2}$, the oscillator strength ratio M_0^2 of bound exciton to the conduction-band–to–valence-band transition, the functional X, and the Huang-Rhys factor S.

Compound	$\sigma = m_e/m_h$	$\mathcal{R} = e^2/2a_D$ (eV)	α_e	M_0^2	10^4X	10^4S
CdS	0.208	0.330	0.613	195	1.73	2.15
CdSe	0.232	0.174	0.580	192	1.80	1.67
CdTe	0.253	0.128	0.269	188	2.05	0.87
ZnSe	0.213	0.235	0.530	194	1.78	1.69
ZnTe	0.15	0.114	0.299	202	1.51	0.58

duction-band–to–valence-band transition[43,44] is $M_0^2 = I^2\omega_g/\omega_0$. Our estimate of $M_0 = 14$ for CdS is about ten times larger than the ratio $I = 1.4$ of Eqs. (A5) and (A9) of Henry and Nassau.[45] They estimated I from the oscillator strength ratio of bound exciton to the free exciton by using the approximate wave function of Rashba and Gurgenishvili[46] to represent the exciton center of mass bound to the crystal defect by short-range potential, and had agreement with the measured[43-45] lifetime of the bound exciton. Our value of M_0 is too large, showing once again that our envelope is too extended in configuration space. Inclusion in the interaction potential of the polaron effects[47,48] would produce larger binding energy, smaller interparticle distances, and smaller values of M_0.

VII. DISCUSSION

Shallow excitons bound to neutral impurities have been until now described by models similar to the one presented here, derived from quantum-chemistry considerations. The underlying effective-mass approximation is a far-reaching simplification. The assumption of a Coulomb potential between the electron and the hole with the impurity may not be in some cases justified. Acceptors are often attributed to vacancies rather than to impurities with a charged center. Also donors may require a more realistic description[49] as they possess their core with a complicated electronic structure. Better models of the excitons bound to impurities are desirable and have to be developed but they necessarily will involve, from the very beginning, calculations still more extensive than those presented here. Our attempt to compute the phonon-replica intensities indicates a path of reasoning which has to be done in order to assess the relation between the bound-exciton envelope and the observable quantities of the complex.

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