PHYSICAL REVIEW B VOLUME 9, NUMBER 4 15 FEBRUARY 1974

Exciton states of semiconductors in a high magnetic field

M. Altarelli*[†]

Department of Physics and Astronomy, University of Rochester, Rochester, New York 14607

Nunzio O. Lipari

Webster Research Center, Xerox Corporation, Webster, New York 14580

(Received 2 May 1973; revised manuscript received 7 September 1973)

Exciton states of diamond and zinc-blende semiconductors in a high magnetic field are investigated taking into full account the degeneracy and anisotropy of the valence bands. An improved version of the adiabatic method introduced by Rees is derived and generalized for arbitrary orientation of the field. Simple one-dimensional adiabatic Hamiltonians which describe the motion component parallel to the magnetic field are obtained. The introduction of a suitable set of Gaussian basis functions is shown to provide exact analytical expressions for the adiabatic-potentials matrix elements. A very accurate procedure is used to diagonalize the Hamiltonians for the various states. Results are obtained for $\vec{H}$ parallel to the [001] and [110] directions and for several materials. The range of validity of the present adiabatic approach is discussed, and the theoretical results are compared to experiment.

I. INTRODUCTION

In the last two decades a considerable amount of experimental and theoretical effort has been devoted to the investigation of the electronic states of solids in the presence of an external magnetic field.[1] In particular, the magnetoabsorption of semiconductors has received great attention because it can provide very important information about the electronic band structure of these materials.[2] However, it has become more and more evident that the various simplifications commonly introduced in the theoretical literature fail to reproduce quantitatively the experimental data, and that a meaningful interpretation of magnetoabsorption experiments is very difficult because of the presence of both the complicated valence-band structure and the electron-hole Coulomb interaction.[3] In fact, it was realized very early that the wealth of the observed structure showing a great number of absorption peaks, unevenly spaced and of different intensities, is a consequence of the complexity of the valence bands.[4]

The theoretical problem of the Landau levels of cubic semiconductors was first satisfactorily treated by Kohn and Luttinger[5] and their solution was later refined by several investigators.[6-8] This Landau-level analysis, although successful in the interpretation of cyclotron-resonance experiments, is not adequate to describe magnetoabsorption near the fundamental edge.[9] This is clearly shown by the measurements of Edwards and Lazazzera on the direct edge of Ge,[10] where the evident nonlinear dependence of the peak positions on magnetic field is in direct contrast with the predictions of the Landau-level theory. In addition, the fact that the lowest peak extrapolates, as the magnetic field $H \rightarrow 0$, to the energy of the direct-exciton ground state is a definite indication of the importance of the electron-hole Coulomb interaction.

This aspect was theoretically supported by the pioneering work of Elliott and Loudon,[11] who treated the case of simple parabolic bands in the high-field limit. They concluded that, associated with each Landau level, there is an exciton series and that the most important absorption peaks in the magnetoabsorption spectrum correspond to the transitions to these exciton levels, with interband Landau absorption as an insignificant shoulder. This work stimulated several theoretical efforts[12-17] aiming both at the extension of the original approach to the whole range of magnetic fields and at the testing of the validity of the adiabatic method used by Elliott and Loudon. In particular, the work by Baldereschi and Bassani[15] provided the first accurate calculation of the four lowest even-parity states for all values of the magnetic field. These calculations account for some qualitative features of the observed magnetoabsorption spectra, such as the nonlinearity of the lowest peaks; however, their common feature and limitation is that they assume simple parabolic bands, so that they predict a simple and polarization-independent spectrum. These features are in sharp contrast with the experimental observation of Johnson and Fan[18] of a different diamagnetic shift of the ground exciton state of GaSb for light polarization parallel or perpendicular to the field, and with the complicated fine structure observed by Johnson[19] in Ge and InSb. It is therefore evident that any theory, aiming at a detailed quantitative interpretation of magnetoabsorption experiments and at an unambiguous determination of band parameters, must incorporate simultaneously the electron-hole Coulomb interaction and the complicated band structure.

The impossibility to work out a unified theoretical treatment, valid for all fields, for the case of simple bands, clearly discourages any such attempt for the realistic case of degenerate and anisotropic bands. The difficulty of the problem lies in the simultaneous presence of the Coulomb attraction and of the localization along the magnetic field lines. When one of the two effects is dominant, it is possible to consider the other as a perturbation and to include it by a suitable approximation. Recently, we have shown[20] that, in the low-field region, where the cyclotron energy is small compared to the Coulomb binding energy of the exciton, a second-order perturbation treatment reproduces the salient features of the observed spectra. In fact, the diamagnetic shift was shown to be the sum of two contributions; the first one corresponding to the familiar hydrogenic result,[21] and the second one depending on the anisotropy of the bands, which is different for the various light polarizations relative to the field. The quantitative agreement with the available experimental data for GaAs[22] and GaSb[18] was quite encouraging, thus pointing out the effectiveness of the inclusion of the realistic band structure. The perturbation treatment, however, is limited for most semiconductors[20] to a small range of magnetic fields; from the experimental point of view, on the other hand, the high-magnetic-field region is the most frequently investigated, and, due to the wealth of clearly resolved fine structure, obviously provides the ideal ground for a detailed comparison between theory and experiment. In this region the magnetic localization predominates over the Coulomb interaction and the adiabatic method, introduced for the case of simple bands by Elliott and Loudon,[11] is an excellent approach.[15]

The extension of the adiabatic method to the realistic case of cubic semiconductors was first considered by Zhilich[23] and by Rees.[24,25] In the analysis by Zhilich,[23] the matrix corresponding to the Landau problem, (i.e., without electron-hole interaction) is diagonalized first, and the Coulomb interaction is then averaged over the previously obtained Landau wave function. This procedure, therefore, neglects completely the admixture among Landau levels, with the same quantum numbers, belonging to different "ladders," which is important for several exciton states. Furthermore, a complicated and approximate method of solution is used to solve the resulting one-dimensional Schrödinger equation. Rees, on the other hand, includes the Coulomb interaction before performing the diagonalization, thus correctly including, in principle, the admixture of Landau levels. His analysis was originally worked out for the acceptor problem[24] and later applied to excitons.[25] For the latter case, however, his approach is invalid, owing to the use of an incorrect effective-mass Hamiltonian for the relative electron-hole motion, as discussed in Sec. II. In addition, the method was not pushed to its full potentiality to provide accurate numerical results, due to approximations to the adiabatic potentials and to the use of oversimplified and unrealistic variational trial functions. Rees's work, however, is important in that it introduces a formalism most convenient for this problem.

In a recent letter,[26] we proposed an improved version of the adiabatic method as applied to the case of cubic semiconductors, which provided the first quantitative interpretation of the fine structure observed in high-resolution measurements of magnetoabsorption in Ge.[19] It is the purpose of the present paper to describe in detail this method and to provide extensive numerical results for several materials for which experimental data are available.

In Sec. II we formulate the problem, briefly outline the method, and give the adiabatic Hamiltonians for the relevant exciton states. The analysis is carried out for the [001] and the [110] directions of the magnetic field. In Sec. III the selection rules for optical transitions from the ground state are obtained and briefly discussed. A Gaussian basis set is introduced in Sec. IV, and the analytical expressions of the matrix elements of the adiabatic potentials are given. In Sec. V the numerical solution of the eigenvalue problem is discussed and results for several materials are obtained and compared with available experimental data. In Sec. VI we summarize the main results of the present investigation and discuss possible future extensions.

II. FORMULATION OF THE PROBLEM: THE ADIABATIC APPROACH

In the presence of an external magnetic field $\vec{H}$ the wave function for a direct exciton at rest in the crystal can be written[27]

$$\Psi_n(\vec{r}_e, \vec{r}_h) = V^{1/2} \exp\left(\frac{ie}{2\hbar c}\vec{H}\cdot(\vec{r}_e \times \vec{r}_h)\right) \times \sum_{i=1}^{r} \sum_{j=1}^{s} \psi_{n,ij}(\vec{r}_e - \vec{r}_h)\phi_{c_i}(\vec{r}_e)\phi_{v_j}(\vec{r}_h), \qquad (1)$$

where V is the volume of the crystal, $\phi_{c_i}(\vec{r}_e)$ and $\phi_{v_j}(\vec{r}_h)$ are the Bloch function of the ith conduction and the jth valence band at the Γ point, respectively, and $\vec{r}_e$ and $\vec{r}_h$ denote the electron and the hole position, respectively.

The summation over i, in the case of interest here, i.e., in cubic semiconductors, includes two terms corresponding to spin up or down in the conduction band; the sum over j includes four terms corresponding to the upper multiplet of the spin-orbit-split valence band. The index n labels all the quantum numbers associated with the relative electron-hole motion. The functions $\psi_{n,ij}(\vec{r})$, where $\vec{r}=\vec{r}_e-\vec{r}_h$, satisfy the effective-mass equation:

$$\mathcal{H}_{\mathrm{ex}}\psi=E\psi\,, \tag{2}$$

where, using the gauge $\vec{A}=\frac{1}{2}(\vec{H}\times\vec{r})$,

$$\mathcal{H}_{\mathrm{ex}}=\mathcal{H}_e\left(-i\vec{\nabla}+\frac{e}{2\hbar c}(\vec{H}\times\vec{r})\right)-\mathcal{H}_h\left(i\vec{\nabla}+\frac{e}{2\hbar c}(\vec{H}\times\vec{r})\right)-\frac{e^2}{\epsilon r}\,. \tag{3}$$

$\vec{A}$ is the vector potential describing the field $\vec{H}$, and ϵ is the static dielectric constant. Since $\psi_{n,ij}$ ($i=1,2$; $j=1,\cdots,4$) is an eight-component wave function, Eq. (2) is an eight-by-eight system of equations; however, states with up or down conduction-band spin are uncoupled, since we neglect, in Eq. (3), the electron-hole exchange coupling whose effect is negligible in comparison with the Coulomb and magnetic terms, and the system splits into two four-by-four systems. $\mathcal{H}_e$ is the conduction-band Hamiltonian and $\mathcal{H}_h$ is the valence-band Hamiltonian. It is important to point out, in Eq. (3), that the gradient operator appears with different sign in the electron and in the hole Hamiltonian, thus giving rise to terms linear in $\vec{H}$. These terms, which are very important for the case of degenerate bands, were omitted by Rees.[25] The explicit expressions for the conduction and valence-band Hamiltonians are

$$\mathcal{H}_e(\vec{k}')=\frac{\hbar^2}{2m_e}k'^2+\bar{\mu}^*\vec{\sigma}\cdot\vec{H} \tag{4}$$

and[27]

$$-\mathcal{H}_h(\vec{k})=\frac{\hbar^2}{m_0}\Big[(\gamma_1+\tfrac{5}{2}\gamma_2)\tfrac{1}{2}k^2-\gamma_2(k_x^2J_x^2+k_y^2J_y^2+k_z^2J_z^2)-2\gamma_3(\{k_x,k_y\}\{J_x,J_y\}+\{k_y,k_z\}\{J_y,J_z\}+\{k_z,k_x\}\{J_z,J_x\}) -\frac{e}{c}\kappa\vec{J}\cdot\vec{H}-\frac{e}{c}q(J_x^3H_x+J_y^3H_y+J_z^3H_z)\Big]\,, \tag{5}$$

where γ_1, γ_2, γ_3, κ, and q are the five valence-band parameters introduced by Luttinger.[28] In Eq. (4), m_e is the conduction-band effective mass and $\bar{\mu}^*$ the effective magnetic moment of the conduction band; in Eq. (5) m_0 is the free-electron mass, J_x, J_y, and J_z are the 4×4 angular-momentum matrices corresponding to a spin-$\frac{3}{2}$ state, and, following Luttinger, we define

$$\{A,B\}=\tfrac{1}{2}(AB+BA)\,. \tag{6}$$

It is important to note that the change of sign of the gradient operator in $\mathcal{H}_h$ implies also a sign inversion for the terms containing κ and q. The choice of the convenient representation for the angular-momentum matrices is suggested by the direction of the magnetic field; in practice it is always convenient to choose a representation for which the component of J along the magnetic field is diagonal.

Let us first consider the case in which the magnetic field is along a cubic axis, for instance, the z axis. We then assume

$$J_x=\begin{pmatrix}0&0&\frac{1}{2}\sqrt{3}\,i&0\\0&0&-i&\frac{1}{2}\sqrt{3}\,i\\-\frac{1}{2}\sqrt{3}\,i&i&0&0\\0&-\frac{1}{2}\sqrt{3}\,i&0&0\end{pmatrix}\,, \tag{7}$$

$$J_y=\begin{pmatrix}0&0&\frac{1}{2}\sqrt{3}&0\\0&0&1&\frac{1}{2}\sqrt{3}\\\frac{1}{2}\sqrt{3}&1&0&0\\0&\frac{1}{2}\sqrt{3}&0&0\end{pmatrix}\,, \tag{8}$$

$$J_z=\begin{pmatrix}\frac{3}{2}&0&0&0\\0&-\frac{1}{2}&0&0\\0&0&\frac{1}{2}&0\\0&0&0&\frac{3}{2}\end{pmatrix}\,. \tag{9}$$

The explicit expression for the effective-mass Hamiltonian (3) is easily obtained using Eqs. (4)–(9) and is very complicated, consisting of two four-by-four operator matrices, which differ only in the sign of the conduction-band spin term.

It is convenient to introduce the operator

$$\vec{K}=i\vec{\nabla}+\frac{e}{2c}(\vec{H}\times\vec{r}) \tag{10}$$

and the following mass parameters:

$$1/\mu_0=\gamma_1/m_0\,, \tag{11}$$

$$1/\mu_1=\gamma_2/m_0\,, \tag{12}$$

$$1/\mu_2=2\sqrt{3}\,\gamma_3/m_0\,, \tag{13}$$

$$\frac{1}{m_h}=\frac{1}{m_0}(\gamma_1+\gamma_2)\,, \tag{14}$$

$$\frac{1}{m_h'}=\frac{1}{m_0}(\gamma_1-\gamma_2), \tag{15}$$

$$\frac{1}{\mu}=\frac{1}{m_e}+\frac{1}{m_h}, \tag{16}$$

$$\frac{1}{\mu'}=\frac{1}{m_e}+\frac{1}{m_h'}, \tag{17}$$

$$\frac{1}{\bar{\mu}}=\frac{1}{2}\,\frac{\gamma_2+\gamma_3}{m_0}, \tag{18}$$

$$\frac{1}{\mu_\delta}=\frac{1}{2}\,\frac{\gamma_3-\gamma_2}{m_0}, \tag{19}$$

and to adopt effective units, i.e., to assume

$$R_0=\frac{\mu_0 e^4}{2\hbar^2\epsilon^2}, \quad a_0=\frac{\hbar^2\epsilon}{\mu_0 e^2} \tag{20}$$

as units of energy and length, respectively, and to introduce the "reduced field"

$$\gamma=e\hbar H/2\mu_0 cR_0 . \tag{21}$$

The explicit expression of the four-by-four Hamiltonian matrices is

$$\mathcal{H}_{ex}=\left|\begin{array}{cccc}
\begin{array}{l}\frac{\mu_0}{\mu}(P_x^2+P_y^2)+(1-2\mu_0/\mu_1)P_z^2\\ +\gamma\left[\left(\frac{\mu_0}{\mu}-\frac{2\mu_0}{m_h}\right)(xP_y-yP_x)\right.\\ \left.-\frac{\mu_0}{m_0}(3\kappa+\frac{27}{4}q)\right]\\ +\frac{1}{4}\frac{\mu_0}{\mu}\gamma^2(x^2+y^2)\pm\bar{\mu}^*\gamma-\frac{2}{r}\end{array} & \frac{\sqrt{3}\,\mu_0}{\bar{\mu}}K_-^2-\frac{\sqrt{3}\,\mu_0}{\mu_\delta}K_+^2 & -i\frac{\mu_0}{\mu_2}K_-P_z & 0\\
\frac{\sqrt{3}\,\mu_0}{\bar{\mu}}K_+^2-\frac{\sqrt{3}\,\mu_0}{\mu_\delta}K_-^2 & \begin{array}{l}\frac{\mu_0}{\mu'}(P_x^2+P_y^2)+(1+2\mu_0/\mu_1)P_z^2\\ +\gamma\left[\left(\frac{\mu_0}{\mu'}-\frac{2\mu_0}{m_h'}\right)(xP_y-yP_x)\right.\\ \left.+\frac{\mu_0}{m_0}(\kappa+\frac{1}{4}q)\right]\\ +\frac{1}{4}\frac{\mu_0}{\mu'}\gamma^2(x^2+y^2)\pm\bar{\mu}^*\gamma-\frac{2}{r}\end{array} & 0 & i\frac{\mu_0}{\mu_2}K_-P_z\\
i\frac{\mu_0}{\mu_2}K_+P_z & 0 & \begin{array}{l}\frac{\mu_0}{\mu'}(P_x^2+P_y^2)+(1+2\mu_0/\mu_1)P_z^2\\ +\gamma\left[\left(\frac{\mu_0}{\mu'}-\frac{2\mu_0}{m_h'}\right)(xP_y-yP_x)\right.\\ \left.-\frac{\mu_0}{m_0}(\kappa+\frac{1}{4}q)\right]\\ +\frac{1}{4}\frac{\mu_0}{\mu'}\gamma^2(x^2+y^2)\pm\bar{\mu}^*\gamma-\frac{2}{r}\end{array} & \frac{\sqrt{3}\,\mu_0}{\bar{\mu}}K_-^2-\frac{\sqrt{3}\,\mu_0}{\mu_\delta}K_+^2\\
0 & -i\frac{\mu_0}{\mu_2}K_+P_z & \frac{\sqrt{3}\,\mu_0}{\bar{\mu}}K_+^2-\frac{\sqrt{3}\,\mu_0}{\mu_\delta}K_-^2 & \begin{array}{l}\frac{\mu_0}{\mu}(P_x^2+P_y^2)+(1-2\mu_0/\mu_1)P_z^2\\ +\gamma\left[\left(\frac{\mu_0}{\mu}-\frac{2\mu_0}{m_h}\right)(xP_y-yP_x)\right.\\ \left.+\frac{\mu_0}{m_0}(3\kappa+\frac{27}{4}q)\right]\\ +\frac{1}{4}\frac{\mu_0}{\mu}\gamma^2(x^2+y^2)\pm\bar{\mu}^*\gamma-\frac{2}{r}\end{array}
\end{array}\right| . \tag{22}$$

In Eq. (22), the ± sign corresponds to the two possible orientations of the conduction-band spin; the operators K_+ and K_- are defined as follows:

$$K_\pm=K_x\pm iK_y . \tag{23}$$

It is important to point out that Eq. (22) contains in all the diagonal elements a term proportional to $L_z\equiv xP_y-yP_x$, which was omitted by Rees.[24] An exact solution of the Schrödinger equation for the Hamiltonian (22) is obviously out of the question. Since we are interested in the high-field region, i.e., $\gamma\gg 1$, we will approach the problem using the adiabatic method. Before considering its application to the case of the complicated band structure, we briefly outline the method as applied in a simple-band case.

It is well known that a free electron in a strong magnetic field tends to move along the field lines and it is confined to a shallow cylinder, whose radius is $\hat{\rho}=\gamma^{-1/2}$. When $\gamma\gg 1$, the localization due to the field is greater than that due to the Coulomb attraction, so that the effect of the latter is mainly in the field direction. One can therefore say that the very rapid x-y motion is insensitive to the presence of the Coulomb field and that the slow z-component motion is determined by a potential which is the average of the Coulomb interaction over the very rapid x-y motion. In the absence of Coulomb interaction the eigenfunctions of the Landau problem are[25]

$$\begin{aligned}\psi_{nl}k_z(x, y, z) &= (2\pi)^{-1/2}\, e^{ik_z z}(N_{nl})^{-1/2} \\ &\quad\times e^{il\phi}\rho^{|l|}\, e^{-(1/4)\gamma\rho^2} L_n^{|l|}(\tfrac{1}{2}\gamma\rho^2) \\ &= (2\pi)^{-1/2}\, e^{ik_z z}\,|n, l\rangle\,. \end{aligned} \tag{24}$$

Here

$$\rho = (x^2 + y^2)^{1/2}, \quad \phi = \tan^{-1}(y/x), \tag{25}$$

$L_n^{|l|}(x)$ is the generalized Laguerre polynomial,[29] and N_{nl} is a normalization constant given by

$$N_{nl} = \frac{\pi(n + |l|)!}{(\frac{1}{2}\gamma)^{|l|+1} n!}\;. \tag{26}$$

Following the physical argument outline above, one replaces $(2\pi)^{-1/2} e^{ik_z z}$ by a function h_{nli} which satisfies a one-dimensional Schrödinger equation whose potential is given by the average of the Coulomb potential over the x-y motion, that is

$$\left(-\frac{d^2}{dz^2} + V_{nl}(z)\right) h_{nli}(z) = E_{nli}\, h_{nli}(z), \tag{27}$$

with

$$V_{nl}(z) = \langle n, l|\frac{-2}{r}|n, l\rangle\;. \tag{28}$$

In the case of degenerate bands, the solution of the Landau problem is known exactly if the small term proportional to μ_δ^{-1} are neglected in the off-diagonal elements of the Hamiltonian (22). In fact, these terms are very small because for all cubic semiconductors with direct exciton spectra the values of $\bar{\gamma} = \frac{1}{2}(\gamma_2 + \gamma_3)$ are very large in comparison to $\delta = \frac{1}{2}(\gamma_3 - \gamma_2)$. In this case the Landau eigenfunctions are conveniently expressed by

$$\Psi_{nlk_z} = \begin{pmatrix} a_1 e^{ik_z z}|n_1, l\rangle \\ a_2 e^{ik_z z}|n_2, l+2\rangle \\ a_3 e^{ik_z z}|n_3, l+1\rangle \\ a_4 e^{ik_z z}|n_4, l+3\rangle \end{pmatrix}, \tag{29}$$

with

$$\sum_{i=1}^{4} |a_i|^2 = (2\pi)^{-1}, \tag{30}$$

and where the four quantum numbers n_1, n_2, n_3, n_4 are expressed in terms of a single quantum number n by simple relations which are listed in Appendix A.

Following the analysis introduced by Rees, the adiabatic method for the degenerate-band case consists of replacing in (29) the plane waves $a_i e^{ik_z z}$ with the functions $h_i(z)$ ($i = 1, 4$), that is, in writing

$$\psi_{nli}(x, y, z) = \begin{pmatrix} h_1(z)|n_1, l\rangle \\ h_2(z)|n_2, l+2\rangle \\ h_3(z)|n_3, l+1\rangle \\ h_4(z)|n_4, l+3\rangle \end{pmatrix}, \tag{31}$$

with the normalization condition

$$\sum_{i=1}^{4} \int |h_i(z)|^2\, dz = 1\,. \tag{32}$$

In Eq. (31) it is understood that, whenever one of the a_i is zero (see Appendix A), the corresponding $h_i(z)$ is also vanishing. Therefore, for any given n and l quantum numbers, there will be as many exciton series as interacting Landau levels.

The functions $h_i(z)$ satisfy a system of coupled differential equations in which the potentials are the average of the Coulomb potential over the x-y motion, that is,

$$\begin{aligned} V_{n_i, l_i}(z) &= \langle n_l, l_i|\frac{-2}{r}|n_i, l_i\rangle \\ &= \frac{-2(n_i!)}{(n_i + |l_i|)!}\int_0^\infty \frac{dr\, r^{|l_i|} e^{-r}[L_{n_i}^{|l_i|}(r)]^2}{(2r/\gamma + z^2)^{1/2}}\;. \end{aligned} \tag{34}$$

In order to investigate the effect of the Hamiltonian (22) on the function (31), we must determine the action of the operators K_+, K_- on the states $|n, l\rangle$:

$$K_+|n, l\rangle = (2\gamma)^{1/2} n^{1/2}|n-1, l+1\rangle, \quad l \geq 0 \tag{35}$$

$$K_+|n, l\rangle = (2\gamma)^{1/2}(n-l)^{1/2}|n, l+1\rangle, \quad l < 0 \tag{36}$$

$$K_-|n, l\rangle = (2\gamma)^{1/2}(n+1)^{1/2}|n+1, l-1\rangle, \quad l > 0 \tag{37}$$

$$K_-|n, l\rangle = (2\gamma)^{1/2}(n-l+1)^{1/2}|n, l-1\rangle, \quad l \leq 0 \tag{38}$$

$$(K_x^2 + K_y^2)|n, l\rangle = \gamma(2n + 2l + 1)|n, l\rangle, \quad l \geq 0 \tag{39}$$

$$(K_x^2 + K_y^2)|n, l\rangle = \gamma(2n + 1)|n, l\rangle, \quad l \leq 0. \tag{40}$$

After straightforward but tedious calculations one obtains the adiabatic Hamiltonians for the z component of the motion, which are different for the various values of the quantum number l. As shown in Sec. III, the only states of interest for optical experiments are those with $l = -3, -2, -1$, or 0. The adiabatic Hamiltonian for $l = 0$ is:

$$\mathcal{H}_{\text{ex}}=\left|\begin{array}{cccc}
\begin{array}{l}\gamma\Big(\frac{2\mu_0}{\mu}(n+\frac{7}{2})-\frac{\mu_0}{m_0}(3\kappa+\frac{27}{4}q)\\ \pm\bar{\mu}^*\Big)+(1-2\mu_0/\mu_1)P_z^2+V_{n_1,0}(z)\end{array} & 2\sqrt{3}\,\gamma\frac{\mu_0}{\bar{\mu}}(n+2)^{1/2}(n+3)^{1/2} & -i(2\gamma)^{1/2}\frac{\mu_0}{\mu_2}(n+3)^{1/2}P_z & 0 \\
2\sqrt{3}\,\gamma\frac{\mu_0}{\bar{\mu}}(n+2)^{1/2}(n+3)^{1/2} & \begin{array}{l}\gamma\Big(\frac{2\mu_0}{\mu'}(n+\frac{7}{2})+\frac{\mu_0}{m_0}(\kappa+\frac{1}{4}q)\\ -4\frac{\mu_0}{m_h'}\pm\bar{\mu}^*\Big)+(1+2\mu_0/\mu_1)P_z^2\\ +V_{n_2,2}(z)\end{array} & 0 & i(2\gamma)^{1/2}\frac{\mu_0}{\mu_2}(n+1)^{1/2}P_z \\
i(2\gamma)^{1/2}\frac{\mu_0}{\mu_2}(n+3)^{1/2}P_z & 0 & \begin{array}{l}\gamma\Big(\frac{2\mu_0}{\mu'}(n+\frac{7}{2})-\frac{\mu_0}{m_0}(\kappa+\frac{1}{4}q)\\ -\frac{2\mu_0}{m_h'}\pm\bar{\mu}^*\Big)+(1+2\mu_0/\mu_1)P_z^2\\ +V_{n_3,1}(z)\end{array} & 2\sqrt{3}\,\gamma\frac{\mu_0}{\bar{\mu}}(n+1)^{1/2}(n+2)^{1/2} \\
0 & -i(2\gamma)^{1/2}\frac{\mu_0}{\mu_2}(n+1)^{1/2}P_z & 2\sqrt{3}\,\frac{\mu_0}{\bar{\mu}}(n+1)^{1/2}(n+2)^{1/2} & \begin{array}{l}\gamma\Big(\frac{2\mu_0}{\mu}(n+\frac{7}{2})+\frac{\mu_0}{m_0}(3\kappa+\frac{27}{4}q)\\ -6\frac{\mu_0}{m_h'}\pm\bar{\mu}^*\Big)\\ +(1-2\mu_0/\mu_1)P_z^2+V_{n_4,3}(z)\end{array}
\end{array}\right| \qquad (41)$$

The adiabatic Hamiltonians for $l=-1,-2,-3$, differ from the Hamiltonian for $l=0$ only in the diagonal elements, the off-diagonal terms being unchanged. We therefore have to specify only the diagonal elements which are:

(a) For $l=-1$:

$$\mathcal{H}_{11}=\gamma\left(\frac{2\mu_0}{\mu}(n+\tfrac{5}{2})-\frac{\mu_0}{m_0}(3\kappa+\tfrac{27}{4}q)+\frac{2\mu_0}{m_h}\pm\bar{\mu}^*\right)+(1-2\mu_0/\mu_1)P_z^2+V_{n_1,-1}(z), \qquad (42)$$

$$\mathcal{H}_{22}=\gamma\left(\frac{2\mu_0}{\mu'}(n+\tfrac{5}{2})+\frac{\mu_0}{m_0}(\kappa+\tfrac{1}{4}q)-\frac{2\mu_0}{m_h'}\pm\bar{\mu}^*\right)+(1+2\mu_0/\mu_1)P_z^2+V_{n_2,1}(z), \qquad (43)$$

$$\mathcal{H}_{33}=\gamma\left(\frac{2\mu_0}{\mu'}(n+\tfrac{5}{2})-\frac{\mu_0}{m_0}(\kappa+\tfrac{1}{4}q)\pm\bar{\mu}^*\right)+(1+2\mu_0/\mu_1)P_z^2+V_{n_3,0}(z), \qquad (44)$$

$$\mathcal{H}_{44}=\gamma\left(\frac{2\mu_0}{\mu}(n+\tfrac{5}{2})+\frac{\mu_0}{m_0}(3\kappa+\tfrac{27}{4}q)-\frac{4\mu_0}{m_h}\pm\bar{\mu}^*\right)+(1-2\mu_0/\mu_1)P_z^2+V_{n_4,2}(z). \qquad (45)$$

(b) For $l=-2$:

$$\mathcal{H}_{11}=\gamma\left(\frac{2\mu_0}{\mu}(n+\tfrac{3}{2})-\frac{\mu_0}{m_0}(3\kappa+\tfrac{27}{4}q)+\frac{4\mu_0}{m_h}\pm\bar{\mu}^*\right)+(1-2\mu_0/\mu_1)P_z^2+V_{n_1,-2}(z), \qquad (46)$$

$$\mathcal{H}_{22}=\gamma\left(\frac{2\mu_0}{\mu'}(n+\tfrac{3}{2})+\frac{\mu_0}{m_0}(\kappa+\tfrac{1}{4}q)\pm\bar{\mu}^*\right)+(1+2\mu_0/\mu_1)P_z^2+V_{n_2,0}(z), \qquad (47)$$

$$\mathcal{H}_{33}=\gamma\left(\frac{2\mu_0}{\mu'}(n+\tfrac{3}{2})-\frac{\mu_0}{m_0}(\kappa+\tfrac{1}{4}q)+\frac{2\mu_0}{m_h'}\right)+(1+2\mu_0/\mu_1)P_z^2+V_{n_3,-1}(z), \qquad (48)$$

$$\mathcal{H}_{44}=\gamma\left(\frac{2\mu_0}{\mu}(n+\tfrac{3}{2})+\frac{\mu_0}{m_0}(3\kappa+\tfrac{27}{4}q)-\frac{2\mu_0}{m_h}\pm\bar{\mu}^*\right)+(1-2\mu_0/\mu_1)P_z^2+V_{n_4,1}(z). \qquad (49)$$

(c) For $l=-3$:

$$\mathcal{H}_{11}=\gamma\left(\frac{2\mu_0}{\mu}(n+\tfrac{1}{2})-\frac{\mu_0}{m_0}(3\kappa+\tfrac{27}{4}q)+\frac{6\mu_0}{m_h}\pm\bar{\mu}^*\right)+(1-2\mu_0/\mu_1)P_z^2+V_{n_1,-3}(z), \qquad (50)$$

$$\mathcal{H}_{22}=\gamma\left(\frac{2\mu_0}{\mu'}(n+\tfrac{1}{2})+\frac{\mu_0}{m_0}(\kappa+\tfrac{1}{4}q)-\frac{2\mu_0}{m_h'}\pm\bar{\mu}^*\right)+(1+2\mu_0/\mu_1)P_z^2+V_{n_2,-1}(z), \qquad (51)$$

$$\mathcal{H}_{33}=\gamma\left(\frac{2\mu_0}{\mu'}(n+\tfrac{1}{2})-\frac{\mu_0}{m_0}(\kappa+\tfrac{1}{4}q)+\frac{4\mu_0}{m_h'}\pm\bar{\mu}^*\right)+(1+2\mu_0/\mu_1)P_z^2+V_{n_3,-2}(z), \qquad (52)$$

$$\mathcal{H}_{44}=\gamma\left(\frac{2\mu_0}{\mu}(n+\tfrac{1}{2})+\frac{\mu_0}{m_0}(3\kappa+\tfrac{27}{4}q)\pm\bar{\mu}^*\right)+(1-2\mu_0/\mu_1)P_z^2+V_{n_4,0}(z). \qquad (53)$$

Equations (42)–(45), (46)–(49), (50)–(53), together with the off-diagonal elements in Eq. (41), allow one to write the adiabatic Hamiltonians for all states of interest, when the magnetic field is parallel to the cubic [001] axis.

The above analysis can be extended to an arbitrary direction of the magnetic field. We now briefly outline this procedure for the case in which $\vec{H}$ is parallel to the [110] direction which is of considerable experimental interest. Let us consider Eq. (3) together with (4) and (5), which provide the Hamiltonian of the problem for an arbitrary direction of the field. When $\vec{H}$ is parallel to [110], it is convenient to choose a new coordinate frame (u, v, w) defined by the transformation:

$$K_x = \frac{1}{\sqrt{2}}(K_w + K_v), \tag{54}$$

$$K_y = \frac{1}{\sqrt{2}}(K_w - K_v), \tag{55}$$

$$K_z = K_u , \tag{56}$$

so that the w direction is along the field. It is easy to show that one gets:

$$\begin{aligned} -\mathcal{H}_h(\vec{\mathrm{K}}) = {} & \frac{\hbar^2}{m_0}\,[(\gamma_1 + \tfrac{5}{2}\gamma_2)\tfrac{1}{2}K^2 - \bar{\gamma}\,(K_u^2 J_u^2 + K_v^2 J_v^2 + K_w^2 J_w^2)] - 2\bar{\gamma}\,(\{K_u, K_v\}\{J_u, J_v\} + \{K_v, K_w\}\{J_v, J_w\} + \{K_w, K_u\}\{J_w, J_u\}) \\ & + \delta[K_u^2 J_u^2 + K_v^2 J_w^2 + K_w^2 J_v^2 + 2(\{K_v, K_w\}\{J_v, J_w\} - \{K_u, K_v\}\{J_u, J_v\} - \{K_u, K_w\}\{J_u, J_w\})] - \frac{e}{c}\kappa H J_w \\ & - \frac{e}{2c}\,qH\,[J_w^3 + J_w J_v^2 + 2J_v\{J_v , J_w\}\,] . \end{aligned} \tag{57}$$

As it was to be expected,[28] Eqs. (57) and (5) are formally identical but for the terms in δ and q. In order to give an explicit expression to (57) we must select a specific representation of the angular-momentum matrices. It is convenient to choose for J_u, J_v, J_w the expressions given for J_x, J_y, J_z, respectively, in Eqs. (7)–(9); this corresponds to a canonical transformation on the Hamiltonian. The explicit expression of (57) thus obtained can be written as the sum of two parts, one not containing δ or q terms which is very similar to (22), except for having different mass parameters; and the second one, which reflects the cubic symmetry of the crystal, and is given by:

$$-\mathcal{H}_h(K) = \left| \begin{array}{cccc} \begin{array}{c} \frac{3}{2}\frac{\mu_0}{\mu_\delta}[K_u^2 + K_w^2 + 3K_v^2] \\ -6\frac{\mu_0}{m_0}q\gamma \end{array} & \begin{array}{c} \frac{\sqrt{3}}{4}\frac{\mu_0}{\mu_\delta}[K_-^2 - 3K_+^2 - 2\{K_+K_-\}] \\ -\frac{3\sqrt{3}}{4}\frac{\mu_0}{m_0}q\gamma \end{array} & -i2\sqrt{3}\frac{\mu_0}{\mu_\delta}K_+K_w & 0 \\ \mathrm{H.c.} & \begin{array}{c} \frac{1}{2}\frac{\mu_0}{\mu_\delta}[7(K_u^2 + K_w^2) + K_v^2] \\ +\frac{5}{2}\frac{\mu_0}{m_0}q\gamma \end{array} & 0 & i2\sqrt{3}\frac{\mu_0}{\mu_\delta}K_+K_w \\ \mathrm{H.c.} & 0 & \begin{array}{c} \frac{1}{2}\frac{\mu_0}{\mu_\delta}[7(K_u^2 + K_w^2) + K_v^2] \\ -\frac{5}{2}\frac{\mu_0}{m_0}q\gamma \end{array} & \begin{array}{c} \frac{\sqrt{3}}{4}\frac{\mu_0}{\mu_\delta}]K_-^2 - 3K_+^2 - 2\{K_+K_-\}] \\ +\frac{3\sqrt{3}}{4}\frac{\mu_0}{m_0}q\gamma \end{array} \\ 0 & \mathrm{H.c.} & \mathrm{H.c.} & \begin{array}{c} \frac{3}{2}\frac{\mu_0}{\mu_\delta}[K_u^2 + K_w^2 + 3K_v^2] \\ +6\frac{\mu_0}{m_0}q\gamma \end{array} \end{array} \right| . \tag{58}$$

In Eq. (58), K_+ and K_- are, in analogy with (23),

$$K_\pm = K_u \pm iK_v . \tag{59}$$

In order to consider the effect of (58), we remind that for all materials of interest, δ is much smaller than $\bar{\gamma}$ and q is very small. Therefore, Eq. (58) can be considered as a perturbation and included to first order. It is important to point out that K_u^2 and K_v^2 appear in the diagonal elements of (58) with different coefficients, so that the diagonal elements of the total Hamiltonian have different mass parameters in front of the K_u^2 and K_v^2 operators. However, a simple rotation by $\frac{1}{4}\pi$ in the u-v plane gives

$$K_u^2 + 3K_v^2 = 2(K_{u'}^2 + K_{v'}^2) + (1/2i)(K_+^2 - K_-^2), \tag{60}$$

$$K_u^2 + K_v^2 = 4(K_{u'}^2 + K_{v'}^2) - (3/2i)(K_+'^2 - K_-'^2) . \tag{61}$$

The first term on the right-hand side of Eqs. (60) and (61) has just the effect of redefining the mass parameters in the diagonal matrix element of $\mathcal{H}_{\mathrm{ex}}$. The eigenstates of the operator so obtained are unaffected by the $\frac{1}{4}\pi$ rotation (except for a phase factor, which, of course, is immaterial). Therefore we use the states $|n, l\rangle$ in terms of unrotated coordinates as our basis set. The second term on the right-hand side of Eqs. (60) and (61) does not contribute to first-order perturbation theory and can therefore be ignored.

The direction w was chosen to be parallel to the external field, so that the corresponding motion component can be decoupled from the motion in the u-v plane by the same adiabatic procedure used for the [001] direction. The method of solution of the adiabatic Hamiltonians for the [001] and [110] directions of the magnetic field will be given in Sec. IV.

III. SELECTION RULES

In Sec. II we obtained the adiabatic Hamiltonians for the exciton states with l ranging from -3 to 0. Clearly these are not all the possible states, but they are the only ones which can be created by one quantum absorption. In fact it is well known[30] that, for an exciton state to be optically allowed, the matrix element

$$\sum_{i=1}^{2}\sum_{j=1}^{4} \psi_{ij}(0)\langle \phi_{c_i}(\vec{r})|\vec{P}+\frac{e}{c}\vec{A}|\phi_{v_j}(\vec{r})\rangle \tag{62}$$

must not vanish. Since the electron-hole exchange interaction has been neglected, the states with conduction-band spin up or down, are uncoupled and (62) reduces to

$$\sum_{j=1}^{4} \psi_{j}(0)\langle \phi_{c_i}(\vec{r})|\vec{P}+\frac{e}{c}\vec{A}|\phi_{v_j}(\vec{r})\rangle \quad (i=1,2). \tag{63}$$

In order for an optical transition to be dipole allowed it is therefore necessary that the jth component of the envelope functions be nonzero at the origin (i.e., $l_j = 0$) and that its correspondent Bloch edge functions be symmetry allowed. Since the four quantum numbers appearing in the envelope function are given by l, $l+2$, $l+1$, and $l+3$, respectively [see Eq. (31)], it is necessary that l be ranging from -3 to 0. Furthermore, for that component of the envelope function with $l_j = 0$, the term in brackets in (62) must be dipole allowed, and this latter requirement specifies the light-polarization condition. The evaluation of $\psi_j(0)$ is easily accomplished by remarking that[29]

$$L_n^{|l_j|}(0) = 1$$

for $l_j = 0$, so that

$$|\psi_j(0)|^2 = |h_j(0)|^2/N_{n_j l_j} .$$

After straightforward considerations, one obtains the selection and intensity rules listed in Table I.

It is useful to recall at this point that in the present analysis we have assumed the same effective-mass Hamiltonian for both diamond and zinc-blende lattices, i.e., we have neglected, for the latter case, the very small linear terms (odd under inversion). This means that the eigenstates have a well-defined parity, so that the over-all exciton envelope function must also have definite parity, since the Bloch edge functions for conduction and valence bands are, respectively, odd and even. Therefore, all components of the envelope function must be of the same parity; for optically allowed states, which are the ones of interest here, each component must be even, because, as shown earlier, one of them must be nonvanishing at the origin.

It is convenient at this point, in order to make the comparison with the results of other authors easier, to establish the connection between our representation, involving the quantum numbers n and l, and the one used in Refs. 4 and 7 and based on one-dimensional harmonic-oscillator wave functions. To this aim, one must remark that the decoupling of the $a^{\pm}$ and $b^{\pm}$ set of levels[4,7] is valid only at $K_z = 0$, and therefore is no longer possible in the presence of the one-dimensional effective Coulomb interaction, when K_z is not a good quantum number. For every n and l value one obtains one, two, three or four exciton series (see Appendix A and Sec. II), which are associated with the Landau edges specified in Table II, in the notation of Refs. 4 and 7. In the table, $c(n)$ ($n = 0, 1, 2, \ldots$) denotes the nth level in the conduction-band ladder with spin up or down.

TABLE I. Selection and intensity rules for optical transitions in the $\sigma_{\pm}$ polarization for Faraday configuration, and in the π polarization in the Voigt configuration. The conduction-band spin characterizing the final state of an allowed transition is given, as well as a relative intensity factor.

	σ_+		σ_-		π	
	Spin	Intensity	Spin	Intensity	Spin	Intensity
$l=0$	$\downarrow$	$\frac{1}{2}\gamma\,|h_1(0)|^2$	Forbidden		Forbidden	
$l=-1$	$\uparrow$	$\frac{1}{6}\gamma\,|h_3(0)|^2$	Forbidden		$\downarrow$	$\frac{2}{3}\gamma\,|h_3(0)|^2$
$l=-2$	Forbidden		$\downarrow$	$\frac{1}{6}\gamma\,|h_2(0)|^2$	$\uparrow$	$\frac{2}{3}\gamma\,|h_3(0)|^2$
$l=-3$	Forbidden		$\uparrow$	$\frac{1}{2}\gamma\,|h_4(0)|^2$	Forbidden	

TABLE II. Correspondence between the notation used in the text and the Landau-level labeling of Ref. 4. The conduction-band ladders are jointly labeled $c(n)$ ($n=0, 1, 2, \cdots$), the $\bar{\mu}^*$ term in Eq. (22) (see text).

l	n	Landau edges
0	−3	$b^+(0)-c(0)$
0	−2	$b^+(1)-c(1)$ $a^+(0)-c(1)$
0	−1	$b^+(2)-c(2)$ $b^-(2)-c(2)$ $a^+(1)-c(2)$
0	0	$b^+(3)-c(3)$ $b^-(3)-c(3)$ $a^+(2)-c(3)$ $a^-(2)-c(3)$
−1	−2	$b^+(1)-c(0)$ $a^+(0)-c(0)$
−1	−1	$b^+(2)-c(1)$ $b^-(2)-c(1)$ $a^+(1)-c(1)$
−1	0	$b^+(3)-c(2)$ $b^-(3)-c(2)$ $a^+(2)-c(2)$ $a^-(2)-c(2)$
−2	−1	$b^+(2)-c(0)$ $b^-(2)-c(0)$ $a^+(1)-c(0)$
−2	0	$b^+(3)-c(1)$ $b^-(3)-c(1)$ $a^+(2)-c(1)$ $a^-(2)-c(1)$
−3	0	$b^+(3)-c(0)$ $b^-(3)-c(0)$ $a^+(2)-c(0)$ $a^-(2)-c(0)$

IV. METHOD OF SOLUTION

In Sec. II the adiabatic Hamiltonians appearing in the one-dimensional Schrödinger equation for the motion along the field were derived. An exact solution of such systems of four coupled differential equations, involving very complicated effective potentials, is clearly out of question. One must therefore resort to numerical methods. We choose to adopt here a method which is of widespread use, for example, in band-structure and molecular calculations; that is, we expand the unknown wave function in terms of a known set of functions. This amounts to transforming the differential problem into a secular determinant for the coefficients of the expansion. The above procedure is exact when the set is complete; in practice, since completeness is achieved only by an infinite set, the use of a finite basis always implies an approximation, which can be made better and better, as the set used is enlarged. The choice of a set of functions is dictated by the physics of the problem and by the simplicity of the Hamiltonian matrix elements. In the present work, we adopt a Gaussian basis set because it conveniently compromises between both features outlined above.

The exciton envelope functions consist of four components, which, as discussed in Sec. III, must be of even parity. This means that the $h_i(z)$ must be even (odd) if l_i is even (odd), so that the expansions are

$$h_i(z)=\sum_{j=1}^{N} c_{ij}\, e^{-\alpha_j z^2} \quad \text{if } l_i \text{ is even}\,, \tag{64}$$

$$h_i(z)=\sum_{j=1}^{N} c_{ij}\, z\, e^{-\alpha_j z^2} \quad \text{if } l_i \text{ is odd}\,. \tag{65}$$

Let us now discuss the choice of the parameters N and α_j ($j=1,\ldots,N$) in Eqs. (64) and (65). The dimension of the basis set N is determined so as to ensure convergence of the eigenvalues and will be discussed in detail later, when numerical results are displayed. The smallest and largest of the α_j's are chosen in such a way as largely to encompass all reasonable values for the extension of the wave function in the z direction; the other α_j's are chosen in geometric progression between the two extreme values. This latter criterion is not critical and any reasonable distribution of the α_j's will be acceptable.

In practice, the problem is reduced to the calculation of the overlap and Hamiltonian matrix elements in the nonorthogonal basis set. Since the basis set includes both even- and odd-parity functions, there are two types of overlap matrix elements; for even functions:

$$S_{ij}^{+}=\int_{-\infty}^{+\infty} dz\, e^{-(\alpha_i+\alpha_j)z^2}=\frac{\sqrt{\pi}}{(\alpha_i+\alpha_j)^{1/2}}\,, \tag{65}$$

and, for odd functions:

$$S_{ij}^{-}=\int_{-\infty}^{+\infty} dz\, z^2\, e^{-(\alpha_i+\alpha_j)z^2}=\frac{\sqrt{\pi}}{2(\alpha_i+\alpha_j)^{3/2}}\,. \tag{66}$$

The matrix elements of the operators appearing in the adiabatic Hamiltonians (except the adiabatic potentials) involve the following integrals:

$$P_{ij}^{+}=-\int_{-\infty}^{+\infty} dz\, e^{-\alpha_i z^2}\frac{d^2}{dz^2}(e^{-\alpha_j z^2})=\frac{2\sqrt{\pi}\,\alpha_i\alpha_j}{(\alpha_i+\alpha_j)^{3/2}}\,, \tag{67}$$

$$P_{ij}^{-}=-\int_{-\infty}^{+\infty} dz\, z\, e^{-\alpha_i z^2}\frac{d^2}{dz^2}(z\, e^{-\alpha_j z^2})=\frac{3\sqrt{\pi}\,\alpha_i\alpha_j}{(\alpha_i+\alpha_j)^{5/2}}\,, \tag{68}$$

$$M_{ij}=\int_{-\infty}^{+\infty} dz\, e^{-\alpha_i z^2}\frac{d}{dz}(z\, e^{-\alpha_j z^2})=\frac{\sqrt{\pi}\,\alpha_i}{(\alpha_i+\alpha_j)^{3/2}}\,. \tag{69}$$

The adiabatic potentials, given by Eq. (34), are very complicated expressions, which, in previous treatments of the problem, were always approximated by simple analytical forms[11] or by numerical interpolation.[15] In the present treatment one needs only the matrix elements of the potentials in the Gaussian basis set. In Appendix B it is shown that, by involved calculations, it is possible to obtain exact analytical expressions for these quantities in terms of elementary functions. It is important to note that, in the present approach we have avoided the difficulties of calculating the adiabatic potentials, because all one needs are their matrix elements and these we calculate exactly in very simple form.

The eigenvalues are obtained by solving, for each l and n, the determinantal equation:

$$\| H_{km} - ES_{km} \| = 0 \quad (k, m = 1, \ldots, 4N) . \tag{70}$$

Here S_{km} is a block diagonal matrix given by

$$S = \begin{pmatrix} S^{\pm}_{ij} & 0 & 0 & 0 \\ 0 & S^{\pm}_{ij} & 0 & 0 \\ 0 & 0 & S^{\mp}_{ij} & 0 \\ 0 & 0 & 0 & S^{\mp}_{ij} \end{pmatrix} \quad (i, j = 1, \ldots, N),$$

where the upper (lower) sign corresponds to even (odd) l. The matrix H_{km} is dependent on l (and also on n); it is obtained by replacing every element of (41) (or the similar adiabatic Hamiltonians for other l's or field directions) by an $N \times N$ matrix, whose entries are given by its matrix elements in the basis set. For convenience we write, as an example, the $l = 0$ matrix for the field along [001] and [110]:

$$H = \begin{vmatrix} \gamma A^{(1)}_n S^{+}_{ij} + B^{(1)} P^{+}_{ij} + V_{n_1, 0; ij} & \gamma C_n S^{+}_{ij} & \gamma^{1/2} D_n M_{ij} & 0 \\ \gamma C_n S^{+}_{ij} & \gamma A^{(2)}_n S^{+}_{ij} + B^{(2)} P^{+}_{ij} + V_{n_2, 2; ij} & 0 & -\gamma^{1/2} D_{n-2} M_{ij} \\ \gamma^{1/2} D_n M_{ji} & 0 & \gamma A^{(3)}_n S^{-}_{ij} + B^{(2)} P^{-}_{ij} + V_{n_3, 1; ij} & \gamma C_{n-1} S^{-}_{ij} \\ 0 & -\gamma^{1/2} D_{n-2} M_{ji} & \gamma C_{n-1} S^{-}_{ij} & \gamma A^{(4)}_n S^{-}_{ij} + B^{(1)} P^{-}_{ij} + V_{n_4, 3; ij} \end{vmatrix} . \tag{71}$$

In Eq. (71), for $\vec{H} \parallel [001]$:

$$A^{(1)}_n = \left(\frac{2\mu_0}{\mu} (n + \tfrac{7}{2}) - \frac{\mu_0}{m_0} (3\kappa + \tfrac{27}{4} q) \pm \bar{\mu}^* \right), \tag{72}$$

$$B^{(1)} = 1 - 2\mu_0 / \mu_1 , \tag{73}$$

$$A^{(2)}_n = \left(\frac{2\mu_0}{\mu'} (n + \tfrac{7}{2}) + \frac{\mu_0}{m_0} (\kappa + \tfrac{1}{4} q) - 4 \frac{\mu_0}{m_h'} \pm \bar{\mu}^* \right), \tag{74}$$

$$A^{(3)}_n = \left(\frac{2\mu_0}{\mu'} (n + \tfrac{7}{2}) - \frac{\mu_0}{m_0} (\kappa + \tfrac{1}{4} q) - \frac{2\mu_0}{m_h'} \pm \bar{\mu}^* \right), \tag{75}$$

$$B^{(2)} = 1 + 2\mu_0 / \mu_1 , \tag{76}$$

$$A^{(4)}_n = \left(\frac{2\mu_0}{\mu} (n + \tfrac{7}{2}) + \frac{\mu_0}{m_0} (3\kappa + \tfrac{27}{4} q) - \frac{6\mu_0}{m_h} \pm \bar{\mu}^* \right), \tag{77}$$

$$C_n = 2\sqrt{3}\, \frac{\mu_0}{\bar{\mu}} (n + 2)^{1/2} (n + 3)^{1/2}, \tag{78}$$

$$D_n = \sqrt{2}\, \frac{\mu_0}{\mu_2} (n + 3)^{1/2} ; \tag{79}$$

and, for $\vec{H} \parallel [110]$:

$$A^{(1)}_n = \left[2\mu_0 \left(\frac{1}{\mu} + \frac{3}{2} \frac{1}{\mu_6} \right) (n + \tfrac{7}{2}) - \frac{\mu_0}{m_0} (3\kappa + \tfrac{51}{4} q) \pm \bar{\mu}^* \right], \tag{80}$$

$$B^{(1)} = 1 - 2\mu_0 \left(\frac{1}{\mu_1} + \frac{3}{2} \frac{1}{\mu_6} \right), \tag{81}$$

$$A^{(2)}_n = \left[2\mu_0 \left(\frac{1}{\mu'} - \frac{3}{2} \frac{1}{\mu_6} \right) + \frac{\mu_0}{m_0} (\kappa + \tfrac{11}{4} q) - 4\mu_0 \left(\frac{1}{m_h'} - \frac{3}{2} \frac{1}{\mu_6} \right) \pm \bar{\mu}^* \right], \tag{82}$$

$$B^{(2)} = 1 + 2\mu_0 \left(\frac{1}{\mu'} + \frac{3}{2} \frac{1}{\mu_6} \right), \tag{83}$$

$$A^{(3)}_n = \left[2\mu_0 \left(\frac{1}{\mu'} - \frac{3}{2} \frac{1}{\mu_6} \right) - \frac{\mu_0}{m_0} (\kappa + \tfrac{11}{4} q) - 2\mu_0 \left(\frac{1}{m_h'} - \frac{3}{2} \frac{1}{\mu_6} \right) \pm \bar{\mu}^* \right], \tag{84}$$

$$A^{(4)}_n = \left[2\mu_0 \left(\frac{1}{\mu} + \frac{3}{2} \frac{1}{\mu_6} \right) + \frac{\mu_0}{m_0} (3\kappa + \tfrac{51}{4} q)$$

$$-6\mu_0\left(\frac{1}{m_h}+\frac{3}{2}\,\frac{1}{\mu_6}\right)\pm\bar{\mu}^*\Bigg], \tag{85}$$

$$C_n=2\sqrt{3}\left(\frac{\mu_0}{\bar{\mu}}+\frac{1}{4}\,\frac{\mu_0}{\mu_6}\right), \tag{86}$$

$$D_n=2\sqrt{6}\,\frac{\mu_0}{\bar{\mu}}(n+3)^{1/2}\,. \tag{87}$$

Similar expressions are easily obtained for all the other values of l.

V. NUMERICAL RESULTS

Before proceeding to the computation of exciton spectra of real semiconductors in a high magnetic field, it is necessary to test the method described in Sec. III in a simpler case, for which numerical results have been obtained in independent investigations. The comparison will determine the convergence and the accuracy of the eigenvalues obtained here, thus allowing a meaningful quantitative comparison of the results with experimental data. This is accomplished by performing a test computation of the exciton levels in the simple hydrogenic model, which has been extensively treated, particularly in the high-field region, by Baldereschi and Bassani.[15] Since in this model every exciton series is associated with a single Landau level, it is convenient to express the results in terms of the binding energy of an exciton with respect to the corresponding Landau edge.

Our first aim is to determine the number N of terms in the expansions (64) and (65) which are necessary to obtain stable and accurate eigenvalues We therefore compute the binding energies of the ground and lower three excited states of the series associated with the $n=0$, $l=0$ Landau edge (Table III). As it was to be expected, the convergence is more rapid for the lowest levels. In fact, the ground and the first excited states are stable, to an accuracy well beyond the experimental resolution, when N is about ten. The higher levels approach stability for larger values of N; in practice $N=15$ represents a convenient choice, since the energy eigenvalues are very accurate and the size of the determinantal equation (70) can be easily handled by any modest computer facility; this is the value that is used to obtain all the results reported hereafter. It is interesting to remark that, before reaching stability, the eigenvalues may not converge monotonically with N. This is not in violation of the variation principle, but is a consequence of the particular criterion used to select the basis set. In fact, going from N to $N+1$ does not simply mean adding a new function to the previous basis set, but corresponds to creating an entirely new set. The amplitude of the resulting oscillations, however, decreases rapidly with N, so that the accuracy of the eigenvalues is not af-

TABLE III. Binding energy (in effective rydbergs) of the ground and lower three excited states of the series $n=0$, $l=0$ of a hydrogenic exciton computed with the present method, with a number N of terms in the expansion (see text). The reduced field γ is equal to 20.

N	E_0	E_1	E_2	E_3
5	4.233 40	0.296 83	0.046 46	−55.440 74
6	4.209 59	0.440 49	0.148 28	−6.0984
7	4.285 16	0.426 87	0.139 57	−0.828 31
8	3.292 53	0.431 96	0.138 54	−0.601 49
9	4.296 83	0.441 85	0.149 92	0.060 81
10	4.298 30	0.443 76	0.157 88	0.078 54
11	3.298 46	0.443 76	0.159 66	0.081 28
12	4.298 60	0.443 86	0.159 77	0.081 53
13	4.298 61	0.444 00	0.159 75	0.081 45
14	4.298 62	0.444 03	0.159 79	0.081 43
15	4.298 62	0.444 03	0.159 84	0.081 47
16	4.298 62	0.444 03	0.159 86	0.081 52
17	4.298 62	0.444 03	0.159 87	0.081 55
18	4.298 62	0.444 03	0.159 88	0.081 57

TABLE IV. Binding energy (in effective rydbergs) of the ground and first excited states of the $n=0$, $l=0$ series of a hydrogenic exciton as a function of the reduced field γ. Second column: theoretical values computed by Baldereschi and Bassani (Ref. 31) with an improved adiabatic scheme. Third column: theoretical values computed in Ref. 31 with the method of Ref. 11. The last column shows the results of the present investigation.

γ	BB	EL	Present calculation
5	2.76 0.384	2.54 0.375	2.57 0.378
10	3.48 0.413	3.31 0.408	3.34 0.411
20	4.42 0.442	4.27 0.439	4.30 0.444
30	5.08 0.461	4.94 0.458	4.97 0.461
40	5.61 0.472	5.47 0.469	5.49 0.474
50	6.05 0.481	5.91 0.478	5.93 0.483
60	6.44 0.488	6.30 0.485	6.31 0.490
70	6.81 0.494	6.64 0.491	6.65 0.497
80	7.14 0.499	6.93 0.496	6.96 0.502
90	7.41 0.503	7.22 0.500	7.24 0.506
100	7.69 0.508	7.48 0.504	7.49 0.510

TABLE V. Binding energy (in effective rydbergs) of the ground states of the $n=0$, 1, 2, and $l=0$ series of hydrogenic exciton as a function of the reduced field γ. In the second column is the theoretical computation by Baldereschi and Bassani (Ref. 31). The last column shows the results of the present investigation.

γ	BB	Present calculation
5	2.76	2.57
	1.77	1.80
	1.43	1.49
10	3.48	3.34
	2.32	2.34
	1.88	1.95
20	4.42	4.30
	2.98	3.04
	2.47	2.53
30	5.08	4.97
	3.49	3.53
	2.86	2.94
40	5.61	5.49
	3.88	3.91
	3.17	3.27
50	6.05	5.93
	4.19	4.24
	3.43	3.55
60	6.44	6.31
	4.47	4.52
	3.58	3.79
70	6.81	6.65
	4.72	4.77
	3.88	4.01
80	7.14	6.96
	4.94	5.00
	4.08	4.20
90	7.41	7.24
	5.09	5.21
	4.25	4.38
100	7.69	7.49
	5.29	5.40
	4.41	4.54

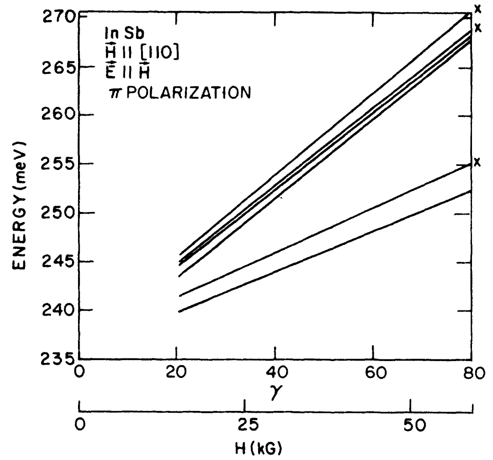

FIG. 1. Energy of the ground and first excited states of the lowest three exciton series of InSb allowed in the π polarization, as a function of the magnetic field. Here the gap is 235 eV and the band parameters are from Ref. 34. The X labels indicate excited states.

fected.

Let us now compare the numerical results for the hydrogenic excitons obtained by the present method with those of other investigators. In Table IV, the results of Baldereschi and Bassani[31] obtained with an improved adiabatic method[15] and with the method of Elliott and Loudon are reproduced. It is clear, by comparing the last two columns, that the present results, obtained without approximating the adiabatic potentials, are more accurate than those obtained using the method of Elliott and Loudon. The results shown in column II are obtained by including the effect of higher Landau levels.[15] A comparison with the last column shows, however, that the extra effect due to this coupling improves the ground-state energies by only a few percent, and is negligible for excited states. In Table V the same conclusion is shown to hold for

TABLE VI. Experimental and theoretical transition energies for InSb, $H=39.1$ kG, $\vec{H} \parallel [110]$, π polarization. All energies are in meV. In the first column the experimental results of Ref. 19 are given; in the second the relative exciton states are labeled by the quantum numbers n and l, the order number of the exciton series for given n and l, the number of the exciton level within the series, and the orientation of the conduction-band spin. Theoretical energy levels are computed with $E_g = 235$ meV and band parameters of: (a) Ref. 34, (b) Ref. 7, (c) Ref. 35, (d) Ref. 33. Theoretical intensities in the last column are in arbitrary units.

Expt. energies	Assignment $(n, l, k, i, \text{spin})$	Theor. energies (*a*)	Theor. energies (*b*)	Theor. energies (c)	Theor. energies (d)	Theor. intensity
244.5	$(-1, -2, 1, 1, \uparrow)$	244.5	244.6	244.8	244.4	1.02
246.3	$(-1, -2, 1, 2, \uparrow)$	246.8	246.9	247.1	246.8	0.022
247.3	$(-1, -2, 1, 3, \uparrow)$	247.0	247.1	247.3	247.0	0.002
254.2	$(-2, -1, 1, 1, \downarrow)$	254.6	255.0	256.0	255.0	1.31
255.5	$(-1, -2, 2, 1, \uparrow)$	255.6	254.5	253.0	255.0	0.001
257.5	$(-2, -1, 1, 2, \downarrow)$	257.2	257.6	257.6	257.6	0.03

TABLE VII. Comparison of the present theory with the data of Ref. 19 for Ge, $H = 72$ kG, $\vec{H} \parallel [110]$ and π polarization. The notation for the exciton levels is the same as in Table VI, and the Landau edges contributing to the exciton series are given in the notation of Roth *et al.*, **Ref.** 4. The value of the energy gap is 889 meV.

Level $(n, l, k, i, \text{spin})$	Landau edges	Theoretical intensities (arbitrary units)	Energy (meV)	Expt. (meV)
$(-1, -2, 1, 1, \uparrow)$	$b^+(2)c^+(0)$ $b^-(2)c^+(0)$ $a^+(1)c^+(0)$	0.71	896.2	896.0
$(-2, -1, 1, 1, \downarrow)$	$b^+(1)c^-(0)$ $a^+(0)c^-(0)$	0.84	897.3	897.5
$(-1, -2, 1, 2, \uparrow)$	$b^+(2)c^+(0)$ $b^-(2)c^+(0)$ $a^+(1)c^+(0)$	0.02	900.3	900.5
$(-2, -1, 1, 2, \downarrow)$	$b^+(1)c^-(0)$ $a^+(0)c^-(0)$	0.03	901.7	901.5
$(-1, -2, 2, 1, \uparrow)$	$b^+(2)c^+(0)$ $b^-(2)c^+(0)$ $a^+(1)c^+(0)$	0.01	906.7	905.7
$(-1, -2, 2, 2, \uparrow)$	$b^+(2)c^+(0)$ $b^-(2)c^+(0)$ $a^+(1)c^+(0)$	0.002	907.4	907.0

excitons originating from higher Landau levels.

The preceding analysis has shown that it is possible to obtain very accurate eigenvalues, and we therefore proceed to investigate exciton levels of real semiconductors. Our attention will be focused on those materials for which detailed experimental information is available, such as InSb[19] and Ge,[19] or for which there has been recent experimental interest.[22]

For InSb, several sets of band parameters have been obtained from the interpretation of different experiments[32] or from theoretical calculations.[33] The use of the various sets of parameters obviously leads to different theoretical exciton spectra, and their comparison with the high-resolution data of Johnson[19] is very useful in providing a good criterion of discrimination among them. In practice, the relative position of two of the observed peaks is critically dependent on the valence-band parameters and only the set of parameters given by Zwerdling *et al.*[34] reproduces the order and the energy splitting of the observed structures. In Table VI, the theoretical spectrum obtained using these parameters is compared with the experimental data by Johnson at $H = 39$ kG, $\vec{H} \parallel [110]$, and π polarization. The results obtained with alternative sets of parameters are also listed to illustrate the argument given above concerning the relative position of the $(-2, -1, 1, 1, \downarrow)$ and $(-1, -2, 2, 1, \uparrow)$ levels. It is important to notice that the assignment of these two structures is quite unambiguous since their intensities are very different. The over-all correspondence between the calculated and the observed spectra is good, except for the relative positions and intensities of the second and third peaks, for which the assignment is not as unambiguous as that of the remaining structure. The agreement between theory and experiment can be very likely improved by fitting the band parameters to the present data rather than using the sets independently proposed by other investigators. In Fig. 1 the fan chart for InSb, with $\vec{H} \parallel [110]$ showing the ground and first excited states of the three lowest series allowed in the π polarization, computed using the parameters of Ref. 34, is displayed.

Another semiconductor for which detailed experimental data are available is germanium.[19] This is one of the most widely investigated materials, and very accurate valence-band parameters were determined by cyclotron resonance.[36] In a recent letter,[26] it was shown that the agreement between theory and experiment is good. The comparison for $H = 72$ kG, $\vec{H} \parallel [110]$, and π polarization is reproduced in Table VII. In Figs. 2 and 3, the ground and first excited states for the two lowest exciton series allowed in σ_+ and σ_- polarization, respectively, are plotted as a function of the magnetic field.

It is interesting to consider, besides the eigenvalues, the behavior of the envelope functions of the exciton states, since they contain information about the intensity of the transitions (see Table I),

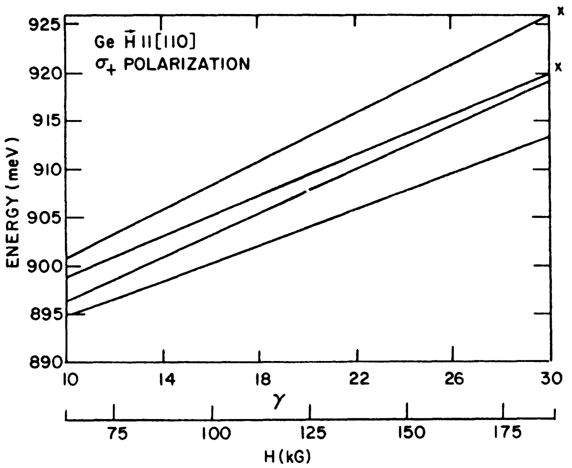

FIG. 2. Energy of the ground and first excited states of the lowest two exciton series of Ge in σ_+ polarization as a function of the magnetic field. Here the gap is 889 meV and the X labels excited states.

the extension of the wave functions in the direction of the field, and the amount of mixing between the four band-edge functions in the exciton state. In Fig. 4 the $h_i(z)$ components of the envelope functions for the ground state of the lowest $l=-2$ series are shown. Note that, as expected, the localization increases with increasing magnetic field.

Very recently, the exciton states of GaAs in low and intermediate magnetic fields were investigated by Dingle.[22] An interesting motivation for the investigation of this material is the disagreement of various experimental and theoretical determinations of the valence-band parameters, and particularly

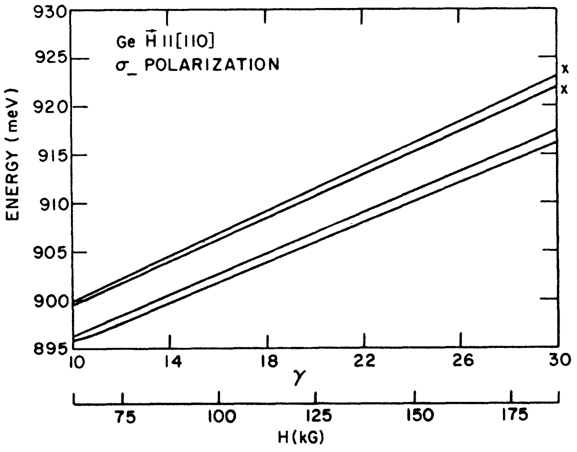

FIG. 3. Energy of the ground and first excited states of the lowest two exciton series of Ge in the σ_- polarization as a function of the magnetic field. Here the gap is 889 meV and the X labels excited states.

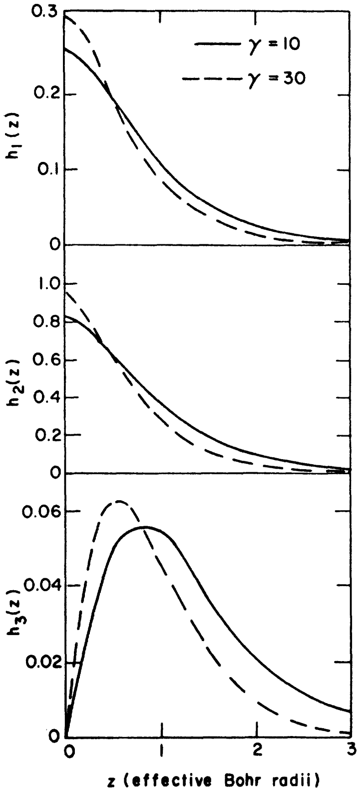

FIG. 4. z-dependent components $h_i(z)$ ($i=1,2,3$) of the ground state of the lowest $l=-2$, $n=-1$ exciton series in germanium for two values of the magnetic field. z is in effective Bohr radii. Notice the different ordinate scale.

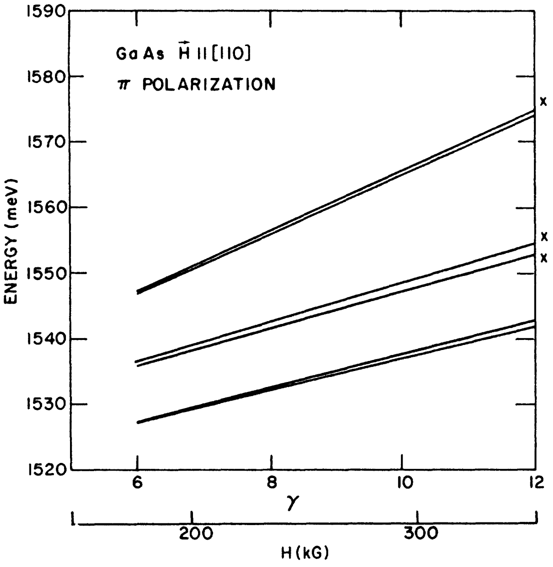

FIG. 5. "Fan" chart of the ground and first excited states of the three lowest exciton series of GaAs allowed in the π polarization. The gap is 1520 meV and the band parameters are those of Ref. 33. X labels the excited states.

of the parameter κ.[2] In Fig. 5 a fan chart for states allowed in the π polarization is shown, using the theoretical parameters of Ref. 33. The extension of experimental measurement to higher fields would indeed provide additional information very useful for a more precise determination of band parameters.

VI. SUMMARY AND CONCLUSIONS

In the present paper we have described a simple method suitable for the computation of extensive excitonic spectra of diamond and zinc-blende semiconductors in a high magnetic field, taking into full account the degeneracy and anisotropy of the valence bands. The adiabatic approach has been used to decouple the motion components parallel and perpendicular to the magnetic field, and no further approximations have been introduced in the theory. The matrix elements of the adiabatic potentials have been calculated analytically and expressed in terms of elementary functions. The method is therefore a simple and accurate procedure to obtain extensive exciton spectra in the high-field region and to analyze magnetoabsorption data of semiconductors.

The comparison of the present theory with the high-resolution data in Ge has shown that, when the band parameters are known with good accuracy, the computed transition energies and intensities are in good agreement with experiment. This suggests that, for other materials, the comparison of experiment with spectra computed with different sets of band parameters can be useful in discriminating among them, and the discussion of the data for InSb has proven that this is indeed the case.

Since the present results are encouraging, it is worthwhile to point out possible lines of future applications and progress. The main motivation for this work was to provide a detailed analysis of magnetoabsorption experiments useful in providing a more accurate determination of band parameters. In the future the method, used in connection with accurate experimental data, could be applied as a best fitting procedure, rather than simply as a test on independently obtained sets of parameters.

The theoretical analysis described above was formulated for diamond and zinc-blende semiconductors whose bands were described in the Kohn-Luttinger scheme.[5] In some narrow-gap materials it may be important to include more correctly the coupling between valence and conduction bands; a good starting point could be the Landau-level theory of Pidgeon and Brown.[7] Furthermore, the investigation of semiconductors with different crystal structures can be approached with essentially the same technique after modifying the symmetry of the effective-mass Hamiltonian.

ACKNOWLEDGMENTS

The authors are indebted to Professor A. Baldereschi for illuminating discussions and for providing them with unpublished results. They are also grateful to Professor D. L. Dexter for discussions and for a critical reading of the manuscript; one of them (M.A.) is indebted to Professor Dexter for his continuing encouragement and support.

APPENDIX A

The relations between the four quantum numbers n_1, n_2, n_3, and n_4 can be obtained from the Hamiltonian

$$\mathcal{H} = \mathcal{H}_e\left(\vec{p} - \frac{e}{c}\vec{A}\right) - \mathcal{H}_h\left(-\vec{p} - \frac{e}{c}\vec{A}\right), \tag{A1.1}$$

where $\mathcal{H}_e$ and $\mathcal{H}_h$ are defined in the text, Eqs. (4) and (5). Using Eqs. (35)–(40), it is easily seen that the quantum numbers and the coefficients a_i satisfy the following relations:

(i) If $l=0$:

$$\begin{aligned} n_1 &= n+3, \\ n_2 &= n+1, \\ n_3 &= n+2, \\ n_4 &= n, \end{aligned} \tag{A1.2}$$

where

(a) $n=-3$ and $a_2=a_3=a_4=0$, or

(b) $n=-2$ and $a_2=a_4=0$, or

(c) $n=-1$ and $a_4=0$, or

(d) $n=0, 1, 2, \ldots$.

(ii) If $l=-1$:

$$\begin{aligned} n_1 &= n+2, \\ n_2 &= n+1, \\ n_3 &= n+2, \\ n_4 &= n, \end{aligned} \tag{A1.3}$$

where

(a) $n=-2$ and $a_2=a_4=0$, or

(b) $n=-1$ and $a_4=0$, or

(c) $n=0, 1, 2, \ldots$.

(iii) If $l=-2$:

$$\begin{aligned} n_1 &= n+1 \\ n_2 &= n+1 \\ n_3 &= n+1 \end{aligned} \tag{A1.4}$$

$n_4 = n$

where

(a) $n = -1$ and $a_4 = 0$, or

(b) $n = 0, 1, 2, \ldots$.

(iv) If $l = -3$:

$n_1 = n_2 = n_3 = n_4 = n$,

where

$$n = 0,\ 1,\ 2, \ldots . \tag{A1.5}$$

APPENDIX B: MATRIX ELEMENTS OF THE ADIABATIC POTENTIALS

The adiabatic potential $V_{nl}(z)$ defined by Eq. (33), is given by

$$V_{nl}(z) = -2\,\frac{n!}{(n+|l|)!}\int_0^\infty d\rho\{\rho^{|l|}\,e^{-\rho}[L_n^{|l|}(\rho)]^2 \times 1/[2\rho/\gamma + z^2]^{1/2}\} . \tag{B2.1}$$

We are interested in the matrix elements of the adiabatic potentials between functions of the Gaussian basis set. These matrix elements are of two different types according to the parity of l, i.e.,

$$[V_{n,l}]_{ij} = \int_{-\infty}^{\infty} e^{-\alpha_i z^2}\, V_{n,l}(z)\, e^{-\alpha_j z^2}\, dz \quad \text{if } l \text{ is even,} \tag{B2.2}$$

and

$$[V_{n,l}]_{ij} = \int_{-\infty}^{\infty} z\, e^{-\alpha_i z^2}\, V_{n,l}(z) z\, e^{-\alpha_j z^2}\, dz \quad \text{if } l \text{ is odd.} \tag{B2.2$'$}$$

Let us consider first the even l matrix element (B2.2). Substituting (B2.1) into (B2.2) and inverting the order of the integrations over ρ and z, one obtains:

$$[V_{nl}]_{ij} = -2\,\frac{n!}{(n+|l|)!}\int_0^\infty d\rho\,\rho^{|l|}\,e^{-\rho}[L_n^{|l|}(\rho)]^2 \times \int_{-\infty}^{+\infty} dz\,\frac{e^{-(\alpha_i+\alpha_j)z^2}}{(2\rho/\gamma + z^2)^{1/2}} . \tag{B2.3}$$

The integral over z gives[37]

$$\int_{-\infty}^{\infty} dz\,\frac{e^{-(\alpha_i+\alpha_j)z^2}}{[2\rho/\gamma + z^2]^{1/2}} = e^{a\rho}\,K_0(a\rho) , \tag{B2.4}$$

where

$$a = (\alpha_i + \alpha_j)/\gamma \tag{B2.5}$$

and K_0 is a modified Bessel function. Equation (B2.3) then becomes

$$[V_{nl}]_{ij} = -2\,\frac{n!}{(n+|l|)!}\int_0^\infty d\rho\, e^{-s\rho}\rho^{|l|}\,L_n^{|l|}(\rho) K_0(a\rho) , \tag{B2.6}$$

where

$s = 1 - a$,

so that the calculation of the matrix elements (B2.2) reduces to the evaluation of the Laplace transform of the product of a polynomial and the modified Bessel function K_0. Therefore all the matrix elements (B2.2) can be expressed in terms of integrals of the type

$$I_m = \int_0^\infty d\rho\, e^{-s\rho}\rho^m K_0(a\rho) , \tag{B2.7}$$

which can be written in terms of a single hypergeometric function[37]

$$I_n = \left(\frac{\pi}{2a}\right)^{1/2} \frac{n!}{\Gamma(n+\frac{3}{2})} F(\tfrac{1}{2}, \tfrac{1}{2}; n+\tfrac{3}{2}; \tfrac{1}{2}(1 - s/a)) . \tag{B2.7$'$}$$

where Γ is Euler's Γ function. For $n = 0$ (B2.7′) reduces to an elementary function since[29]

$$F(\tfrac{1}{2}, \tfrac{1}{2}; \tfrac{3}{2}; \tfrac{1}{2}(1 - s/a)) = \begin{cases} \dfrac{\arcsin[\frac{1}{2}(1 - s/a)]^{1/2}}{[\frac{1}{2}(1 - s/a)]^{1/2}} , & |s| < a \\[2ex] \dfrac{\ln\{[\frac{1}{2}(s/a - 1)]^{1/2} + [\frac{1}{2}(s/a + 1)]^{1/2}\}}{[\frac{1}{2}(s/a - 1)]^{1/2}} , & |s| > a . \end{cases} \tag{B2.8}$$

For $n \neq 0$, the following recursion relation applies:

$$F(\tfrac{1}{2}, \tfrac{1}{2}; n+\tfrac{3}{2}; \tfrac{1}{2}x) = \frac{4n^2 - 1}{4n^2 x}[(1 - x)F(\tfrac{1}{2}, \tfrac{1}{2}; n - \tfrac{1}{2}; x) + (2x - 1)F(\tfrac{1}{2}, \tfrac{1}{2}; n + \tfrac{1}{2}; x)] . \tag{B2.9}$$

Furthermore, the following relation holds

$$F(\tfrac{1}{2}, \tfrac{1}{2}; \tfrac{1}{2}; \tfrac{1}{2}(1 - s/a)) = [\tfrac{1}{2}(1 + s/a)]^{-1/2} . \tag{B2.10}$$

Equation (B2.9) together with Eqs. (B2.8) and (B2.10) allows one to express all I_n's in terms of elementary functions. After lengthy calculations one finds:

$$[V_{00}]_{ij} = -2I_0 , \tag{B2.11a}$$

$$[V_{10}]_{ij} = -2I_0 - 4I_1 - 2I_2 , \tag{B2.11b}$$

$$[V_{20}]_{ij} = -2I_0 + 8I_1 - 10I_2 + 4I_3 - \tfrac{1}{2}I_4 , \tag{B2.11c}$$

$$[V_{30}]_{ij} = -2I_0 + 12I_1 - 24I_2 + \tfrac{56}{3}I_3 - \tfrac{13}{2}I_4 + I_5 - \tfrac{1}{18}I_6 , \tag{B2.11d}$$

$$[V_{02}]_{ij} = -I_2 , \tag{B2.11e}$$

$$[V_{12}]_{ij} = -3I_2 + 2I_3 - \tfrac{1}{3}I_4 . \tag{B2.11f}$$

The matrix elements (B2.2′) involve an integral over z which is easily shown to be[37]

$$\int_{-\infty}^{\infty} dz\, z^2 \frac{e^{-(\alpha_i+\alpha_j)z^2}}{[2\rho/\gamma + z^2]^{1/2}} = \frac{\rho}{\gamma} e^{-a\rho}[K_1(a\rho) - K_0(a\rho)] . \tag{B2.12}$$

In analogy to the procedure used for even l's, the matrix elements (B2.2′) can be expanded in terms of integrals of the type

$$J_m = \int_0^{\infty} d\rho\, e^{-s\rho} \rho^m [K_1(a\rho) - K_0(a\rho)] , \tag{B2.13}$$

where $m \geqslant 2$. We then obtain

$$J_m = \left(\frac{\pi}{2a}\right)^{1/2} \frac{(m!)^2}{\Gamma(m+\frac{3}{2})} \left(\frac{m+1}{m} F(-\tfrac{1}{2}, \tfrac{3}{2}; m+\tfrac{3}{2}; \tfrac{1}{2}(1-s/a)) - F(\tfrac{1}{2}, \tfrac{1}{2}; m+\tfrac{3}{2}; \tfrac{1}{2}(1-s/a))\right) . \tag{B2.14}$$

The hypergeometric function $F(\frac{1}{2}, \frac{1}{2}; m+\frac{3}{2}; \frac{1}{2}(1-s/a))$ has been already reduced to elementary functions in the treatment of the even l's. The following recursion relation holds[29]:

$$F(-\tfrac{1}{2}, \tfrac{3}{2}; m+\tfrac{3}{2}; x) = \frac{4m^2-1}{4(m^2-1)x} [(1-x)F(-\tfrac{1}{2}, \tfrac{3}{2}; m-\tfrac{1}{2}; x) + (2x-1)F(-\tfrac{1}{2}, \tfrac{3}{2}; m+\tfrac{1}{2}; x)] . \tag{B2.15}$$

For the $m=2$ case, (B2.15) involves

$$F(-\tfrac{1}{2}, \tfrac{3}{2}; \tfrac{5}{2}; x) = (3/4x)[\tfrac{1}{2}F(\tfrac{1}{2}, \tfrac{1}{2}; \tfrac{3}{2}; x) + \tfrac{1}{2}(1-x)F(\tfrac{1}{2}, \tfrac{3}{2}; \tfrac{3}{2}; x) - (1-x)F(-\tfrac{1}{2}, \tfrac{3}{2}; \tfrac{3}{2}; x)] . \tag{B2.16}$$

It can be shown that[29]

$$F(\pm\tfrac{1}{2}, \tfrac{3}{2}; \tfrac{3}{2}; x) = (1-x)^{\mp 1/2} . \tag{B2.17}$$

Expression (B2.15), together with (B2.16), (B2.17), and (B2.8) allows one to express all J_m's in terms of elementary functions. After lengthy calculations one finds

$$[V_{01}]_{ij} = -\frac{2}{\gamma} J_2 , \tag{B2.18a}$$

$$[V_{11}]_{ij} = \frac{-1}{\gamma}(4J_2 - 4J_3 + J_4), \tag{B2.18b}$$

$$[V_{21}]_{ij} = \frac{-1}{\gamma}(6J_2 - 12J_3 + 8J_4 - 2J_5 + \tfrac{1}{6}J_6) , \tag{B2.18c}$$

$$[V_{03}]_{ij} = \frac{-1}{3\gamma} J_4 . \tag{B2.18d}$$

---

*Supported by USAF-Aerospace Research Laboratory.

†Present address: Dept. of Physics, University of Illinois, Urbana, Ill. 61801.

[1] See, for example, J. G. Mavroides, in *Optical Properties of Solids*, edited by F. Abelès (North-Holland, Amsterdam, 1972).

[2] R. G. Aggarwal, in *Semiconductors and Semimetals*, edited by R. K. Willardson and A. C. Beer (Academic, New York, 1972), Vol. 9, p. 151, and references therein.

[3] B. P. Zakharchenya and R. P. Seisyan, Usp. Fiz. Nauk 97, 193 (1969) [Sov. Phys.-Uspekhi 12, 70 (1969)].

[4] L. M. Roth, B. Lax, and S. Zwerdling, Phys. Rev. 114, 90 (1959).

[5] W. Kohn and J. M. Luttinger, Phys. Rev. 96, 529 (1954); J. M. Luttinger and W. Kohn, Phys. Rev. 97, 869 (1955); J. M. Luttinger, Phys. Rev. 102, 1030 (1956).

[6] R. R. Goodman, Phys. Rev. 122, 397 (1961).

[7] C. R. Pidgeon and R. N. Brown, Phys. Rev. 146, 575 (1966).

[8] E. Kazmarek, Phys. Rev. 132, 1929 (1963).

[9] B. P. Zakharchenya and R. P. Seisyan, Usp. Fiz. Nauk 97, 193 (1969) [Sov. Phys.-Uspekhi 12, 70 (1969)], and references therein.

[10] D. F. Edwards and V. J. Lazazzera, Phys. Rev. 120, 420 (1960).

[11] R. J. Elliott and R. Loudon, J. Phys. Chem. Solids 8, 382 (1959); J. Phys. Chem. Solids 15, 196 (1960).

[12] A. G. Zhilich and B. S. Monozon, Fiz. Tverd. Tela 8, 3559 (1966) [Sov. Phys.-Solid State 8, 2846 (1967)].

[13] D. M. Larsen, J. Phys. Chem. Solids 29, 271 (1968).

[14] E. P. Pokatilov and M. M. Rusanov, Fiz. Tverd. Tela 10, 3117 (1968) [Sov. Phys.-Solid State 10, 2458 (1969)].

[15] A. Baldereschi and F. Bassani, in *Proceedings of the Tenth International Conference on the Physics of Semiconductors, Cambridge, Mass.*, 1970, edited by S. P. Keller, J. C. Hensel, and F. Stern CONF-700801 (U. S. AEC Division of Technical Information, Springfield, Va., 1970), p. 191.

[16] D. Cabib, E. Fabri, and G. Fiorio, Nuovo Cimento B 10, 185 (1972).

[17] See also H. Hasegawa, in *Physics of Solids in Intense Magnetic Fields*, edited by E. D. Haidemenakis (Plenum, New York, 1969), p. 246.

[18] E. J. Johnson and H. Y. Fan, Phys. Rev. 139, A1991 (1965).

[19] E. J. Johnson, Phys. Rev. Lett. 19, 352 (1967); and in *Proceedings of the Ninth International Conference on the Physics of Semiconductors, Moscow*, 1968 (VINITI, Leningrad, 1968).

[20] M. Altarelli and N. O. Lipari, Phys. Rev. B 7, 3798 (1973).

[21] L. I. Schiff and H. Snyder, Phys. Rev. 55, 59 (1939).

[22] R. Dingle, Bull. Am. Phys. Soc. 18, 437 (1973); and private communication.

[23] A. G. Zhilich, Fiz. Tver. Tela 13, 2883 (1971) [Sov. Phys.-Solid State 13, 2425 (1972)].

[24] G. J. Rees, J. Phys. C 4, 2822 (1971).

[25] G. J. Rees, J. Phys. C 5, 549 (1972).

[26] N. O. Lipari and M. Altarelli, Solid State Commun. 13, 1791 (1973).

[27] J. O. Dimmock, in Ref. 2, Vol. 3, p. 259.

[28] J. M. Luttinger, Phys. Rev. 102, 1030 (1956).

[29] W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Springer-Verlag, Berlin, 1966).

[30] R. J. Elliott, Phys. Rev. 108, 1384 (1957).

[31] See Ref. 15; and A. Baldereschi (private communication).

[32] See J. G. Mavroides, Ref. 1.

[33] P. Lawaetz, Phys. Rev. B 4, 3460 (1971).

[34] S. Zwerdling, W. H. Kleiner, and J. P. Theriault, J. Appl. Phys. Suppl. 32, 2118 (1961); and in *Proceedings of the International Conference on the Physics of Semiconductors, Exeter*, 1962 (The Institute of Physics, London, 1962), p. 455.

[35] D. N. S. Bagguley, N. L. A. Robinson, and R. A. Stradling, Phys. Lett. 6, 143 (1963).

[36] J. C. Hensel and K. Suzuki, Phys. Rev. Lett. 22, 838 (1969).

[37] A. Erdélyi, W. Magnus, F. Oberhettinger, and F. Tricomi, *Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. I.