Fine structure of the levels of a bound exciton and multiexciton complexes in germanium

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A model, discovered recently by Mayer and Lightowlers,[1] which can explain the fine structure of an exciton bound by a neutral donor in germanium, is proposed. The indicated level splitting is attributable to the fact that, in addition to orbit-valley interaction, the exchange-valley splitting and crystalline splitting, play an essential role in germanium, in contrast with silicon.

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At the present, a one-electron model, called a shell model in the theory of bound multiexciton complexes (BMEC)[2], is used to describe the states of a bound exciton and of multiexciton complexes. According to Ref. 2, the electrons in the BMEC in germanium successively fill the Γ_1 and Γ_5 ND states, which are split by the amount Δ as a result of orbit-valley interaction. The ground state of a bound NDE_1 exciton is the $\Gamma_1 \times \Gamma_1$ state and one or two electrons fill the Γ_5 state in the $\Gamma_1 \times \Gamma_5$ and $\Gamma_5 \times \Gamma_5$ excited states. A fine structure of the $\Gamma_1 \times \Gamma_5$ state has recently been observed elsewhere.[1]

In an earlier paper, published jointly with one of the authors of this paper, it was assumed that one- and two-valley, two-electron states, just as the doubly charged D^- states,[4] must have different energies. This exchange-valley splitting is attributable to a reduction of the Coulomb interaction of two-valley states due to a strong anisotropy of the effective masses in each valley, which gives rise to a corresponding anisotropy of the electron wave functions.

Taking into account the exchange-valley splitting, the energy of the $\Gamma_1 \times \Gamma_1$ state is

$$E = \frac{1}{2}\left[(\delta - 2\Delta) - 2\left(\Delta^2 + \frac{\delta^2}{4} + \frac{\Delta\delta}{2}\right)^{1/2}\right]. \qquad (1)$$

The $\Gamma_1 \times \Gamma_5$ state must be split into two terms Γ_5^c and Γ_5^a with energies

$$E_c = -\Delta + \frac{1}{2}\left[(\delta + \Delta) - (\Delta^2 + \delta^2)^{1/2}\right],$$

$$E_a = -\Delta \,. \qquad (2)$$

The lower state is the antisymmetrized Γ_5^a state without single-valley functions.

The $\Gamma_5 \times \Gamma_5$ state is split into four terms: $\Gamma_5^c, \Gamma_4^a, \Gamma_1^c, \Gamma_3^c$ with energies

$$E_{\Gamma_3^c} = 0; \; E_{\Gamma_4^a} = 0; \; E_{\Gamma_5^c} = \frac{1}{2}\left[(\delta - \Delta) + (\Delta^2 + \delta^2)^{1/2}\right],$$

$$E_{\Gamma_1^c} = \frac{\delta}{2} - \Delta + \left(\Delta^2 + \frac{\delta^2}{4} + \frac{\Delta\delta}{2}\right)^{1/2}. \tag{3}$$

Here, δ is the difference in energies of the two-valley and one-valley states.

The total electron spin is $S = 0$ for all symmetrized states, and it is $S = 1$ and $S_z = 0, \pm 1$ for antisymmetrized states. As is known, the Γ_8 hole state of a free exciton, because of the anisotropy of the electron wave function, is split into two terms with spins $J_{z'} = \pm 3/2$ and $J_{z'} = \pm 1/2$, where the z' axis is oriented in the direction of the major axis of the corresponding extremum. The crystalline splitting $\Delta_{cr} = E_{\pm 3/2} - E_{\pm 1/2}$ for a free exciton in germanium is equal to about 1 meV.[5] A crystalline splitting should also lead to a splitting of the states $\Gamma_{5(4)} \times \Gamma_8 = \Gamma_6 + \Gamma_7 + 2\Gamma_8$ and $\Gamma_3 \times \Gamma_8 = \Gamma_6 + \Gamma_7 + \Gamma_8$ of a bound exciton in the BMEC and to a partial mixing of identical representations derived from different

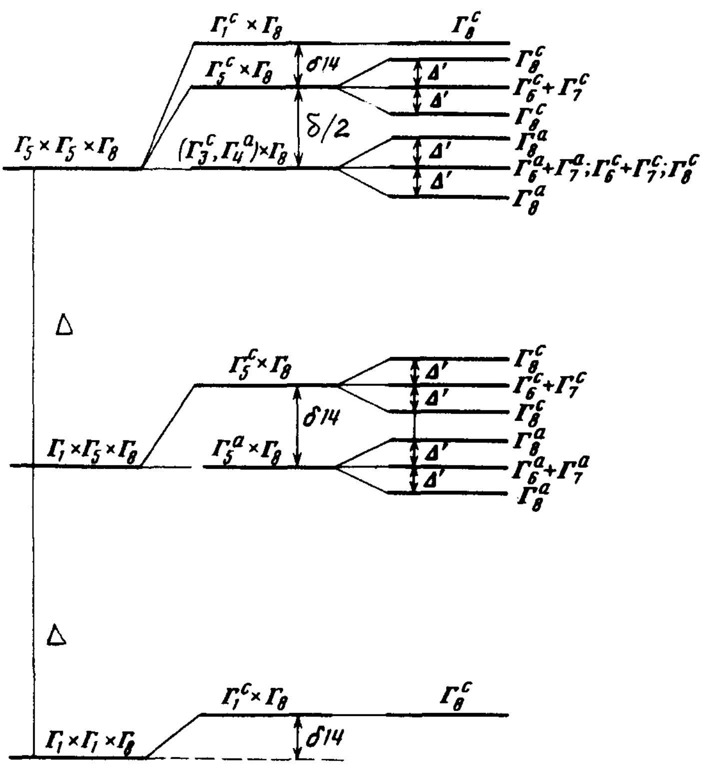

FIG. 1. A scheme for level splitting of an exciton bound by ND in germanium. $\Delta' = \Delta_{cr}/2$.

terms.

The scheme for splitting of the NDE_1 levels with allowance for the orbit-valley, exchange-valley, and crystalline splittings is shown in Fig. 1. The energy of the corresponding states calculated in the δ approximation, $\Delta_{cr} \ll \Delta$, is also shown in Fig. 1; we assumed that $\Delta_{cr} \ll \delta$ for the $\Gamma_5 \times \Gamma_5$ states. If these conditions are not satisfied, then the triply degenerate states $\Gamma_6^a + \Gamma_7^a, \Gamma_6^c + \Gamma_7^c$, and Γ_8^c will be split into three terms. Note that allowance for only the crystalline splitting for Δ_{cr}, which is comparable with Δ and $\delta = 0$, also leads to a splitting of the $\Gamma_1 \times \Gamma_5 \times \Gamma_8$ states into six terms and $\Gamma_5 \times \Gamma_5 \times \Gamma_8$ states into nine terms.

The selection rules for the *NP* transitions for free excitons in germanium coincide with those for the *LA* line. These selection rules, determined in Table I of Ref. 5, differ only in the subsitution of $\bar{\lambda}$ and $\bar{\eta}$ constants for λ and η. The selection rules for the *LA* lines of a bound exciton, which are independent of the state, coincide with the selec-

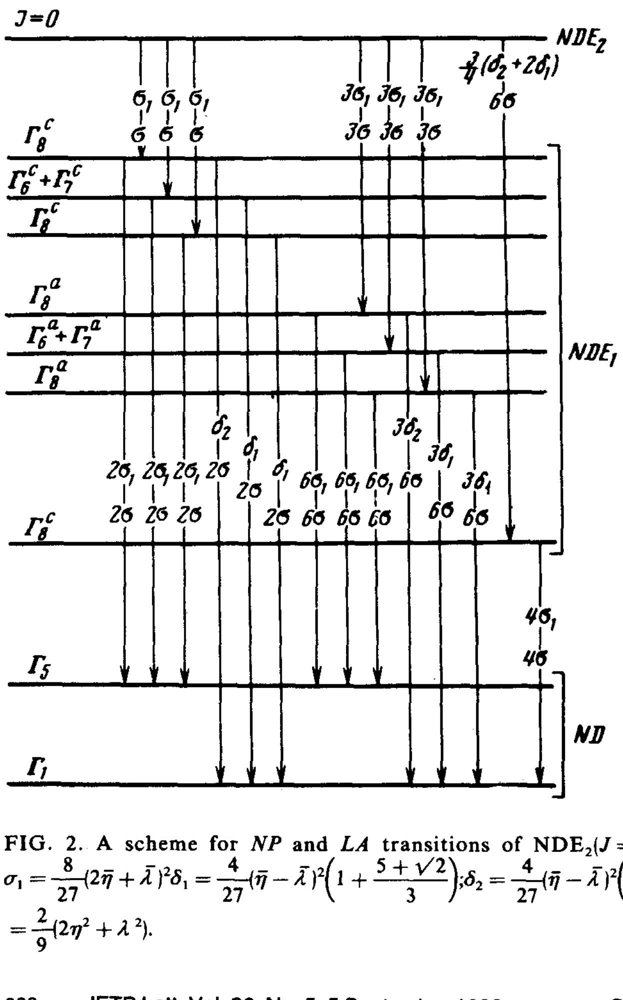

FIG. 2. A scheme for *NP* and *LA* transitions of $NDE_2(J=0) \rightarrow NDE_1 \rightarrow ND$ in germanium: $\sigma_1 = \frac{8}{27}(2\bar{\eta} + \bar{\lambda})^2 \delta_1 = \frac{4}{27}(\bar{\eta} - \bar{\lambda})^2\left(1 + \frac{5+\sqrt{2}}{3}\right); \delta_2 = \frac{4}{27}(\bar{\eta} - \bar{\lambda})^2\left(1 + \frac{5-2\sqrt{2}}{3}\right); \sigma = \sigma_{LA} = \frac{2}{9}(2\eta^2 + \lambda^2)$.

tion rules (averaged over all four valleys) for a free exciton. Just as in silicon,[6] the selection rules for the *NP* lines of the Γ_1 state differ from those of the Γ_5 state. Figure 2 shows the relative abundance of transitions from the split NDE_1 states to the Γ_1 and Γ_5 states of ND and the transitions from a NDE_2 ground state to an NDE_1 state, which were also observed in Ref. 1. We have assumed that the lower NDE_2 level is the $\Gamma_1 \times \Gamma_1 \times \Gamma_5$ electronic state and the Γ_1 hole state with total spin $J = 0$.

As a result of transitions across the nearest band $\Gamma'_2 \bar{\eta} = \lambda$ and $\eta = \lambda$.[5] The ratio $(\bar{\eta} - \bar{\lambda})/\bar{\eta}$ is small not only because of an increase of the energy denominator in the transitions across the more remote bands but also because these transitions are associated with the scattering of Γ'_{25} or Γ_{15} electrons by the impurity potential at the L point. The wave functions for all the representations except Γ_1 and Γ'_2 are equal to zero at the ion center, where its potential is maximum. Therefore, the *NP* transitions with Γ_5-electron and Γ_8-hole recombinations are almost forbidden, and the indicated transitions were observed[1] only in the *LA* absorption spectra.

According to Fig. 1, the $\Gamma_1 \times \Gamma_5 \times \Gamma_8$ NDE_1 state in germanium must split into six sublevels. In Ref. 1, four levels were observed for arsenic and five levels for phosphorus.

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