Excited states of donors in quantum wells in a magnetic field

David M. Larsen
Department of Physics and Applied Physics, University of Lowell, Lowell, Massachusetts 01854
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Calculations of energy levels of a hydrogenic donor in the center of a quantum well show that, although the energy of the lowest-lying state of each symmetry tunes with the magnetic field much like its bulk counterpart, energies of the excited states in the well and in bulk have entirely dissimilar behaviors. Plots of energy versus magnetic field for these former states show a Landau-level fanlike structure starting near the lowest or first excited subband energy but interrupted by anticrossings with fans originating from alternating higher subbands. One interesting consequence is that certain states (the $2s$ and $2p_{+1}$ levels, for example), which in bulk become widely separated in energy with increasing magnetic field, may remain close together over a wide range of fields in quantum wells.

INTRODUCTION

Recent experimental advances have stimulated interest in the excited states of shallow donors in quantum wells. Since the initial magnetospectroscopic study of Jarosik *et al.*[1] on the "$1s$-$2p_{+1}$" transition for shallow donors in quantum wells, improvements in sample quality and experimental sensitivity have revealed a number of much weaker transitions,[2,3] which have been attributed to final states of higher energy than $2p_{+1}$. Very recently anticrossings involving the $2p_{+1}$ and $2p_0$ levels have been observed in magnetic fields which are tipped away from the normal to the quantum-well planes.[4] These latter experiments suggest that the strong $1s \rightarrow 2p_{+1}$ absorption line can be used as a probe to explore higher excited states of the well donors, states to which transitions from the ground state may be parity forbidden in fields normal to the well planes. In general one expects that n-doped molecular-beam epitaxy GaAs will have significant compensation and that therefore there will be internal random electric fields throughout the quantum-well samples, arising from donor and acceptor ions present in the wells. Such fields produce Stark shifts of neutral donor levels, broadening the spectral transitions. It is necessary to know the energy levels and wave functions of the excited states, especially those in close proximity to the $2p_{+1}$, if one wishes to understand fully the spectral line shapes observed in magnetic fields. For all these reasons it is of interest to develop a scheme for practical calculations of the magnetic-field dependence of excited-state levels for donors in a quantum well. Such a scheme is presented in this paper.

Let us begin with the simplest possible model for a donor in a quantum well in the presence of a magnetic field. We take the quantum well to be a square well with infinite walls, place the donor at its center, and assume that the magnetic field points normal to the plane of the well. In this model all states can be labeled by the quantum number M for the component of orbital angular momentum along the magnetic field, and by a parity quantum number P_z, which is $+1$ if the wave function does not change sign upon the reflection carrying z into $-z$ and -1 otherwise. We employ the effective-mass Hamiltonian

$$H=-\nabla^2-\frac{2}{r}+\frac{\gamma}{i}\left[x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right]+\tfrac{1}{4}\gamma^2\rho^2+V(z)\ , \qquad V(z)=0 \ \text{ for } |z|<L/2, \quad V(z)=\infty \ \text{ for } |z|>L/2\ , \tag{1}$$

where $r=(\rho^2+z^2)^{1/2}$, and all lengths and energies are taken in units of the bulk donor Bohr radius, a_0, and rydberg, $\mathcal{R}$, respectively, where $a_0=\hbar^2\epsilon_0/m^*e^2$, $\mathcal{R}=\hbar^2/2m^*a_0^2=e^2/2\epsilon_0 a_0$, m^* is the bulk electron conduction-band mass, and ϵ_0 is the bulk static dielectric constant. The magnetic field in (1) is contained in the dimensionless constant γ, where $\gamma=\hbar\omega_c/2\mathcal{R}$ and $\omega_c=eB/m^*c$ is the bulk cyclotron resonance frequency.

Consider the case in which both the subband splittings and the Landau-level splittings are not small compared to $\mathcal{R}$. Then one might expect that a useful basis set for expanding eigenfunctions of H would be the eigenstates of (1) with the Coulomb term set equal to zero. For $P_z=+1$ these are product states of the form

$$\Psi_{N,M,n}=L_N^M(\xi)\exp(-\xi^2/2)\cos(k_n z)\exp(-iM\phi) \tag{2}$$

with unperturbed energies

$$E_{N,M,n}=(2N+1)\gamma+k_n^2\ . \tag{3}$$

In (2) L_N^M is an associated Laguerre polynomial,[5] $\xi^2=0.5\gamma\rho^2$, and $k_n=n\pi/L$ with n an odd integer. [For $P_z=-1$ one replaces the cosine by the sine function in (2) and allows only even values of n.] The lowest-order eigenvalues of H in the wave functions of (2) can be found by taking expectation values of (1) in those wave functions. Figure 1 shows the unperturbed spectrum obtained in this way for levels with $M=0$ and $P_z=+1$ using a well of width $L=6$ (in units of a_0). Qualitatively similar spectra are obtained for other values of M and P_z. Energies in Fig. 1 and elsewhere in this paper are measured relative to E_{free}, the lowest energy level of a free electron in the quantum well, given by

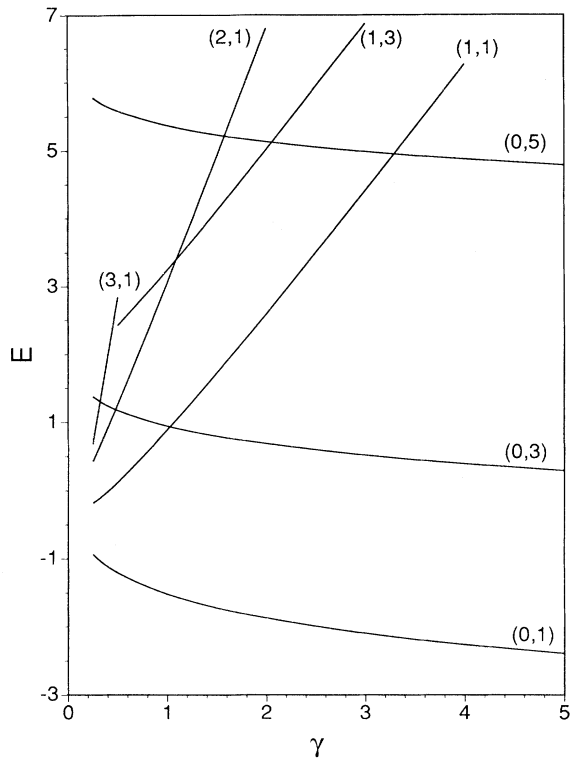

FIG. 1. Magnetic-field dependence of diagonal matrix elements of H defined by Eq. (1) in basis states of the form given by Eq. (2) with $\mathcal{H}$ in Eq. (5) taken equal to 0.5γ. The basis states considered have $M=0$ and $P_z=1$ and are labeled (N,n) on the figure. Energies on the vertical axis are measured relative to E_{free} given by Eq. (4).

$$E_{\text{free}}=(\pi/L)^2+\gamma \ . \tag{4}$$

To obtain a more realistic level spectrum one must, of course, include the off-diagonal matrix elements of the Coulomb potential. These do not permit the level crossings evident in Fig. 1, in accordance with the no-crossing rule, which asserts that levels with the same good quantum numbers (M and P_z in the present case) cannot cross. In addition, the off-diagonal elements couple together an infinite number of states; thus an exact solution of the eigenvalue problem involves diagonalizing an infinite matrix. For practical calculations one circumvents this difficulty by diagonalizing H in a finite subspace of states—a procedure which, of course, introduces errors in the eigenvalues found. This paper describes a method, based on the foregoing discussion, which appears to give quite accurate eigenvalues for well widths and values of γ of experimental interest and yet presents a very manageable computational problem.

CALCULATIONS AND RESULTS

A major weakness of the basis set given by (2) is that the Ψ functions defined there are poorly suited for describing the exact wave function at weak magnetic fields ($\gamma \ll 1$). To remedy this problem we introduce a single variational parameter $\mathcal{H}$ into Ψ by redefining ξ as

$$\xi^2=\mathcal{H}\rho^2 \ . \tag{5}$$

Each eigenvalue of the matrix of H in a finite set of wave functions (2) now becomes a function of $\mathcal{H}$. We know that for any value of $\mathcal{H}$ the functions (2) form a complete set for this problem so that including all such functions would give the exact answer. If one has constructed an appropriate basis set for a given eigenvalue one can show that appending any additional state to the initial basis set chosen can only lower the calculated energy of that eigenvalue (see the Appendix). For such eigenvalues we thus have a variational principle which states that for any value of $\mathcal{H}$ the resulting approximate eigenvalue is an upper bound to the exact value. To obtain the most accurate eigenvalue possible with an appropriate basis set of fixed dimension we should then minimize the approximate eigenvalue with respect to $\mathcal{H}$. As a rule this process results in different optimum values of $\mathcal{H}$ for different states with the same good quantum numbers. States so generated that share these quantum numbers are not, therefore, exactly orthogonal to each other. A virtue of the basis set defined by Eqs. (2) and (5) is that all matrix elements of the Coulomb potential can be reduced to one-dimensional integrals (over z), facilitating rapid computation of the Hamiltonian matrix.

One might anticipate that this method would produce its most accurate energies in states for which the magnetic field dominates the Coulomb field. Thus a searching test of the accuracy of the method would be to compare eigenvalues obtained at zero magnetic field with corresponding eigenvalues from other variational trial functions which might reasonably be expected to yield accurate results for the zero-field problem. To accomplish this I have taken basis sets comprised of wave functions of the type given in (2) with $0\le N\le 4$ and n running from zero to a value as high as required for convergence; I have then calculated, by varying $\mathcal{H}$, energies of various states with $M=0$ and -1 and with $P_z=1$ and -1. For purposes of comparison I have computed also energies obtained from the following multiparameter trial functions.

$M=0$, $P_z=+1$ ($1s$-like states):

$$\begin{aligned}\Phi_1(\mathbf{r})&=F_0(\mathbf{r})\cos(k_1 z) \ ,\\ \Phi_2(\mathbf{r})&=F_0(\mathbf{r})\sum_{n=1}^{4} A_n\cos(k_{2n-1}z) \ .\end{aligned} \tag{6a}$$

$M=-1$, $P_z=+1$, ($2p_{-1}$-like states):

$$\begin{aligned}\Phi_1(\mathbf{r})&=F_1(\mathbf{r})\cos(k_1 z)\\ \Phi_2(\mathbf{r})&=F_1(\mathbf{r})\sum_{n=1}^{4} A_n\cos(k_{2n-1}z) \ .\end{aligned} \tag{6b}$$

$M=0$, $P_z=-1$ ($2p_0$-like states):

$$\begin{aligned}\Phi_1(\mathbf{r})&=F_0(\mathbf{r})\sin(k_2 z) \ ,\\ \Phi_2(\mathbf{r})&=F_0(\mathbf{r})\sum_{n=1}^{5} A_n\sin(k_{2n}z) \ .\end{aligned} \tag{6c}$$

$M=-1$, $P_z=-1$ ($3d_{-1}$-like states):

$$\Phi_1(\mathbf{r})=F_1(\mathbf{r})\sin(k_2 z)\ ,$$
$$\Phi_2(\mathbf{r})=F_1(\mathbf{r})\sum_{n=1}^{5} A_n \sin(k_{2n} z)\ , \tag{6d}$$

where

$$F_{|M|}(\mathbf{r})=\rho^{|M|}\exp[-\eta\rho^2-K(\rho^2+\alpha z^2)^{1/2}]\exp(iM\phi)\ ,$$

$k_n=n\pi/L$, and η, K, α, and A_n are parameters which are optimized for each state calculated.

Comparisons of variational energies are presented in Tables I–IV, where entries E_P are calculated from the above-described matrix, and entries E_1 and E_2 are associated with Φ_1 and Φ_2, respectively. Notice that E_P improves relative to E_1 and E_2 with increasing fields. Notice also that E_P is relatively better for p-like and d-like states than for s-like states. It is to be expected that this improvement will be even more marked for states of higher $|M|$. It is of interest to note that the energy obtained by the ansatz of Bastard[6] in his pioneering paper on this subject is -1.2152 for the $\gamma=0$ $1s$-like state as compared to -1.2255 found here for E_P. Energies for states with $M=|M|$ can be found from their counterparts with $M=-|M|$ by adding $2|M|\gamma$ to the latter energies, just as in bulk.

Errors in the energies E_P are due primarily to the truncation of the expansion of the wave functions in Landau levels ($N<5$ in the present calculations). One expects that if the admixture of the Nth Landau level into the optimized trial function declines rapidly as N increases the energy E_P will be relatively accurate. For my apparently least accurate E_P value ($\gamma=0$ in Table I) the probability that the $N=4$ Landau level is occupied is 2×10^{-2}. For my seemingly most accurate energy, E_P at $\gamma=5$ in Table IV, that probability is only 7×10^{-7}. In general it would appear that for low-lying excited states the amplitude of the highest Landau level admixed in the optimized trial function is a useful indicator of the accuracy of the energy obtained.

Comparisons are presented only for wells with $L=6$ in Tables I–IV. The deviations of energies E_P from energies E_2 are, however, not very sensitive to L for $L>1$, being usually not much greater for $L=1$ than for $L=6$. (At $\gamma=0$ we find, for example, that $E_P-E_2=0.0275$ for the $1s$ state at $L=1$.) On the other hand, in the limit $L\to0$, E_P becomes quite poor, giving, for example, a ground-state energy of -3.781 versus the exact energy (approached by E_1 and E_2) of -4.000. (This large discrepancy is presumably due to the difficulty of representing accurately the exact two-dimensional $1s$ wave function, which has a nonvanishing ρ derivative at $\rho=0$, by a small number of Landau wave functions, each of which has zero ρ derivative at $\rho=0$.)

The anticrossing structure of the lowest-lying excited state energies for the $[M,P_z]$ pairs $[0,+1]$, $[-1,+1]$, and $[0,-1]$ are presented in Figs. 2–4, respectively. To understand the anticrossing behavior displayed in those plots one should compare them to Fig. 1. For example, the bending of the curve representing level 4 in Fig. 3 near $\gamma=1$ is an effect of the crossing of the $N=1$ Landau level associated with the $n=3$ subband [denoted (1,3) in Fig. 1] with the $N=2$ Landau level associated with the $n=1$ subband [denoted (2,1)] illustrated in Fig. 1. Excited levels 2 and 3 have reached their high-field limiting behavior in Fig. 3; level 4 will eventually become pinned below the $n=7$ subband at higher fields.

The energies of the first eleven excited states with $P_z=+1$ and $|M|<2$ are listed in order of increasing energy in Table V for $\gamma=1$ and $L=3$. The states denoted in parentheses are the bulk states into which the corresponding well states evolve as $L\to\infty$. Notice that, unlike in the bulk, the $2p_{+1}$, $2s$, and $3p_{-1}$ levels form a closely spaced cluster beneath the $N=1$ free-particle Landau level (of energy $2N\gamma=2$); levels labeled $3p_{+1}$, $3s$-$3d_0$, and $4p_{-1}$-$4f_{-1}$ form a similar cluster below the

TABLE I. Comparison of upper bounds to the energy of the lowest-lying donor level with $M=0$ and $P_z=1$ as calculated from the Hamiltonian matrix (E_P) and from the trial functions of Eqs. (6a) (E_1 and E_2) with $L=6$. The zero of energy is taken as E_{free}, given, relative to the bottom of the square well, by Eq. (4).

	(1s-like states)		
γ	E_P	E_1	E_2
0	−1.2255	−1.2343	−1.2430
1.0	−1.9074	−1.9119	−1.9183
5.0	−3.0251	−3.0290	−3.0306

TABLE II. Comparison of upper bounds to the energy of the lowest-lying donor level with $M=-1$ and $P_z=1$ as calculated from the Hamiltonian matrix (E_P) and from the trial functions of Eqs. (6b) (E_1 and E_2) with $L=6$. The zero of energy is taken as E_{free}, given, relative to the bottom of the square well, by Eq. (4).

	($2p_{-1}$-like states)		
γ	E_P	E_1	E_2
0	−0.3560	−0.3573	−0.3580
1.0	−1.1110	−1.1098	−1.1112
5.0	−1.9737	−1.9725	−1.9737

TABLE III. Comparison of upper bounds to the energy of the lowest-lying donor level with $M=0$ and $P_z=-1$ as calculated from the Hamiltonian matrix (E_P) and from the trial functions of Eqs. (6c) (E_1 and E_2) with $L=6$. The zero of energy is taken as E_{free}, given, relative to the bottom of the square well, by Eq. (4).

	($2p_0$-like states)		
γ	E_P	E_1	E_2
0	0.1112	0.1134	0.1109
1.0	−0.3276	−0.3240	−0.3275
5.0	−0.6533	−0.6477	−0.6529

TABLE IV. Comparison of upper bounds to the energy of the lowest-lying donor level with $M=-1$ and $P_z=-1$ as calculated from the Hamiltonian matrix (E_P) and from the trial functions of Eqs. (6d) (E_1 and E_2) with $L=6$. The zero of energy is taken as E_{free}, given, relative to the bottom of the square well, by Eq. (4).

	($3d_{-1}$-like states)		
γ	E_P	E_1	E_2
0	0.515 6	0.515 6	0.515 3
1.0	−0.073 05	−0.072 05	−0.072 78
5.0	−0.467 7	−0.465 3	−0.467 3

$N=2$ Landau level. These clusters and those attached to higher Landau levels persist to higher fields until perturbations due to anticrossings become important. States of higher $|M|$ values, not explicitly calculated in this paper, are expected also to appear in the above-described clusters.

It is to be expected that in the limit of infinite magnetic field the lowest-lying states of arbitrary M and $P_z=+1$ will shrink to a point just as ground states of the same symmetry do in bulk.[7] This effect is a consequence of the singular behavior of the Coulomb potential in the infinite-field limit, the effective potential being proportional to $-1/|z|$ in that limit. This shrinkage of the wave function eliminates contact between the electron and the wall, causing the well donor state to become indistinguishable from the analogous bulk donor level and producing, as in bulk, an unbounded increase in binding energy with increasing magnetic field. In contrast, excited states of the same M with $P_z=+1$ and all states with $P_z=-1$ retain, in the infinite-field limit, a finite extension in the z direction and a finite binding to the $N=0$ Landau level associated with the appropriate subband level.

Since quantum-well donor electrons in a magnetic field are fully quantized, there are no metastable resonant states associated with $N=1$ and higher Landau levels of the type appearing for bulk semiconductors.[8] Nevertheless, the quantum-well problem may provide an interesting model for studying such resonant levels. As the well width is increased one expects that precursors of these resonant states will, for a given magnetic field, appear as bound states which are clustered in energy and are built from wave functions of the form given in Eq. (2) containing predominantly the same function $L_N^M(\xi)$ (i.e., the same Landau level).

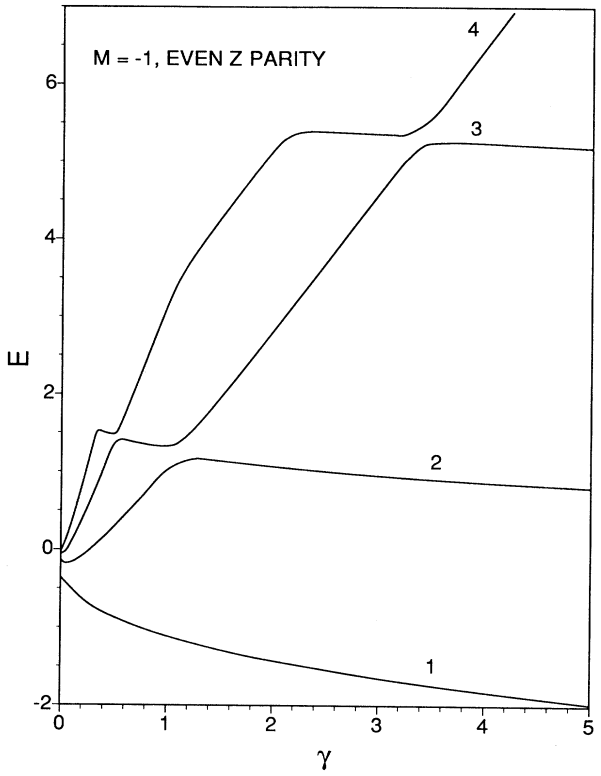

FIG. 3. Energy vs magnetic field for the four lowest-energy donor states with $M=-1$ and $P_z=1$. The donor ion is in the center of a quantum well with $L=6$. Energies are measured relative to E_{free} given by Eq. (4).

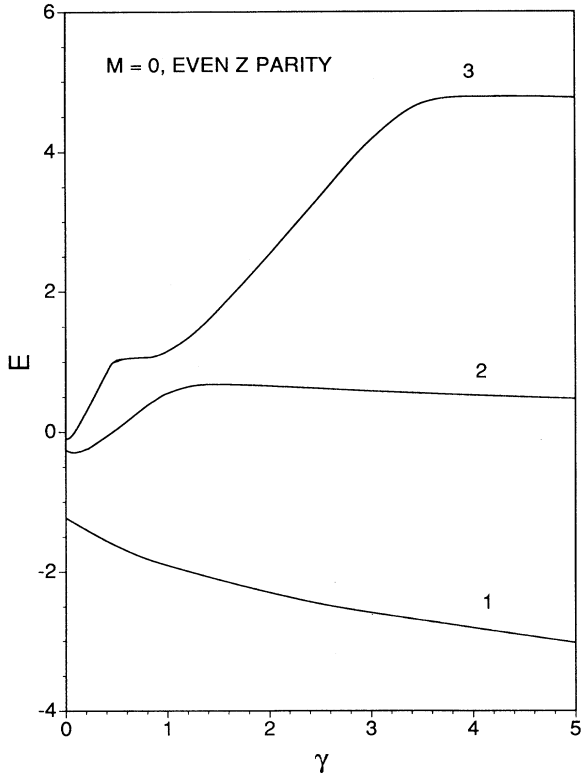

FIG. 2. Energy vs magnetic field for the three lowest-energy donor states with $M=0$ and $P_z=1$. The donor ion is in the center of a quantum well with $L=6$. Energies are measured relative to E_{free} given by Eq. (4).

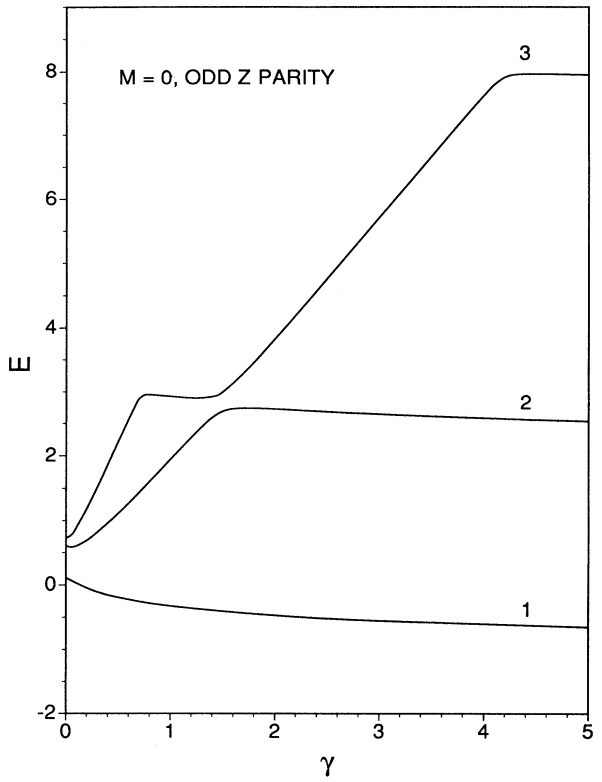

FIG. 4. Energy vs magnetic field for the three lowest-energy donor states with $M=0$ and $P_z=-1$. The donor ion is in the center of a quantum well with $L=6$. Energies are measured relative to E_{free} given by Eq. (4).

CONCLUSION

A method of calculating excited states of a donor in the center of a quantum well in a magnetic field is described, which, though expected to be most accurate for states with high $|M|$ values and $P_z=-1$, is argued to give moderate accuracy even for $M=0$ and $P_z=+1$ at zero magnetic field for a modest calculational effort. The method is variational for each of the excited-state energies provided that enough of the lowest-lying basis states are employed. By systematically increasing the size of the basis set the accuracy of the calculations can in principle be improved as much as required. The method can be trivially extended to calculations of donors located anywhere in the well or in the barrier and can be modified to account for finite barrier height (including different effective masses in the barrier and in the well). The problem of the Stark effect on donor levels in a magnetic field can also be treated conveniently and with an accuracy which is anticipated to be comparable to that obtained in the absence of electric fields.

TABLE V. Energies of the eleven lowest-lying donor states with even z parity ($P_z=1$) and $|M|\leq 1$ in a quantum well with $L=3$ as calculated from the Hamiltonian matrix of this paper with $\gamma=1$. States indicated in parentheses are those into which the corresponding well states evolve when $L\rightarrow\infty$ adiabatically with the donor remaining in the center of the well. The zero of energy is taken as E_{free}, given, relative to the bottom of the square well, by Eq. (4).

M	E
0 ($1s$)	−2.3157
−1 ($2p_{-1}$)	−1.2554
0 ($2s$)	0.6180
1 ($2p_{+1}$)	0.7446
−1 ($3p_{-1}$)	0.9690
0 ($3s$-$3d_0$)	2.8605
1 ($3p_{+1}$)	2.9690
−1 ($4p_{-1}$-$4f_{-1}$)	3.0871
0	5.0329
1	5.0871
−1	5.1872

APPENDIX

Let $E_j(s)$ be the set of (discrete) approximate eigenvalues of H determined by diagonalizing H in an s-dimensional basis set of given functions [for example, functions defined by Eqs. (2) and (5)]. Assume that these eigenvalues are nondegenerate and are labeled in order of increasing energy with $j=1$ corresponding to the lowest eigenvalue, $j=2$ to the next lowest, etc. We show that augmenting the original basis set by adding an additional basis vector produces a new set of approximate energies $E_j(s+1)$, such that, if the inequality (A9) is satisfied,

$$E_j(s+1)<E_j(s)\ .$$

Associated with each eigenvalue $E_j(s)$ in the original set is a normalized eigenfunction $\chi_j(r)$. To the set χ_j we append an additional normalized basis vector $\phi(r)$ which is orthogonal to all of the χ_j's. In the new, $(s+1)$-dimensional basis, the new eigenfunctions have the form

$$\psi=\sum_{i=1}^{s} a_i\chi_i+a_{s+1}\phi\ , \tag{A1}$$

which must satisfy, in the $(s+1)$-dimensional subspace,

$$H\psi=E\psi\ . \tag{A2}$$

Substituting into (A2) from (A1) leads to

$$\begin{aligned} &E_i(s)a_i+M_ia_{s+1}=Ea_i \quad (i<s+1)\ , \\ &\sum_{i=1}^{s} a_iM_i+\varepsilon a_{s+1}=Ea_{s+1}\ , \end{aligned} \tag{A3}$$

where we have assumed that M_i is real and

$$\varepsilon=\langle\phi|H|\phi\rangle,\quad M_i=\langle\chi_i|H|\phi\rangle\ .$$

Solving in the case $|M_i|>0$ for all values of i gives

$$\begin{aligned} &a_i=-M_ia_{s+1}/[E_i(s)-E]\ , \\ &E-\varepsilon=\sum_{i=1}^{s}\frac{|M_i|^2}{E-E_i(s)}\ . \end{aligned} \tag{A4}$$

Consider the lowest-lying solution for E in (A4). If it should be true that

$$\varepsilon > E_1(s) ,$$

then the left-hand side of (A4) will be negative for solutions with $E < E_1(s)$. If we imagine that E sweeps from $E_1(s)$ to $-\infty$, the left-hand side of (A4) sweeps from a finite negative value to $-\infty$ whereas the right-hand side of (A4) sweeps at the same time from $-\infty$ to zero. Thus a solution must exist with $E < E_1(s)$. This solution is denoted $E_1(s+1)$.

Let us now search for a solution of (A4) obeying

$$E_1(s) < E < E_2(s) . \tag{A5}$$

For this purpose it is convenient to rewrite (A4) in the form

$$E - \varepsilon - \frac{|M_1|^2}{E - E_1(s)} = \sum_{i=2}^{s} \frac{|M_i|^2}{E - E_i(s)} . \tag{A6}$$

In (A6) the left-hand side is guaranteed to be negative if (A5) holds and

$$\varepsilon > E_2(s) . \tag{A7}$$

As E sweeps from $E_2(s)$ to $E_1(s)$ the left-hand side of (A6) varies from a finite negative value to $-\infty$ whereas the right-hand side sweeps from $-\infty$ to a finite negative value. Thus a solution obeying (A5) must exist. This solution is denoted $E_2(s+1)$.[9]

By continuing the above argument one can show that the solution $E_j(s+1)$ obeys

$$E_{j-1}(s) < E_j(s+1) < E_j(s) \tag{A8}$$

if

$$\varepsilon > E_j(s) . \tag{A9}$$

[Condition (A9) is clearly sufficient to ensure (A8) but may not always be necessary.]

If, for a given $E_j(s)$, every allowed choice of $\phi(r)$ [allowed choices satisfying the requirement that $\phi(r)$ be orthogonal to all of the χ_j's] results in a value of ε obeying (A9), then $E_j(s)$ is an upper bound to the exact value of the jth eigenvalue and the basis set from which $E_j(s)$ is calculated is an "appropriate basis set" for the jth eigenvalue. Intuitively, we see from (A4) that E on the left-hand side is increased by those terms in the sum for which E_j lies below E. We must take care not to omit any such terms in order to be assured that the E in the range of interest is an upper bound. For the problem discussed in this paper it is very easy to order the successive $\phi(r)$'s to achieve this end since unperturbed Landau and subband levels with successively higher quantum numbers N and n, respectively, have successively higher energies.

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[9]It is to be expected that for all i, $|M_i| > 0$ since the states χ_i and ϕ have the same good quantum numbers. In the event that $|M_i| = 0$, in addition to the solutions of (A4) there is an additional solution $E = E_i$.