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## Calculation of exchange energy in quantum dots: application to porous silicon

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**ABSTRACT:** We present a variational calculation of the envelope wave function of an exciton inside a cube, in the effective mass approximation, with one parameter which plays the part of a Bohr radius. This geometry allows one to reduce the sixfold integrals to threefold integrals which shortens tremendously computer calculations. This wave function is used to obtain the exchange energy and the oscillator strength. The limiting cases (large or small cubes) are recovered. We show that recent experimental results in porous silicon can be explained without further hypothesis.

### 1. INTRODUCTION

In a quantum dot it is well known that the hamiltonian describing an exciton, i.e. an electron-hole pair correlated by the Coulomb interaction, has no analytical solution[1]. As a consequence it is necessary to look for approximate solutions. Inside the effective mass approximation framework, which we use in the present paper, it is possible either to develop the (envelope) wave function on a appropriate basis[2] or to use a trial function[3]. Here we shall adopt this last approach. To simplify the calculation as much as possible we describe the electron of the conduction band and the hole of the valence band by a average mass  $m_e$  and an average mass  $m_h$  respectively. Furthermore we assume infinite potential barriers, which is not a bad approximation for the case of porous silicon which will be considered more specifically later.

### II. WAVE FUNCTION

In the quantum dot the hamiltonian is (with standard notations):

$$H = p_e^2/2m_e + p_h^2/2m_h - e^2/\epsilon r_{eh} \quad (1)$$

We are looking for the ground state of this hamiltonian and we will consider the case of a cubic quantum dot as this is easier to solve for than a sphere. Inside a cube of side  $2Q$  we will use the function ( $q = \pi / 2Q$ ):

$$\Phi_c(\mathbf{r}) = \cos qx \cos qy \cos qz \quad (2)$$

and the normalized wave function

$$\Psi_c(\mathbf{r}) = Q^{-3/2} \Phi_c(\mathbf{r}) \quad (3)$$

The trial wave function for the exciton in the cube is then:

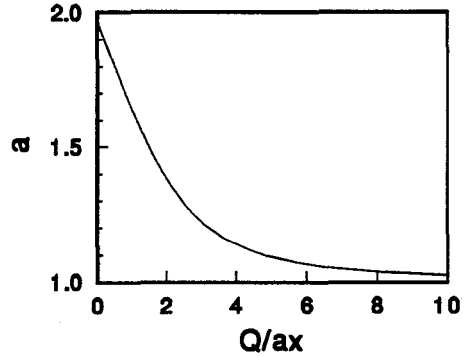
$$\Phi_{x,c}(\mathbf{r}_e, \mathbf{r}_h) = \Phi_c(\mathbf{r}_e) \cdot \Phi_c(\mathbf{r}_h) \cdot \exp(-r_{eh}/a) \quad (4)$$

where  $a$  plays the part of an effective Bohr radius. We have to minimize:

$$\langle \Phi_{x,c} | H | \Phi_{x,c} \rangle / \langle \Phi_{x,c} | \Phi_{x,c} \rangle \quad (5)$$

The results are given Fig.1. If  $Q/a_x$  is very large,  $a/a_x$  tends to one as expected ( $a_x$  is the Bohr radius of the 1s bulk exciton). The limit is less obvious when  $Q/a_x$  is very small: in this case the limit of  $a/a_x$  is equal to 1.97 while in a sphere [4] the limit is equal to 2.01: this indicates the small importance of the shape of the quantum dot.

Fig.1 Effective Bohr radius  $a$  of an exciton in a cube of half-side  $Q$ . The length unit is  $a_x$ , the Bohr radius of the 1s bulk exciton.



This leads to a normalized wave function:

$$\Psi_{x,c}(\mathbf{r}_e, \mathbf{r}_h) = N^{-1/2} \Phi_c(\mathbf{r}_e, \mathbf{r}_h) \quad (6)$$

where

$$N = \langle \Phi_{x,c} | \Phi_{x,c} \rangle = \int \int d^3r_e d^3r_h |\Phi_{x,c}(\mathbf{r}_e, \mathbf{r}_h)|^2 \quad (7)$$

All the integrals are analogous to that of Eq.7. (Details of calculation will be published elsewhere.) In a cube the limits of the integral are independent so that we have to calculate integrals of the shape:

$$I = \int_{-\pi/2}^{\pi/2} d\xi_e \int_{-\pi/2}^{\pi/2} d\xi_h \cos^2 \xi_e \cos^2 \xi_h f(|\xi_e - \xi_h|) \quad (8)$$

We put:  $u = \xi_e - \xi_h$  and  $v = \xi_e + \xi_h$  so that two lines of algebra show the twofold integral is equal to the simple integral:

$$I = \frac{1}{4} \int_0^\pi du \left\{ [(\pi - u) \cos 2u + 2(\pi - u) + \frac{3}{2} \sin 2u] f(u) \right\} \quad (9)$$

Thus the sixfold integrals are reduced to threefold integrals. It is worth to note that this transformation is equally possible in case of a parallelepiped.

The difference between the description by an exciton  $\Psi_{x,c}(\mathbf{r}_e, \mathbf{r}_h)$  and by an uncorrelated electron-hole pair  $\Psi_{eh,c}(\mathbf{r}_e, \mathbf{r}_h)$  where

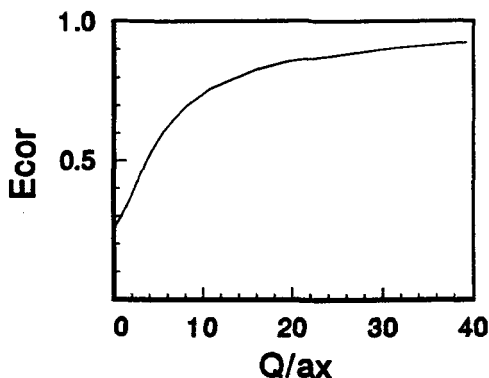
$$\Psi_{eh,c}(\mathbf{r}_e, \mathbf{r}_h) = Q^{-6} \Phi_c(\mathbf{r}_e) \Phi_c(\mathbf{r}_h) \quad (10)$$

is usefully described by the correlation energy

$$E_{cor} = \langle \Phi_{x,c} | H | \Phi_{x,c} \rangle - \langle \Phi_{eh,c} | H | \Phi_{eh,c} \rangle \quad (11)$$

$E_{\text{cor}}/E_{x,1s}$  is given in Fig.2;  $E_{x,1s}$  is the binding energy of the 1s bulk exciton. Although, in the limit  $Q/a_x = 0$ ,  $\Psi_{x,c}$  tends to  $\Psi_{\text{eh},c}$ ,  $E_{\text{cor}}$  does not tend to zero but to  $0.251 E_{x,1s}$ . Again this points out the slight difference between the cube and the sphere where this limit is equal to  $0.248 E_{x,1s}$ [4].

Fig.2 Correlation energy versus the half-side of the cube. The energy unit is the binding energy of the 1s bulk exciton.  $a_x$  is the same as in Fig.1.



### 3. EXCHANGE ENERGY AND OSCILLATOR STRENGTH

We are now in position to calculate the exchange energy[5]. For an uncorrelated electron hole pair the exchange energy is:

$$E_{\text{eh},c} = \pi a_x^3 E_x \int d^3r |\Psi_{\text{eh},c}(\mathbf{r},\mathbf{r})|^2 \quad (12)$$

where  $E_x$  is the exchange energy of the 1s bulk exciton. Now

$$\int d^3r |\Psi_{\text{eh},c}(\mathbf{r},\mathbf{r})|^2 = \int d^3r |\Psi_c(\mathbf{r})|^4 = \frac{27}{64} \frac{1}{Q^3} \quad (13)$$

In a cube the exchange energy of an exciton is:

$$E = \int d^3r |\Psi_{x,c}(\mathbf{r},\mathbf{r})|^2 \pi a_x^3 E_x \quad (14)$$

Finally we obtain:

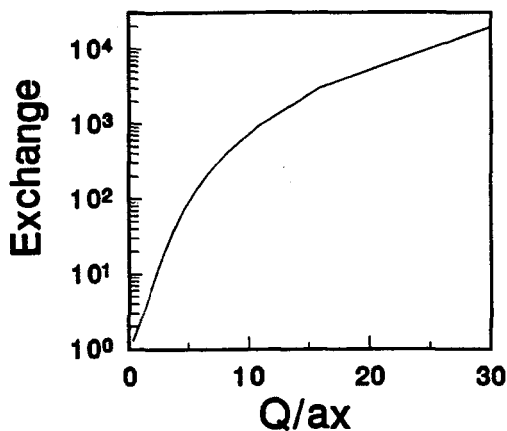
$$\frac{E}{E_{\text{eh},c}} = \frac{64}{27 \pi} \left( \frac{Q}{a_x} \right)^3 \frac{E}{E_x} \quad (15)$$

The ratio  $E/E_{\text{eh},c}$  is plotted in Fig.3 and allows one to know the exchange energy  $E$  for an exciton for any value of  $Q/a_x$ . This ratio can be also be written as:

$$\frac{E}{E_{\text{eh}}} = \frac{Q^6}{N} \quad (16)$$

It is straightforward to verify that i) if  $Q/a_x$  tends to zero,  $E$  tends to  $E_{\text{eh}}$  and ii) if  $Q/a_x$  tends to infinite,  $E$  tends to  $E_x$ . This is what we expect.

Fig.3 Vertical axis: ratio of the exchange energy  $E$  of an exciton to the exchange energy  $E_{\text{eh},c}$  of an uncorrelated electron-hole pair in a cube of half-side  $Q$ . Horizontal axis: ratio of half-side  $Q$  to  $a_x$ , the Bohr radius of the 1s bulk exciton. The vertical axis gives also the envelop function dependent part of the oscillator strength (see text).



Incidentally we can note that the envelope function dependent part  $F_0$  of the oscillator strength[6], i.e.:

$$F_0 = \left| \int d^3r \Psi_{x,c}(r,r) \right|^2 \quad (17)$$

is equal to  $Q^6/N$  so that the Fig.3 gives also  $F_0$ .

#### 4. POROUS SILICON

We can now use the above results to explain recent experimental results in porous silicon[7,8]. For a luminescence energy equal to 1.77 eV, which corresponds roughly to a crystallite of 25 Å [9], the exchange energy is equal to 10 meV. In Ref.7 this result was interpreted as being the exchange energy of uncorrelated electron-hole pair, which leads to  $2Q = 24$  Å (see Eq.12 and 13), using known values  $a_x = 43$  Å [10] and  $E_x = 0.15$  meV [11]. Now we can comment on whether this approximation is justified or not. Using the results given in Fig.3, we obtain  $2Q = 26$  Å. (A discussion on the validity of all the values given here is postponed in a further publication). This shows that, in this particular case, a description of the exciton as an uncorrelated electron-hole pair is well justified.

#### 5. CONCLUSION

We have shown that it is more simple to study the exciton inside a cube than inside a sphere, at least from the viewpoint of the unavoidable numerical calculation. We have pointed out the similarities (exchange energy, oscillator strength) and the differences (correlation energy) between an exciton and an uncorrelated electron hole-pair in very small crystallites. Finally we have applied our calculation to porous silicon and confirmed that the measured splittings can be due to exchange energy.

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#### REFERENCES

- 1 G.W.Bryant, *Optics of Excitons in Confined Systems*, edited by A.D'Andrea, R.Del Sole, R.Girlanda and A.Quattropani, (Int.Phys.Conf.Ser. n°123, IOP Publishing, 1991) p.131.
- 2 Y.Kayanuma, Phys.Rev. B 38 (1988) 9797 .
- 3 T.Takagahara and K.Takeda, Phys.Rev.B 46 (1992) 15578 .
- 4 Y.Kayanuma, Solid State Commun. 59 (1986) 405 .
- 5 C.H.Henry, R.A.Faulkner and K.Nassau, Phys.Rev. 183 (1969) 798.
- 6 C.H.Henry and K.Nassau, Phys.Rev.B 1 (1970) 1628.
- 7 P.D.J. Calcott, K.J. Nash, L.T. Canham, M.J. Kane and D. Brumhead, J.Phys.: Condensed Matter 5 (1993) L 91 .
- 8 J.C. Vial, A. Bsiesy, G. Fishman, F. Gaspard, R. Hérino, M. Ligeon, F. Muller and R. Romestain, in *Microcrystalline Semiconductors-Material Science and Device*, P.Fauchet, Y.Aoyagi, L.T.Canham, I.Shimizu and C.C.Tsai Ed. (Mater.Res. Soc. Symposium Proc., Vol 283, 1993), to be published.
- 9 G. Fishman, I. Mihalcescu, and R. Romestain, Phys.Rev. B to be published.
- 10 N.O.Lipari and M.Altarelli, Phys.Rev.B 15 (1977) 4883.
- 11 J.C.Merle, M.Capizzi, P.Fiorini and A.Frova, Phys.Rev.B 17 (1978) 4821.