

type samples in that the peak is much higher and they approach the  $T^{-1/2}$  dependence from above rather than below.

The temperature dependence of the dielectric constant will affect the ionized-impurity limited mobility in the following way. As the temperature increases, thermally excited carriers increase the intraband screening and tend to raise the mobility. The dielectric constant decreases tending to increase the mobility through more efficient intraband screening and decrease the mobility through less efficient dielectric screening. Preliminary calculations indicate that the 300 K ionized-impurity limited mobility of, for example, an  $n$ -type sample with a  $10^{15}$ - $\text{cm}^{-3}$  donor-acceptor difference will be slightly less than one-third that which would be expected using the degenerate dielectric constant. This temperature dependence should be most easily observable in heavily double-doped samples, i.e.,

$$0 < Z_D N_D - Z_A N_A \ll Z_D N_D,$$

because under these conditions ionized-impurity scattering will dominate neutral-defect scattering and, to fairly high temperatures, acoustic-phonon scattering, while still allowing a large low-temperature dielectric constant. A calculation of this effect will be shown in a later publication.

It would also appear that the interband part of

$\epsilon_1(\omega)$  should have a temperature dependence similar to  $\epsilon_I(0)$ . A numerical calculation of this is under way, and it is likely that this is the reason that the 300 K optical data<sup>12</sup> do not show the  $\omega$  dependence predicted by Sherrington and Kohn<sup>13</sup> in the degenerate limit.

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<sup>1</sup>L. Liu and D. Brust, Phys. Rev. Lett. 20, 651 (1968).

<sup>2</sup>P. Nozières and D. Pines, Nuovo Cimento 9, 470 (1958).

<sup>3</sup>L. Liu and E. Tosatti, Phys. Rev. Lett. 23, 772 (1969).

<sup>4</sup>J. G. Broerman, Phys. Rev. Lett. 24, 450 (1970).

<sup>5</sup>J. G. Broerman, Phys. Rev. B 1, 4568 (1970).

<sup>6</sup>J. G. Broerman, Phys. Rev. B 2, 1818 (1970).

<sup>7</sup>J. G. Broerman, to be published.

<sup>8</sup>J. G. Broerman, Phys. Rev. 183, 754 (1969).

<sup>9</sup>J. McDougall and E. C. Stoner, Phil. Trans. Roy. Soc. London, Ser. A 237, 350 (1938).

<sup>10</sup>C. F. Lavine and A. W. Ewald, to be published.

<sup>11</sup>B. L. Booth and A. W. Ewald, Phys. Rev. 168, 805 (1968).

<sup>12</sup>D. Sherrington and W. Kohn, Phys. Rev. Lett. 21, 153 (1968).

<sup>13</sup>R. E. Lindquist and A. W. Ewald, Phys. Rev. 135, A191 (1964).

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## Angular Momentum Theory and Localized States in Solids. Investigation of Shallow Acceptor States in Semiconductors\*

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We show that localized states in solids can be conveniently investigated using techniques which are widely applied in the theory of atomic and nuclear spectra. The effective-mass theory for shallow acceptor states is formulated in a simple way and a meaningful classification of these states is obtained. The eigenvalue problem is reduced to simple radial Hamiltonians which are solved for the most important acceptor states.

All semiconductors with the diamond and zinc-blende structure have a simple conduction-band minimum and a degenerate valence-band maximum.<sup>1</sup> Therefore, donor states are easily investigated<sup>2</sup> whereas a complex analysis is required for acceptor states.<sup>3,4</sup>

A formal treatment for impurity states originating from degenerate bands has been derived by Kittel and Mitchell<sup>5</sup> and Luttinger and Kohn<sup>6</sup> within the effective-mass theory. Approximate solutions for acceptors in Si and Ge have been obtained by Kohn and Schecter<sup>3</sup> and Mendelson and James.<sup>4</sup> Although useful in the interpretation of the experimental results, these solutions involve elaborate computations and do not provide a clear picture of the acceptor problem.

Experimental data on acceptor states are available for several diamond and zinc-blende crystals.<sup>7-10</sup>

These results show that the effective-mass approximation is satisfactory for excited states whereas, for the ground state, central-cell effects<sup>11</sup> must be included. Since the magnitude of central-cell corrections is of great interest, accurate solutions for the effective-mass ground state are useful too.

The purpose of the present Letter is to achieve a clear insight into the acceptor problem through a more powerful and elegant procedure than that used in the previous investigations. To this goal, we make use of the strong similarity between impurity centers and atomic and nuclear systems. So far, this similarity has not been fully exploited. In fact, the only attempt in this direction has been in describing the impurity center as a particle with effective mass, spin, and charge which is bound to the impurity site through a screened Coulomb potential. It seems reasonable to assume that more profit can be obtained from this similarity if, in addition, one investigates the impurity problem using techniques of atomic and nuclear spectroscopy. The present Letter shows the soundness of this assumption.

The acceptor Hamiltonian in the strong spin-orbit coupling limit, as written by Luttinger,<sup>12</sup> is

$$H = (\gamma_1 + \frac{5}{2}\gamma_2) \frac{\vec{p}^2}{2m_0} - \frac{\gamma_0}{m_0} (\vec{p}_x^2 J_x^2 + \vec{p}_y^2 J_y^2 + \vec{p}_z^2 J_z^2) - \frac{2\gamma_3}{m_0} [\{p_x p_y\} \{J_x J_y\} + \{p_y p_z\} \{J_y J_z\} + \{p_z p_x\} \{J_z J_x\}] - \frac{e^2}{\epsilon_0 r} \quad (1)$$

when terms linear in  $\vec{p}$  are neglected for zinc-blende crystals. Here  $\{ab\} = (ab + ba)/2$ ,  $m_0$  is the free-electron mass,  $\epsilon_0$  is the static dielectric constant,  $\vec{p}$  is the hole linear momentum operator, and  $\vec{J}$  is the angular momentum operator for a particle with spin  $\frac{3}{2}$ . The above Hamiltonian can be thought of as describing a particle with spin  $\frac{3}{2}$  in a Coulomb potential. The first term is the kinetic energy, the second and third represent a "spin-orbit" interaction, and the last term is the external potential.

The operators  $\vec{p}$  and  $\vec{J}$  appear in Hamiltonian (1) in second order only. It is therefore convenient to introduce the following symmetric second-rank tensor operators<sup>13</sup> with vanishing trace:

$$P_{ik} = 3p_i p_k - \delta_{ik} p^2 \quad (2)$$

and

$$J_{ik} = \frac{3}{2}(J_i J_k + J_k J_i) - \delta_{ik} J^2, \quad (3)$$

where the indices  $i, k = 1, 2, 3$  mean  $x, y, z$ , respectively. Using the tensor operators  $P_{ik}$  and  $J_{ik}$ , the Hamiltonian (1) can be written as

$$H = \left[ \frac{\gamma_1}{2m_0} p^2 - \frac{e^2}{\epsilon_0 r} \right] - \frac{1}{9m_0} [\gamma_3 - (\gamma_3 - \gamma_2)\delta_{ik}] P_{ik} J_{ik} \quad (4)$$

with the Einstein convention on repeated indices.

The operators  $P_{ik}$  and  $J_{ik}$  are reducible tensors of the second rank. Therefore they can be decomposed into irreducible tensors of rank  $k = 0, 1, 2$ . Such decomposition contains neither the  $k = 0$  nor the  $k = 1$  components. In fact, the former does not appear because  $P_{ik}$  and  $J_{ik}$  have vanishing trace, the latter because of the symmetry properties

$$P_{ik} = P_{ki}; \quad J_{ik} = J_{ki}. \quad (5)$$

As a result, the tensor operators in Hamiltonian (4) can be expressed in terms of their second-rank irreducible components  $P_q^{(2)}$  and  $J_q^{(2)}$  ( $q = -2, 1, 0, 1, 2$ ) as follows:

$$H = \left[ \frac{\gamma_1}{2m_0} p^2 - \frac{e^2}{\epsilon_0 r} \right] - \frac{3\gamma_3 + 2\gamma_2}{45m_0} (P^{(2)} \cdot J^{(2)}) - \frac{\gamma_3 - \gamma_2}{18m_0} \left\{ [P^{(2)} \times J^{(2)}]_{-4}^4 + \frac{\sqrt{70}}{15} [P^{(2)} \times J^{(2)}]_0^4 + [P^{(2)} \times J^{(2)}]_4^4 \right\}, \quad (6)$$

where the usual definitions of scalar and vector products of irreducible tensor operators have been used.<sup>13</sup>

Expressions (1) and (6) are equivalent ways of writing the same acceptor Hamiltonian but they reflect two different points of view as far as symmetry is concerned. Luttinger<sup>12</sup> looked at the problem having in mind the point group of the crystal and as a consequence he considered all the terms which appear in (1) as having the same cubic symmetry properties. On the contrary, our approach is based

Table I. Theoretical and experimental ionization energies of acceptor impurities.  $\epsilon_0$  is the static dielectric constant;  $\gamma_1$ ,  $\gamma_2$ , and  $\gamma_3$  are the Luttinger valence-band parameters. The parameters  $\mu$  and  $\delta$  are defined in the text by expressions (7) and (8), respectively. The symbols in parentheses refer to the kind of impurity.

Crystal	$\epsilon_0$	$\gamma_1$	$\gamma_2$	$\gamma_3$	$\mu$	$\delta$	$E_{inz}$ Theor	$E_{inz}$ Exp
Ge	15.36 <sup>a</sup>	13.23 <sup>d</sup>	4.27 <sup>d</sup>	5.61 <sup>d</sup>	0.767	0.102	9.9	10.8 <sup>e</sup> (Ga)
Si	11.4 <sup>a</sup>	4.23 <sup>d</sup>	0.38 <sub>5</sub> <sup>d</sup>	1.44 <sup>d</sup>	0.481	0.249	31	68.9 <sup>f</sup> (Al)
AlSb	9.9 <sup>b</sup>	5.26 <sup>d</sup>	1.37 <sub>5</sub> <sup>d</sup>	2.15 <sup>d</sup>	0.700	0.147	49	33 <sup>g</sup> (?)
GaP	10.75 <sup>c</sup>	3.83 <sup>d</sup>	0.86 <sup>d</sup>	1.48 <sub>5</sub> <sup>d</sup>	0.645	0.163	50	64 <sup>h</sup> (Zn)

<sup>a</sup>From Ref. 2.

<sup>b</sup>W. J. Turner and W. E. Reese, Phys. Rev. **127**, 126 (1962).

<sup>c</sup>L. Patrick and P. J. Dean, Phys. Rev. **188**, 1254 (1970).

<sup>d</sup>From Ref. 14.

<sup>e</sup>From Ref. 7.

<sup>f</sup>From Ref. 8.

<sup>g</sup>From Ref. 9.

<sup>h</sup>From Ref. 10.

on the full rotation group and therefore we have separated in (6) the last term, which is cubic, from the first two which, besides having cubic symmetry, are also spherically invariant.

This rearrangement of terms suggests a more convenient set of parameters for the description of the acceptor problem. Together with  $\gamma_1$ , we use

$$\mu = (6\gamma_3 + 4\gamma_2)/5\gamma_1 \quad (7)$$

which gives the strength of the spherical spin-orbit interaction, and

$$\delta = (\gamma_3 - \gamma_2)/\gamma_1 \quad (8)$$

which measures the cubic contributions. In Table I we give the values of  $\mu$  and  $\delta$  for a few substances as obtained from the valence band parameters  $\gamma_1$ ,  $\gamma_2$ , and  $\gamma_3$  given by Lawaetz.<sup>14</sup> As one can see, the cubic term in Hamiltonian (6) is small and therefore its effects can be considered as a perturbation. This justifies our idea of looking at the problem from the full rotation group point of view. In fact, by doing so, we are able to write the acceptor Hamiltonian as the sum of a spherical term and a small cubic contribution.

We first consider the case  $\delta = 0$ . The Hamiltonian (6) becomes spherically symmetric and the total angular momentum  $\vec{F} = \vec{L} + \vec{J}$  is a constant of the motion. Accordingly, we can classify the acceptor eigenstates in exactly the same way and notation used for atoms with spin-orbit interaction ( $L$ - $S$  coupling). Without the spin-orbit interaction the eigenstates can be classified with the usual hydrogenic quantum numbers. When the spin-orbit interaction is included, a fine structure is produced. The  $nS$  states give rise only to  $nS_{3/2}$  states while the  $nP$  states split into  $nP_{1/2}$ ,  $nP_{3/2}$ , and  $nP_{5/2}$ .

We now analyze the  $nS_{3/2}$  states. The most general wave function for such states is

$$f(\mathbf{r})|L=0, J=\frac{3}{2}, F=\frac{3}{2}, F_z\rangle + g(\mathbf{r})|L=2, J=\frac{3}{2}, F=\frac{3}{2}, F_z\rangle, \quad (9)$$

where  $f(\mathbf{r})$  and  $g(\mathbf{r})$  are radial wave functions which have to be determined. The projection of the total Hamiltonian (6) onto the  $S_{3/2}$  subspace can be written as a  $2 \times 2$  matrix whose elements are easily evaluated using the "reduced matrix element" technique<sup>13</sup>:

$$\langle L', J, F, M | Q^{(2)} \cdot J^{(2)} | L, J, F, M \rangle = (-)^{L+J+F} \begin{Bmatrix} F & L' & J \\ 2 & J & L \end{Bmatrix} \langle J || J^{(2)} || J \rangle \langle L' || Q^{(2)} || L \rangle. \quad (10)$$

The evaluation of the  $6-j$  symbol and of the reduced matrix elements which appear on the right-hand side of expression (10) is straightforward and will not be given here. As a result we obtain the following  $2 \times 2$  matrix Hamiltonian for the radial wave functions  $f(\mathbf{r})$  and  $g(\mathbf{r})$ :

$$\begin{bmatrix} \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \frac{2}{r} & -\mu \left( \frac{d^2}{dr^2} + \frac{5}{r} \frac{d}{dr} + \frac{3}{r^2} \right) \\ -\mu \left( \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} \right) & \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{6}{r^2} + \frac{2}{r} \end{bmatrix} \begin{bmatrix} f \\ g \end{bmatrix} = E \begin{bmatrix} f \\ g \end{bmatrix}, \quad (11)$$

where effective atomic units have been used. Following the same procedure, we obtain Hamiltonians for  $P_{1/2}$ ,  $P_{3/2}$ , and  $P_{5/2}$  states. These Hamiltonians are similar to (11) and their expression will be published elsewhere.<sup>15</sup>

Exact solutions of the Hamiltonians for the  $S_{3/2}$ ,  $P_{3/2}$ , and  $P_{5/2}$  states have not been found. We have studied the lowest state of each Hamiltonian using the variational technique and assuming as trial functions exponentials times the lowest possible polynomials which behave correctly at the origin. As an example, for the ground state of Hamiltonian (11) we used the trial wave functions

$$\begin{aligned} f(r) &= 2\alpha^{3/2} \exp(-\alpha r); \\ g(r) &= (2/\sqrt{3})\beta^{5/2} r \exp(-\beta r). \end{aligned} \quad (12)$$

The Hamiltonian for the  $P_{1/2}$  states reduces to that of the hydrogen atom for  $P$  states and therefore can be solved exactly.

The energies of the lowest  $S_{3/2}$ ,  $P_{1/2}$ ,  $P_{3/2}$ , and  $P_{5/2}$  states are shown in Fig. 1 as a function of the parameter  $\mu$  over the range of interest for all diamond and zinc-blende crystals. These results represent the first theoretical investigation of acceptor energy levels as functions of the valence-band parameters. While the energy of the  $P_{1/2}$  state decreases very slowly with increasing  $\mu$ , the energies of the other states show the opposite behavior and increase very rapidly for  $\mu \geq 0.5$ . Using the results of Fig. 1, we have evaluated the ionization energies of the substances shown in Table I. A comparison of these effective-

mass ionization energies with the experimental values allows the appreciation of central-cell corrections.

We now consider the small cubic term which appears in Hamiltonian (6). This low-symmetry term shifts the energy levels and in addition can remove some degeneracies. For the  $S_{3/2}$ ,  $P_{1/2}$ , and  $P_{3/2}$  states no splitting is produced and, furthermore, selection rules on the angular momenta show that the first nonvanishing contribution comes from second-order perturbation theory. The sixfold degenerate  $P_{5/2}$  states have a nonvanishing first-order contribution and split into a fourfold  $P_{5/2}(\Gamma_8)$  and a twofold  $P_{5/2}(\Gamma_7)$  states. Since for all the diamond and zinc-blende crystals the parameter  $\delta$  is small, we consider only first-order contributions in  $\delta$ . Following a procedure similar to that used for the case  $\delta=0$ , the Hamiltonians for the  $P_{5/2}(\Gamma_8)$  and the  $P_{5/2}(\Gamma_7)$  states are obtained.<sup>15</sup> In Fig. 1 we give the splitting of the  $2P_{5/2}$  state for  $\delta=0.15$ .

From the point of view of numerical accuracy, our results are not expected to improve those obtained in the previous investigations. In effect, for Si and Ge, they are in agreement with those reported by Schechter<sup>3</sup> and Mendelson and James.<sup>4</sup> However, having chosen a better set of parameters to describe the valence band, we are able to give results which can be easily adapted to any cubic semiconductor. An even greater advantage of our approach is in the simple formulation which, without introducing any explicit representation for the Hamiltonian, allows a general understanding of the problem and explains the validity of several assumptions made in the previous investigations in the construction of the trial wave functions. In fact, the assumed mixing of a limited number of angular momenta is now understood from the small size of the cubic term. Furthermore, our new point of view makes possible a meaningful classification of the acceptor states and therefore a general picture of the acceptor spectrum.

It is reasonable to suppose that the present method can be extended to other localized states in solids. The only condition for its applicability is that the low-symmetry terms of the Hamiltonian must be sufficiently small and this condition is often verified.

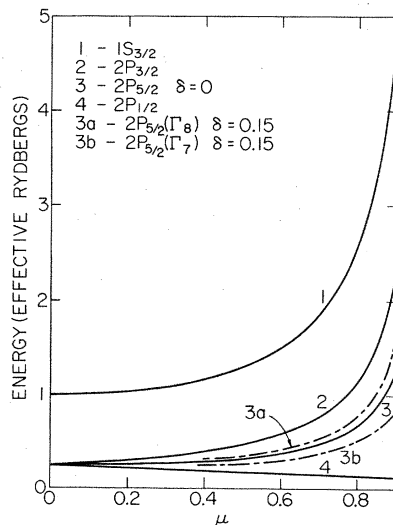


FIG. 1. Energy levels of the most important acceptor states as functions of the valence-band parameter  $\mu$ . The dotted lines show the splitting of the  $2P_{5/2}$  state produced by the cubic term for  $\delta=0.15$ .

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<sup>1</sup>See, for example, M. L. Cohen and T. K. Bergstresser, *Phys. Rev.* **141**, 789 (1966).

<sup>2</sup>R. A. Faulkner, *Phys. Rev.* **184**, 713 (1969).

<sup>3</sup>W. Kohn and D. Schechter, *Phys. Rev.* **99**, 1903 (1955); D. Schechter, *J. Phys. Chem. Solids* **23**, 237 (1962).

<sup>4</sup>K. S. Mendelson and H. M. James, *J. Phys. Chem. Solids* **25**, 729 (1964).

<sup>5</sup>C. Kittel and A. H. Mitchell, *Phys. Rev.* **96**, 1488 (1954).

<sup>6</sup>W. Kohn and J. M. Luttinger, *Phys. Rev.* **97**, 869 (1955).

<sup>7</sup>P. Fisher and H. Y. Fan, *Phys. Rev. Lett.* **2**, 456 (1959); R. L. Jones and P. Fisher, *J. Phys. Chem. Solids* **26**, 1125 (1965).

<sup>8</sup>A. Onton, P. Fisher, and A. K. Ramdas, *Phys. Rev.* **163**, 686 (1967).

<sup>9</sup>R. J. Stirn and W. M. Becker, *Phys. Rev.* **148**, 907 (1966); B. T. Ahlburn and A. K. Ramdas, *Phys. Rev.* **187**, 932 (1969).

<sup>10</sup>P. J. Dean, C. J. Frosh, and C. H. Henry, *J. Appl. Phys.* **39**, 5631 (1968).

<sup>11</sup>J. C. Phillips, *Phys. Rev. B* **1**, 1540, 1545 (1970).

<sup>12</sup>J. M. Luttinger, *Phys. Rev.* **102**, 1030 (1956).

<sup>13</sup>See, for example, A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton Univ., Princeton, N. J., 1960).

<sup>14</sup>P. Lawaetz, private communication.

<sup>15</sup>A. Baldereschi and N. O. Lipari, to be published.

## Classical Analog of the Variable Moment of Inertia Formulas for Rotational States in Even-Even Nuclei\*

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A simple mechanical model has been found which gives the same angular velocity dependence of energy and angular momentum as postulated in the variable moment of inertia description of rotational states. The possibility for one of the two coefficients of this description to adopt negative values follows naturally from this model. Also the nonzero ground-state energies, which in some cases result from the variable moment of inertia description, are easily understood.

One explanation which has been advanced for the departure from the  $J(J+1)$  energy formula for rotational states is the classical, rotation-dependent, elastic deformation ( $\beta$  stretching).<sup>1</sup> Much greater success has recently been obtained using the formulas

$$E = \frac{1}{2}\omega^2(\mathcal{J}_0 + 3C\omega^2), \quad (1)$$

$$\hbar[J(J+1)]^{1/2} = \omega(\mathcal{J}_0 + 2C\omega^2) = \omega\mathcal{J}, \quad (2)$$

where  $\omega$  is the angular frequency,  $\mathcal{J}$  is the moment of inertia, and  $\mathcal{J}_0$  and  $C$  are constants. These expressions were first derived by Harris<sup>2</sup> from an extension of the cranking model,<sup>3</sup> and then shown to be equivalent to the variable moment of inertia (VMI) description.<sup>4</sup>

The striking success of these formulas in fitting the energy levels of ground-state rotational bands<sup>4</sup> was recently extended to an even wider range of nuclei by allowing the parameter  $\mathcal{J}_0$  to become negative.<sup>5,6</sup> Thus, most, and perhaps all, even-even nuclei are now included in this description. The introduction of negative values of  $\mathcal{J}_0$  also leads to an accurate prediction of a distinct discontinuity<sup>5,6</sup> in the so-called "Mallmann" plots,<sup>7</sup> the graphs of  $E_8/E_2$  and  $E_6/E_2$

versus  $E_4/E_2$ .

Harris's model, however, does not allow negative values for  $\mathcal{J}_0$ . Furthermore, the fact that a nonzero ground-state energy is obtained for some of the solutions<sup>5,6</sup> requires clarification. The purpose of the present work was to search for a classical model, similar to the centrifugal stretching model, which would be described not by the equations of that model but by Eqs. (1) and (2).

In the hydrodynamical model, on which the centrifugal stretching model is based, all the elements of mass in the nucleus take part in the motion contributing to the total angular momentum and energy. For real nuclei, however, only certain nucleons give rise to the total angular momentum while the rest, forming closed  $j$  shells, do not contribute. It seems, therefore, appropriate to search for a model in which the total mass  $M_T$  of a nucleus is divided into a rotating portion of mass  $M$  and a stationary part of mass  $M_T - M$ . In such a model the increase of the moment of inertia with angular momentum can be due either to a variation of the mass  $M$  or to a change of its orbit, or to a combination