

GROUND-STATE ENERGY OF A DONOR-BOUND EXCITON COMPLEX IN SEMICONDUCTORS

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The ground-state energy of a system consisting of an exciton in the presence of a neutral donor in semiconductors is calculated for an arbitrary value of the electron to the hole mass ratio using a variational approach. The energy bands for the electron and for the hole are assumed to be parabolic. The system is found to be bound for all values of the electron to the hole mass ratio.

Introduction

Since Lampert [1] first suggested the possibility of an exciton binding to a neutral donor impurity, several theoretical attempts [2] have been made to calculate the binding energy of this system for various values of the electron to the hole mass ratio (σ). Hopfield [3] using known values of the energies of the hydrogen molecule and negative hydrogen ion, estimated this binding energy as a function of σ by interpolation. Sharma and Rodriguez [4] using a variational approach, found that the binding energy dropped sharply at first and then increased as a function of σ . Munsch and co-workers [5,6] have reported that the exciton-neutral impurity complex is not bound for $\sigma_c < \sigma < 3$ where σ_c is some constant between 1 and 2. Two recent calculations, one using the local density approximation [7] and the other using perturbation theory [2], show that the system is bound for all values of σ . A third calculation due to Herbert [8], using the configuration interaction approach, shows extremely large binding energies.

In view of the conflicting results obtained using different approaches, we decided to undertake a variational calculation for the ground-state energy of this complex. Our results show that the system is bound for all values of σ . This is the first truly variational calculation which shows binding for all values of the mass ratio. The procedure we follow consists of two parts. In the first part which is more appropriate for $\sigma \lesssim 10$, we derive an effective potential between the positive ion and the hole using a trial wave function which is a product of generalized Hylleras-Ore type wave function [9] and an envelope function which depends on the positive ion-hole distance. This potential is then solved variationally assuming for the envelope function the ground-state solution of the Morse potential. In the second part which is appropriate for $\sigma > 10$, we calculate the ground-state energy using a variational function which is a product of the hole wave function and Chandrasekhar [10] wave function for the D^- system, similar to what was done in Reference [5].

Method

Within the effective mass approximation assuming parabolic bands, the Hamiltonian of two electrons of mass m_e and a hole of mass m_h in the presence of a positive ion is

$$H = -(\Delta_1^2 + \Delta_2^2) - \sigma \Delta_3^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_3} - \frac{2}{r_{13}} - \frac{2}{r_{23}} + \frac{2}{r_{12}}, \quad (1)$$

where the positive ion is assumed to be at the origin and r_1 , r_2 , and r_3 are the distances of the two electrons and a hole, respectively, from the positive ion. All energies and distances are expressed in terms of the impurity Rydberg $R = m_e e^4 / 2 \epsilon_0 \hbar^2$ and Bohr radius $a_0 = \epsilon_0 \hbar^2 / m_e e^2$, respectively, where ϵ_0 is the static dielectric constant of the medium.

For $\sigma \leq 10$ we calculate the ground-state energy following a variational approach and choose a trial wave function of the form

$$\phi = [\psi(r)/N(r_3)]G(r_3), \quad (2)$$

with

$$N^2(r_3) = \int |\psi(r)|^2 d\tau_r. \quad (3)$$

Here $\psi(r)$ is a function of electron-hole distances only; single index r is used to designate these distances. The expectation value of the Hamiltonian with respect to ϕ is then calculated in two steps. First, we integrate over the electron coordinates to obtain the equation of motion of the hole in an effective potential, $U(r_3)$. This potential is evaluated using the following form of ψ

$$\psi = e^{-(\alpha r_1 + \beta r_{13} + \nu r_2 + \delta r_{23})} + e^{-(\alpha r_2 + \beta r_{23} + \nu r_1 + \delta r_{13})} \quad (4)$$

and following a procedure similar to that outlined in Reference [11]. Here α , β , ν , and δ are variational parameters. For a given set of values of these parameters, the function $U(r_3)$ has a form similar to that of a Morse potential. The function $G(r_3)$ is, therefore, chosen to have the form of the ground-state eigenfunction of the Morse Potential with three variational parameters. The ground-state energy E is then obtained by minimizing the expectation value of H with respect to seven variational parameters for a given value of σ . We find that the value of E thus calculated is very close to that obtained by using a much simpler form of $G(r_3)$, i.e.,

$$G(r_3) \sim r_3^n e^{-\epsilon r_3}, \quad (5)$$

where ϵ is a variational parameter and n is found to be of the order unity. For $\sigma > 10$ we calculate the ground-state energy using a trial wave function which is a product of the hole wave function and Chandrasekhar [10] wave function for the D^- system. We define the binding energy E_D (also called the dissociation energy) as

$$E_D = -E - \frac{2 + \sigma}{1 + \sigma}. \quad (6)$$

Results and Discussion

The values of E_D as a function of σ were calculated using the first wave function, and the system was found to be bound for $\sigma \sim 10$. This calculation was extended upto $\sigma = 20$, and the system was still bound. The values of E_D for $\sigma > 10$ were determined using the second wave function and the system was bound for this range of values of σ . Also the values of E_D for σ between 10 and 20 were larger than those obtained by using the first wave function. Thus, we find that the system is bound for all values of σ , i.e., there are no regions where the complex is unstable. In Fig. (1) we display the variation of E_D as a function of σ and stop at $\sigma = 5$ for convenience. The value of E_D at $\sigma = 1$ is calculated to be 0.036 which compares quite favorably with a very accurately determined value of 0.058 for positronium hydride by Navin, *et al.* [12], who used an approach specifically designed for $\sigma = 1$. For comparison we have also plotted the results of some other calculations. Our results compare rather well with those of Wunsche, *et al.* [7], who use the local density approximation, although our values of E_D are somewhat lower than theirs. We have not displayed the results of Reference [2] which shows that the system is bound for all σ since there is a serious question about the convergence of its perturbation expansion.

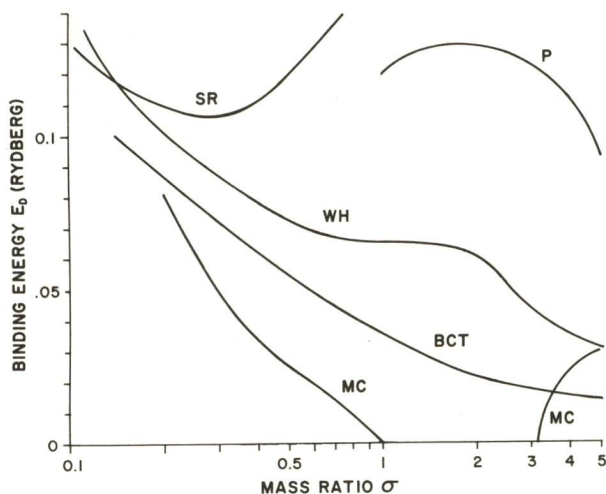


Fig. 1 Variation of the binding energy of E_D expressed in terms of the impurity Rydberg as a function of the mass ratio σ :

SR - Sharma, *et al.* [4], WH - Wunsche, *et al.* [7],
MC - Munchy, *et al.* [5], P - Pan, *et al.* [13], and
BCT - Present Calculation

To conclude, we have calculated the ground-state energy of an exciton-donor complex as a function of σ using a variational approach. We find that the system is bound for all values of σ . This is the first truly variational calculation which shows binding for all σ . Our values of E_D represent lower bounds and are sometimes lower than those of others in some regions of σ . The appropriate inclusion of electron-electron correlations in the first wave function and the electron-hole correlations in the second wave function will increase the values of E_D . Calculations which include such effects are in progress.

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