

# Letters to the Editor

## THE ENERGY OF AN EXCITON IN ALKALI-HALIDE CRYSTALS

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IN Ref. 1 a model for excitons in alkali-halides crystals was constructed, according to which the exciton excitation was connected with the transition of one of the six p-electrons of the outer shell of the halide ion to the s-shell of the nearest alkali ions. Such a model made it possible, even without knowing the electronic functions, to calculate the change in polarization energy of the lattice, the half-width of the band of exciton absorption and its temperature dependence, the field mass of the exciton,<sup>2</sup> and a number of other quantities characterizing, on the whole, an excited state, but not the ground state of the crystal. However, to evaluate the energy of an exciton transition and its probability, the interaction cross section of excitons with different impurity centers, and so on, it is necessary to use the eigenfunctions of the system both in an excited, and in the ground state.

In Ref. 3 the wave function  $\Psi_0$  of the ground state of the system (corresponding to a non-excited crystal) was chosen in the form of an antisymmetrized product of electron functions at the various ions. To describe the exciton state of the crystal, the wave function  $\Psi_{\text{exc}}$  was also written as an antisymmetrized product of electron functions, in correspondence with the model considered in Ref. 1, but it was assumed that in one, say the  $l$ -th, elementary cell one of the external p-electrons was absent from a halide ion, and at the six nearest alkali ions there was, with equal probability, an extra electron.

Substituting  $\Psi_0$  and  $\Psi_{\text{exc}}$  into the Hamiltonian of the system, which describes all possible electrical pair interactions between the electrons and the atomic nuclei of the crystal, we are able to evaluate the energies  $E_0$  and  $E_{\text{exc}}$  of the ground state and excited (exciton) state, respectively. Their difference determines the energy of the exciton excitation and can be transformed to the form

$$\begin{aligned}
 E_{\text{exc}} - E_0 = & \varepsilon_2 - \varepsilon_1 - \frac{e^2}{1 + 4A + B} \\
 & \times \sum'_{(s', l'+1, l_1)} \sum_{l_1=1}^6 \int V_{s'}^{l'}(\rho) \varphi_{l_1}^{l'}(\rho) \varphi_{l_1}^{l'}(\rho) d\tau - \text{exch. term} \\
 & - \frac{e^2}{3} \sum'_{(s', l'+2, l)} \int V_{s'}^{l'}(\rho) |\varphi_{2p}^l(\rho)|^2 d\tau + \text{exch. term} \\
 & - \frac{1}{6(1 + 4A + B)} \sum_{\alpha, \beta} \sum_{l_1=1}^6 \int [\varphi_{l_1}^{*l_1}(\rho) \varphi_{2\alpha}^{*l}(\rho') \varphi_{l_1}^{l_1}(\rho) \varphi_{2\beta}^l(\rho') \\
 & - \varphi_{l_1}^{*l_1}(\rho) \varphi_{2\alpha}^{*l}(\rho') \varphi_{l_1}^{l_1}(\rho') \varphi_{2\beta}^l(\rho)] \frac{e^2}{|\rho - \rho'|} d\tau d\tau'. \quad (1)
 \end{aligned}$$

In this equation A and B are constants occurring in the normalization of  $\Psi_{\text{exc}}$  and equal to the overlap integrals of the s-functions of different alkali ions at distances  $a\sqrt{2}$  and  $2a$  apart, where  $a$  is the lattice constant. The index 1 refers everywhere to an atom (ion) of the metal, and 2 to those of the halides:  $\varepsilon_1$  is the ionization energy of an alkali atom,  $\varepsilon_2$  is the affinity energy of a halide atom,  $\varphi_{l_1}^{l_1}(\rho)$  is the wave function of a valence electron of an alkali atom in the  $l_1$ -th elementary cell,  $\varphi_{2\alpha}^l(\rho)$  the p-electron function of a halide atom ( $\alpha$  indicates the magnetic and spin quantum numbers),  $\varphi_{2p}^l(\rho)$  is the radial part of the p-electron wave function, and  $V_s^l(\rho)$  is the potential of the ion  $s, l$  at a point with radius vector  $\rho$ .

Equation (1) was numerically evaluated for an NaCl crystal. We took for  $V_s^l(\rho)$  and  $\varphi_{2\alpha}^l(\rho)$  Hartree functions.<sup>4</sup> In the evaluation of  $E_0$  and  $E_{\text{exc}}$  we can use here these functions as the functions of the zeroth approximation because the overlap integrals of even the nearest ions in the NaCl lattice are very small ( $\sim 10^{-2}$ ). However, we can not use directly the Hartree function for the 3s-electron of atomic Na since the corresponding overlap integrals are not small. For the functions  $\varphi_{l_1}^{l_1}(\rho)$  we took thus the functions found by Tolpygo and Tomasevich.<sup>5</sup> After evaluating the polarization of the electronic shells of the ions without inertial effects, we got for the energy of the exciton transition in NaCl  $\Delta E = 7.5$  ev. The exchange terms which were not written down explicitly in Eq. (1) turned out to have practically no influence on the final value of  $\Delta E$ .

Muto and Okuno<sup>6</sup> have evaluated by numerical methods the energy of the exciton transition in KCl and NaCl crystals. They were, however, not able to determine the absolute value of the energy but only the distance of the exciton energy level from the bottom of the conduction band, the position of which was found in addition from experi-

mental data. To get agreement with experiment they could essentially still use two parameters. The method proposed by us is free of these shortcomings and enables us to consider the interaction of excitons with light and various centers. One can consider that the result obtained is in satisfactory agreement with the experimental value of  $\Delta E$  determined from the position of the maximum of the exciton absorption band at  $\lambda = 1580 \text{ \AA}$  ( $\sim 7.85 \text{ eV}$ ).

In conclusion we note that if we take the translational symmetry of our problem into consideration we can write the wave function in the following form

$$\Psi_h = N^{-1/2} \sum_l \exp(ikr_l^l) \Psi_h^l. \quad (2)$$

Expression (2) determines the exciton band, whose width is of the order of

$$\frac{1}{36(1+4A+B)} \sum_{l'(+l)}^6 \sum_{l_1, l_1'}^6 \sum_{x\alpha, y\beta} \int \varphi_{l_1}^{*l_1'}(\rho) \varphi_{2x\alpha}^{*l'}(\rho') \times \frac{e^2}{|\rho-\rho'|} \varphi_{2y\beta}^l(\rho) \varphi_{l_1'}^l(\rho') d\tau d\tau' - \text{exch. term.} \quad (3)$$

The width (3) of the exciton band is, as follows from a numerical calculation, far smaller than  $\Delta E$ . This is, though, clear from the fact that in (3) functions occur referring to different halide ions and the integrals in (3) are thus much less than the analogous integrals in (1).

Since the width of the exciton band is much smaller than  $\Delta E$ , the energy of the excitation can be evaluated using the simpler function  $\Psi_{\text{exc}}$  as was done in the foregoing calculations. In those cases, however, where one is interested in effects which depend essentially on the form and width of the exciton band, it is necessary to use the more exact function (2).

<sup>1</sup>I. M. Dykman, J. Exptl. Theoret. Phys. (U.S.S.R.) **26**, 307 (1954).

<sup>2</sup>Dykman, Kaplunova, and Tolpygo, J. Tech. Phys. (U.S.S.R.) **26**, 2459 (1956), Soviet Phys. JTP **1**, 2376 (1956).

<sup>3</sup>A. A. Tsetsvadze, Труды Тбилисск. ун-та (Trans. Tbilisi Univ.) **62**, 149 (1957).

<sup>4</sup>D. Hartree and W. Hartree, Proc. Roy. Soc. **166**, 450 (1938).

<sup>5</sup>O. F. Tomasevich and K. B. Tolpygo, Укр. физ. журн. (Ukrainian Phys. Journal) (in press).

<sup>6</sup>T. Muto and H. Okuno, J. Phys. Soc. Japan **11**, 633 (1956); **12**, 108 (1957).

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261

## CONSEQUENCES OF THE TWO-COMPONENT BEHAVIOR OF THE ELECTRON IN THE BETA INTERACTION

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THE latest measurements<sup>1-3</sup> of the longitudinal polarization of the electrons emitted in  $\beta$  decay show that the values of the longitudinal polarization  $\langle \sigma_{\parallel} \rangle$  in cases of allowed transitions and first-forbidden transitions in heavy nuclei are to good accuracy equal to  $v/c$ . As can be rigorously proved from the formulas<sup>4</sup> for the longitudinal polarization of the electrons from such transitions, a necessary and sufficient condition for the relation  $\langle \sigma_{\parallel} \rangle = v/c$  is the existence of the following relations between the interaction constants conserving parity and violating its conservation:

$$C_S = -C'_S, \quad C_T = -C'_T, \quad C_A = C'_A, \quad C_V = C'_V. \quad (1)$$

With these conditions the interaction Hamiltonian takes the form

$$H = \sum_{\alpha} C_{\alpha} (\bar{\Psi}_p O_{\alpha} \Psi_n) (\bar{\psi}_e (1 - \gamma_5) O_{\alpha} \psi_{\nu}) + \text{c. c.}, \quad (2)$$

and the electronic  $\psi$  function is involved in all the types of  $\beta$  interaction through only two components.

Let us examine the consequences of the relations (1), i.e., of the two-component behavior of the electron in the  $\beta$  interaction. When the conditions (1) hold the expressions for the various effects in  $\beta$  decay are decidedly simplified, so that in the case of allowed transitions there remain all told just six independent combinations of the constants and matrix elements:

$$\begin{aligned} N_0 &= (|C_S|^2 + |C_V|^2) |M_F|^2 + (|C_T|^2 + |C_A|^2) |M_{GT}|^2, \\ N_1 &= -\lambda_{jj'} (|C_T|^2 + |C_A|^2) |M_{GT}|^2 \\ &\quad - 2\delta_{jj'} \sqrt{j/(j+1)} \text{Re}(C_S C_T^* + C_V C_A^*) M_F M_{GT}^*, \\ N_3 &= (|C_V|^2 - |C_S|^2) |M_F|^2 + 1/3 (|C_T|^2 - |C_A|^2) |M_{GT}|^2, \\ N_4 &= 2\delta_{jj'} \sqrt{j/(j+1)} \text{Im}(C_V C_A^* - C_S C_T^*) M_F M_{GT}^*, \\ N_5 &= -\lambda_{jj'} (|C_T|^2 - |C_A|^2) |M_{GT}|^2 \\ &\quad + 2\delta_{jj'} \sqrt{j/(j+1)} \text{Re}(C_S C_T^* - C_V C_A^*) M_F M_{GT}^*, \\ N_6 &= 2\delta_{jj'} \sqrt{j/(j+1)} \text{Im}(C_V C_A^* + C_S C_T^*) M_F M_{GT}^*. \end{aligned} \quad (3)$$

Here

$$\lambda_{jj'} = [j(j+1) - j'(j'+1) + 2]/2(j+1),$$