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Resonant impurity states in semiconductors in a strong magnetic field

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We present a theory of magnetically induced resonance states in narrow-gap semiconductors and apply it to study the resonance states in InSb. By expanding the impurity wave functions in terms of the free-electron Landau wave functions, we obtain an infinite set of coupled equations. If the magnetic field is sufficiently large, i.e., $\gamma > 1$ (here, $\gamma = \hbar\omega_c/2\mathrm{Ry}^*$), only a small number of Landau levels need be solved self-consistently because for any energy to a good approximation, the coupling need be considered only between the adjacent Landau level and all the lower ones. The calculation of the energy and width can be made using a multicomponent generalization of the Kohn variational method for phase shifts. We have made detailed calculations for the lowest resonant state associated with the $n=1$ Landau level. Screened potentials were used primarily because they simplify the numerical calculation, but the procedure is applicable without modification to any potential $V(z)$ which goes to zero faster than $1/z$. Furthermore, although we have used the parabolic band model, the method can be readily modified to include nonparabolicity.

I. INTRODUCTION

It is well known[1,2] that in zero-gap semiconductors resonant states in impurity scattering arise from the overlap of the bound state of the impurity with the continuum states of the conduction or the valence band of the semiconductor. Such an overlap invariably broadens the impurity state and if the width Γ is small, the state is called a resonance which can manifest itself either as an extra peak in optical absorption or as a sharp increase in the electrical resistivity when the Fermi surface is close to the resonance energy. In semiconductors such as InSb where the band gap is large compared with the impurity energy, a similar mechanism, although instrinsically absent, can be induced[1] by the application of a magnetic field which is high enough that the separation between the Landau levels is greater than the impurity energy. In this case the impurity states associated with each Landau level (except the lowest) would overlap with the continuum of the lower level(s), once again giving rise to the possibility of resonance states.[3(a)] Extensive work, which has been reviewed by Kaplan,[3(b)] has been done on the energy of these states, treating them as bound. Some model calculations have also been done by Bastard[4] on their width. The purpose of this paper is to present a theory which calculates the resonance energy and the width using realistic potentials. We use the one-band effective-mass approximation although the method can be readily modified to include the effect of nonparabolicity.

In the simplest version of the effective mass approximation, the one band isotropic case, the problem of the impurity states in a magnetic field is the same (except for the screening) as the classic problem of the hydrogen atom in a magnetic field, discussed by various authors, e.g., Schiff and Snyder.[5] The resulting Schrödinger equation being a partial differential equation in two variables which are not separable, has not been solved exactly. Certain approximation schemes, applicable under different conditions, can be devised to separate the variables. The most widely explored is the so-called adiabatic approximation[6] (AA), valid

under high magnetic fields where the rapid transverse motion of the electron can be decoupled from the longitudinal motion in the same spirit as the decoupling of the motion of the electrons in a lattice from that of the slow moving ions. Shinada and Sugano[7] proposed another scheme called the "two-dimensional" model in which the longitudinal motion is suppressed by taking $m_\perp/m_{||}\to 0$ which, although valid only for highly anisotropic semiconductors, has the advantage of being able to treat the transverse motion in the presence of arbitrary magnetic fields (plus, of course, the Coulomb field). While each of these approximations under their respective conditions of applicability is expected to give reasonable results for the Coulomb states associated with the lowest Landau level, neither of them is suitable for the study of magnetically induced resonances because of their inability to include an essential ingredient of the problem, namely the interaction (arising from overlap, or even just the proximity) of the longitudinal states associated with *different* transverse states. The longitudinal motion, if considered, is taken to be affected by one or more Landau levels only through the potential presented to the longitudinal motion, but *different longitudinal motions themselves are never mixed.* We present a scheme which takes this interaction into account and which reduces to the adiabatic approximation when this interaction is neglected. The scheme is based on an expansion of the impurity wave function in terms of the free-electron Landau wave function which yields an infinite set of coupled equations because the impurity potential mixes the longitudinal part of any Landau state to that of *all* others. The coupling between different levels can be truncated to a finite number which depends upon the values of the magnetic field and energy and upon the accuracy desired. For the case of one open channel, this finite set of coupled equations can be solved by the multicomponent generalization of the Kohn variational method for phase shifts, as in Ref. 2.

In Sec. II we obtain the infinite set of coupled equations. In Sec. III we discuss the application of a truncated set of these equations to the study of resonance. In Sec. IV we discuss the variational methods for the phase shifts and in Sec. V the boundary conditions for the wave function and the consequent modifications in the Kohn expression for the phase shift. In Sec. VI we give the results of a numerical calculation for the resonant level below the $n=1$ Landau level for InSb assuming the coupling only between $n=0$ and $n=1$. Throughout we have assumed a parabolic band but the treatment can readily be extended to include the effect of nonparabolicity. For the numerical calculation we have used screened potentials calculated from the theory of Jog and Wallace.[8]

II. IMPURITY ATOM IN A MAGNETIC FIELD

In the parabolic band model, the Schrödinger equation for the impurity wave functions in the presence of the magnetic field and a spherically symmetric impurity potential $V(r)$ is[9,10]

$$\left[-L_{\rho\theta}-\frac{\partial^2}{\partial z^2}+\frac{2m^*}{\hbar^2}V(r)\right]\psi=\epsilon\psi, \tag{1}$$

where

$$L_{\rho\theta}=\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right]+\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{i\rho}{2l^2}\right]. \tag{2}$$

l represents the cyclotron radius and is equal to $\sqrt{\hbar c/eH}$, $\epsilon=2m^*E/\hbar^2$. To solve (1), we expand ψ in terms of the free-electron Landau wave functions

$$\psi=\frac{1}{\sqrt{2\pi}}\sum_{n,l}\chi_{nl}(\rho)e^{il\theta}Z_{nl}(z), \tag{3}$$

where

$$Z_{nl}(z)=\frac{1}{\sqrt{2\pi}}\sum_{k_z}a_{nlk_z}e^{ik_z z}. \tag{4}$$

Substituting (3) into (1), and noting that[11]

$$-L_{\rho\theta}\chi_{nl}(\rho)e^{il\theta}=\epsilon^0_{nl}\chi_{nl}(\rho)e^{il\theta}, \tag{5}$$

where

$$\epsilon^0_{nl}=\frac{2m^*}{\hbar^2}\hbar\omega_c\left[n+\frac{1}{2}+\frac{l+|l|}{2}\right], \tag{6}$$

we get

$$-\sum_{n',l'}\chi_{n'l'}(\rho)e^{il'\theta}Z''_{n'l'}+\frac{2m^*}{\hbar^2}V(\sqrt{\rho^2+z^2})\sum_{n',l'}\chi_{n'l'}(\rho)e^{il'\theta}Z_{n'l'}=\sum_{n'l'}(\epsilon-\epsilon^0_{n'l'})\chi_{n'l'}e^{il'\theta}Z_{n'l'},\quad Z''_{n'l'}=\frac{d^2}{dz^2}Z_{n'l'}. \tag{7}$$

Multiplying (7) by $\rho\,\chi_{nl}(\rho)\,e^{-il\theta}$ and integrating over ρ and θ, we get

$$-Z''_{nl}-\sum_{n'} I_{nn'l}Z_{n'l}=\epsilon_{nl}\chi_{nl}, \tag{8}$$

where

$$I_{nn'l}=-\frac{2m^*}{\hbar^2}\int \rho\,d\rho\; V(\rho^2+z^2)\chi_{n'l}\chi_{nl} \tag{9}$$

and

$$\epsilon_{nl}=\epsilon-\epsilon^0_{nl}. \tag{10}$$

(Note that V is an attractive potential, so $I_{nn'}>0$.) The simultaneous equations (8) which have to be solved self-consistently, from the basis of our analysis of the resonance states. But before we proceed to study resonances in Sec. III, we note the following points.

(1) The coupling in (8) is between longitudinal "wave functions" Z_{nl} with "energies" ϵ_{nl} where, as is evident from (10), ϵ_{nl} is the residual energy obtained by subtracting the energy ϵ^0_{nl} of the transverse motion from the total energy ϵ.

(2) The coupling in (8) is only between states of the *same l*. This is expected because the coupling potential is spherically symmetric. Note that although there is no coupling between states of different l, the coupling potential itself does depend upon l.

(3) The adiabatic approximation roughly corresponds to replacing $Z_{n'l'}$ $(n'\neq n)$ in (8) by $Z_{nl}I_{nn'l}/(\epsilon^0_{nl}-\epsilon^0_{n'l})$ for $\epsilon\approx\epsilon^0_{nl}$. Thus, the AA consists in considering that the dominant contribution to the impurity wave function of azimuthal quantum number l and energy ϵ comes from the band nl for which ϵ^0_{nl} is closest to ϵ; the contribution from the other bands is smaller in the ratio of the mixing integral $I_{nn'}$ and the energy difference $(E^0_n - E'^0_n)$. As $\gamma\to\infty$, $Z_{n'l}/Z_{nl}\to 0$ for $n'\neq n$, which is the approximation considered by Yafet *et al.*[6] However, it is important to note that the final equation for the longitudinal state in the adiabatic approximation involves only *one* value of n and l. Thus, the limited mixing, considered in AA, amounts simply to a *renormalization*[12] *of the original state without permitting its free mixing with other states.* Depending upon the sophistication of the adiabatic procedure followed by different authors, this renormalization has been carried anywhere from the lowest order of perturbation (Yafet *et al.*[6]) to all orders.[13] However, this clinging of a longitudinal state to its parent Landau state is hardly likely to be satisfactory when there are overlapping bands, an essential feature of the resonance under study.

(4) The Z_{nl}'s obtained by solving (8) self-consistently will give an exact solution of the problem for any magnetic field. However, the computational effort increases greatly with the number of Z_{nl}'s included in the self-consistent scheme. To keep this number small, one must restrict oneself to high fields and low energies. The field must be high in order that the Coulomb energy is small compared with $\hbar\omega_c$ which reduces the effect of Landau levels on each other, brought about by the impurity potential. Furthermore, the energy must be small because for any energy, the coupling between the adjacent Landau level and all the lower ones has to be considered in any case.

In the following three sections we discuss the solution of these coupled equations for a two-component system. From the presentation, it would be evident that the method applies equally well to a multicomponent system with one open channel.[14]

III. APPLICATION TO RESONANCE

All that there is to know about the impurity states is contained in the self-consistent equations (8). Equations of this type are well known[15] in the study of the scattering (resonant or nonresonant) of electrons from atoms and a great variety of methods have been developed to solve them. The problem of resonance may be approached in essentially two different ways. One, due to Fano,[16] consists in considering a resonant state as nearly bound and to study its decay into the various continua. The other is to consider it as a continuum state which becomes nearly bound by the scattering potential. For the case of parabolic band and two Landau levels ($n=0$ and $n=1$) for which we have carried out the numerical calculations, the two approaches give consistent results. However, below we discuss only the scattering approach because it is broader in scope: Firstly, it is free from the restriction of narrow widths. Secondly, it can be readily generalized to the case of multiple open channels.

In (8), taking $l=0$ and ignoring all coupling except between $n=0$ and $n=1$, we get

$$\begin{aligned} -Z'_0{}' - I_{00}Z_0 - I_{01}Z_1 &= k^2 Z_0\,, \\ -Z'_1{}' - I_{11}Z_1 - I_{10}Z_0 &= (k^2-2S)Z_1\,, \end{aligned} \tag{11}$$

where

$$S=\frac{m^*\omega_c}{\hbar}$$

and

$$k^2=\epsilon-S.$$

It is convenient to rewrite (11) in the matrix notation

$$\underline{L}\,\underline{u}=0,$$

where

$$\underline{L}=\left[-\frac{d^2}{dz^2}-k_z^2\right]\underline{1}+\begin{bmatrix}-I_{00} & -I_{01}\\ -I_{10} & 2S-I_{11}\end{bmatrix} \quad (12)$$

and

$$\underline{u}=\begin{bmatrix}Z_0\\ Z_1\end{bmatrix}.$$

Since the potentials $I_{nn'}$ are symmetrical about the origin, parity commutes with the Hamiltonian and all the information about the scattering is contained in two phase shifts δ_0 and δ_1 corresponding, respectively, to even and odd parity. Let us concentrate only on the even case which should yield the ground quasilocalized state. To find resonance, we study δ_0 as a function of energy. If $\delta_0(E)$ increases rapidly through $\pi/2$, the resonant energy E_R is given by the value of E at which $\delta_0=\pi/2$ and the width Γ is given by

$$\Gamma^{-1}=\left.\frac{\partial\delta}{\partial E}\right|_{E=E_R} \quad (\Gamma>0)$$

(here the subscript 0 has been dropped from δ). For the study of scattering from realistic potentials, variational methods have been found to be particularly useful. These methods are briefly discussed next.

IV. VARIATIONAL METHODS FOR THE CALCULATION OF THE PHASE SHIFT

In variational methods the phase shift is calculated by estimating the stationary value of a certain functional J of the wave function within the space spanned by the trial wave functions. Two of these methods, due to Kohn and due to Harris, have recently been used by Joos, Das, and Wallace[2] for the study of resonance in zero-gap semiconductors where the coupled equations are similar to (11). In the present problem we have used the Kohn method. Computational difficulties, commonly associated with this method, were avoided by introducing nonlinear parameters in the wave function (WF) as in Joos *et al.*[2] We found it possible to choose nonlinear parameters for which the Kohn method was free from such computational difficulties over a very wide range of energy for all the values of magnetic fields and screening parameter for which the calculations were made. Furthermore, the second-order Kohn correction was rather small, lending confidence to the suitability of the trial WF. In Sec. V we discuss the boundary conditions satisfied by the even-parity solution of (11) and the functional J (which turns out to be the same as for solutions of odd parity). The potential used and the trial WF used are discussed in Sec. VI.

V. BOUNDARY CONDITIONS AND THE FUNCTIONAL J

Even-parity solutions of (11) satisfy the boundary conditions

$$\psi(z)=\psi(-z), \quad (13a)$$

$$\left.\frac{d\psi}{dz}\right|_{Z=0=0}, \quad (13b)$$

where ψ stands for either Z_0 or Z_1 (or any other component included in the coupled equations). In view of the evenness condition (13a), we will restrict the remaining discussion only to $z>0$ and denote $|z|$ by r.

If Z_0 is the only open channel, we must also have

$$Z_1\underset{r\to\infty}{\longrightarrow}0, \quad (14a)$$

$$Z_0\underset{r\to\infty}{\longrightarrow}\cos(kr+\delta). \quad (14b)$$

A solution of the form of (14b) can, of course, occur only if the potentials asymptotically approach zero faster than $1/r$.

In order that the phase shift enter as a linear parameter in the trial WF, it is convenient to rewrite (14b) as

$$Z_0\underset{r\to\infty}{\longrightarrow}\cos kr-\lambda\sin kr \quad (15)$$

where $\lambda=\tan\delta$.

With the boundary condition at the origin and (15), it is easy to see that if $\bar{u}$ is the true WF and δu any variation in $\bar{u}$ subject to the same boundary conditions as $\bar{u}$ itself, then we get

$$\delta I=I[\bar{u}+\delta u]-I[\bar{u}]=k\delta\lambda, \quad (16)$$

where

$$I[u]=\int_0^\infty dr\ \underline{u}^\dagger\underline{L}\,\underline{u}.$$

Thus, the stationary functional J is given by

$$J=I-k\lambda. \tag{17}$$

As in Joos *et al.*,[2] the variational WF can be written in the spinor form

$$\underline{u}=\sum_{i=1}^{2n} C_i\underline{\chi}_i+\underline{C}-\lambda\underline{S},$$

where

$$\begin{aligned}
\underline{\chi}_i &= \eta_i\begin{bmatrix}1\\0\end{bmatrix}\text{(odd } i\text{)},\\
\underline{\chi}_i &= \eta_i\begin{bmatrix}0\\1\end{bmatrix}\text{(even } i\text{)},\\
\underline{C} &= C\begin{bmatrix}1\\0\end{bmatrix},\\
\underline{S} &= S\begin{bmatrix}1\\0\end{bmatrix},
\end{aligned} \tag{18}$$

with C having the asymptotic form $\cos kr$ and S the form $\sin kr$ in accordance with (15). Thus, all the formalism of the Kohn method goes through by changing S and C of the usual theory to C and $-S$, respectively. In particular, we find the following.

(i) $\partial J/\partial c_i = 0$ leads to two systems of $2n$ linear equations: Two systems because each of the $2n$ c_i's is written as $C_i^c-\lambda C_i^s$, the superscripts C and S corresponding to cos and sin terms in (15), the values of C_i^c and C_i^s separately being required for the evaluation of λ.

(ii) If the equations for C_i^c and C_i^s can be solved (failure would occur when the energy at which the phase shift is being calculated, happens to be very close to an eigenvalue of the Hamiltonian in the space spanned by the η_i's), we get

$$J(\lambda)=M_{00}+(M_{01}+M_{10})\lambda+M_{11}\lambda^2-k\lambda, \tag{19}$$

where

$$\begin{aligned}
M_{00} &= \left(\underline{C}\,|\,\underline{L}\,|\,\sum_{i=1}^{2n} C_i^c\underline{\chi}_i+\underline{C}\right),\\
M_{10} &= \left(-\underline{S}\,|\,\underline{L}\,|\,\sum_{i=1}^{2n} C_i^c\underline{\chi}_i+\underline{C}\right),\\
M_{01} &= \left(\underline{C}\,|\,\underline{L}\,|\,\sum_{i=1}^{2n} -C_i^s\underline{\chi}_i-\underline{S}\right),\\
M_{11} &= \left(-\underline{S}\,|\,\underline{L}\,|\,\sum_{i=1}^{2n} -C_i^s\underline{\chi}_i-\underline{S}\right).
\end{aligned} \tag{20}$$

(iii) Using $\partial J/\partial\lambda = 0$ in (19) we get

$$\lambda_{\text{Kohn}}=-\frac{M_{10}}{M_{11}}. \tag{21}$$

(iv) λ given by (21) is the value of $\tan\delta$ for the optimum WF. If I is the value of the integral in (16) using the optimum WF, a still better estimate of λ can be obtained by using

$$[\lambda]_{\text{Kohn}}=\lambda_{\text{Kohn}}-\frac{1}{k}\frac{\det M}{M_{11}}, \tag{22}$$

where $\det M=M_{00}M_{11}-M_{10}M_{01}$. $(\det M)/M_{11}$ is the value of I for the optimum WF. The term $-I/k$ essentially amounts to modifying the optimum WF to bring the value of I closer to zero (which is the value of $I[\bar{u}]$).

The simplest choice for C is

$$C=\cos kz, \tag{23}$$

which is acceptable because it satisfies the boundary condition at $z=0$. If, on the other hand, we were to choose S to be $\sin kz$, the derivative at the origin would not be zero. An acceptable choice is

$$S=(1-e^{-zd})\sin kz, \tag{24}$$

where d is a nonlinear parameter. The choice of η's depends not only on boundary conditions at $z=0$ but also on the $I_{nn'}$'s. These will be discussed in Sec. VI following the discussion of the potentials. It may be mentioned that for odd parity, J is still given by (17) and (19); in (20), C and S are replaced by S and $-C$ (just as in the usual Kohn formalism); (21) and (22) remain unchanged.

VI. NUMERICAL CALCULATION

For the purpose of numerical calculation, we chose InSb primarily because of the small effective mass and large dielectric constant so that γ may be large enough for moderate magnetic fields. We confine the calculation to the case where only the $n=0$ Landau state is occupied[17] and all the spins are aligned (which is readily achieved because of the large spin splitting in InSb). The spins are taken to be aligned to justify neglecting spin-orbit interactions.

The potential used was the screened potential calculated from the theory of Jog and Wallace.[8] The unscreened potential, although closer to the conditions which one would choose for optical experiments[3(b)] (which usually are for low densities where screening is not very important), could not

be used because of the requirement (see Sec. V) that the $I_{nn'}$'s must go to zero faster than $1/z$. Screening may, however, be very weak, and the unscreened case can, in principle, be obtained by extrapolation.

In the theory of Jog and Wallace,[8] screening depends only on one dimensionless parameter p which, for a given material, depends upon temperature and on the *ratio* of N/H where N is the number density of carriers. We calculated Γ and E_R for three different values of p (=0.332, 0.193, and 0.1) and three fields (25, 50, and 100 kG) for each p. The first two values of p correspond to $T=2$ k, $N=10^{15}$ carriers/cm^3, and $H=50$ and 100 kG.

In terms of p, $I_{nn'}$'s are given by[18]

$$I_{nn'}(\xi)=\frac{\sqrt{2}m^{*}e^{2}}{\epsilon_0\hbar^2 l}\mathscr{I}_{nn'}(\xi)$$

$$=(a^{*})^2\sqrt{2\gamma}\,\mathscr{I}_{nn'}(\xi) \tag{25}$$

where

$$\mathscr{I}_{nn'}(\xi)=\int_0^{\infty}dx\;P_{nn'}(x)e^{-x}\exp\frac{[-2\xi(x+pe^{-x})^{1/2}]}{(x+pe^{-x})^{1/2}}$$

and

$$\xi=z/l\sqrt{2}.$$

$P_{nn'}$ are polynomials, a few of which are given by

$$P_{00}=1,\quad P_{01}=P_{10}=x,\quad P_{11}=(1-x)^2,$$

$$P_{02}=\tfrac{1}{2}x^2,\quad P_{12}=P_{21}=x(2-2x+\tfrac{1}{2}x^2),$$

$$P_{22}=(1-2x+\tfrac{1}{2}x^2)^2.$$

For a given p, $\mathscr{I}_{nn'}(\xi)$ may be calculated once and for all, different values of H affecting $I_{nn'}(z)$ only through scaling (which enters in two places: in $\sqrt{2}l\xi$ and in γ). $\mathscr{I}_{nn'}(\xi)$ was found to have a feature which considerably reduced the computer time. It was noted that unless p was very small, the integral could be written as a sum of exponentials of the form

$$\mathscr{I}_{nn'}(\xi)=C_1e^{-b_1\xi}+C_2e^{-b_2\xi}+\cdots. \tag{26}$$

Three exponentials were found to fit for $\xi\leq 11$ with an error of less than 0.1% for $p=0.332$ and 0.193. For $p=0.1$, the error was about 1% at certain points but much less for the important region of small ξ (less than 0.1% for $\xi\leq 3$). The form (26) results in a saving of the computer time because the integrals in (20) can be performed analytically.

Now we discuss the choice of the localized functions η needed for representing the inner part of u. These functions are determined primarily by the behavior of Z_1 close to the origin. The solution of Z_1 in which we are interested is one which would be a bound state in the absence of mixing. For a single exponential potential of the form $\alpha e^{-\beta r}$, ($\alpha<0$), the one-dimensional bound-state problem can be solved exactly. The solution is a Bessel function $J_\nu(X)$ with $\nu\propto\sqrt{|E|}/\beta$ ($|E|$ is the binding energy measured from the bottom of the $n=1$ continuum) and $X=\nu e^{-\beta r/2}$. The various terms in the expansion of the Bessel function have the form $e^{-\alpha' r}e^{-\beta(i-1)r}$ with i an integer taking different values from 1 to ∞ and $\alpha'=(2m|E|/\hbar^2)^{1/2}$. Since η's are determined primarily from the behavior of Z_1 close to the origin where the potential (26) can be written as a single exponential, the most suitable form of η_i must be

$$\eta_i=e^{-\alpha' r}e^{-\beta(i-1)r}.$$

But η_i given above does not satisfy the boundary condition (13b), so we modify the above η_i to the form

$$\eta_i=\left[\frac{1}{\alpha'+(i-1)\beta}+r\right]e^{-\alpha' r}e^{-\beta(i-1)r}$$

or (27)

$$\eta_i=\left[\frac{1}{\alpha'+(i-1)}+x\right]e^{-\alpha'' x}e^{-(i-1)x}$$

where $\alpha''=\alpha'/\beta$ and $x=\beta r$.

Therefore, the variational WF has three nonlinear parameters: α' and β in (27) and d in (24). With $\beta=1$ and $d=10$, values of δ were found to be stable with respect to variation of α' and with respect to the number of η's used in u for all the calculations made. The best value of α' varied from 0.5 to 1.0. For each p and H, the search for E_R was found to be considerably simplified by finding E_{RO}, an approximate value of E_R, by direct integration of the Schrödinger equation for Z, with no mixing. From $\delta=\delta(E)$ with $E\approx E_{RO}$, we obtained $d\delta/dE$ (hence, Γ) analytically by fitting $\delta(E)$ with a polynomial. The results for Γ and E_R for different values of p and H using nine exponentials for the inner part of each Z_0 and Z_1 are given in Table I.

It may be noted that as p is increased, the resonant level becomes shallower since the binding potential becomes weaker because of more effective screening. As H is increased, the resonance be-

TABLE I. Results for Γ and E_R for different values of p and H. E_R is measured from the bottom of $n=1$ band *downwards*. Units of E_R and Γ are effective Rydbergs.

H (kG)	25	50	100
p	E_R	E_R	E_R
	(Γ)	(Γ)	(Γ)
0.1	0.711	0.852	0.923
	(0.025)	(0.020)	(0.015)
0.193	0.556	0.641	0.721
	(0.027)	(0.022)	(0.018)
0.332	0.382	0.434	0.482
	(0.028)	(0.024)	(0.019)

comes deeper primarily because of the presence of γ in $I_{nn'}$ [see (25)].

The width Γ is found to increase with p but to decrease with H. An increase of p, on the one hand, tends to decrease Γ because of a decrease in the strength of the mixing potential; on the other hand, it tends to increase Γ because a given mixing potential causes a greater spread of a shallower level. Evidently, in the range under investigation, the latter effect dominates.

With H, the mixing potential increases but it becomes less effective in spreading the level both because of the increased gap between $n=0$ and $n=1$ and because of the resonant level having become deeper. The net effect is a decrease of Γ with H: This feature may turn out to apply more generally than just to the range considered.

It was also noted that for all p and H, the value of Γ is comparable with the difference of E_R and E_{RO}, as is expected from the Kramer-Kronig relation.

For $p=0.332$ and $H=50$ kG, we also compared the results of Γ and E_R with those obtained from the Fano method. E_R^F, the superscript denoting Fano, is, of course, the same as E_{RO}, discussed above. Γ^F was calculated by taking the unmixed Z_0 to be just a plane wave, i.e., ignoring the effect of I_{00} on the unmixed Z_0. This gave Γ^F to be about 20% larger than Γ^V (V denotes variational). To check the consistency of the results, we recalculated Γ^V by artificially setting $I_{00}=0$ and by reducing I_{01} by a factor of 10. In this case, Γ^V and Γ^F matched almost exactly although Γ^F was still too high by about 2%. E_R and E_{RO} were also in almost perfect agreement because their difference is comparable with Γ which is reduced by a factor of about 100 when the mixing potential is reduced by a factor of 10. It may be mentioned that restoring I_{00} to its actual value in the variational calculation increases Γ slightly although the effect (on Γ or E_R) is very small.

For comparison with the experimental results of Kaplan,[3(b)] we approximated the unscreened potential by a series of exponentials which agreed with the exact numerical values of the potential to within 2% up to $\xi=12$. At 50 kG, the resonance energy was 3.42 Ry* but no reliable estimate of Γ could be made because unlike the case of screened potentials, the value of δ was not stable with respect to variation of α'. The value of the resonance energy compares favorably with the experimental result of about 4.8 Ry* (read approximately from Kaplan's diagram[3(b)]) at 77 kG. We plan to pursue the problem of the unscreened potential by a direct integration of the two-component Schrödinger equation.

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[3](a) In spite of the overlap in energy space, truly bound states are indeed possible if the impurity potential does not mix these states with any continuum states, e.g., the Coulombic states below $n=0$ and $l=1$ are bound whereas those below $n=1$ and $l=0$ are resonant. Although both overlap with the continuim of $n=0$ and $l=0$, a spherically symmetric potential mixes only states of the same l. (b) R. Kaplan, *Proceedings of the International Summer School on Narrow Gap Semiconductors,* edited by W. Zawadski

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$$V(r)=\int v(\vec{q})e^{i\vec{q}\cdot\vec{r}}d^3\vec{q}.$$

Substituting this in Eq. (12) we integrate over ρ which gives

$$I_{nn'}(Z)=-\frac{2m^*}{\hbar^2}\int v(q_\rho,q_z)P_{nn'}(q_\rho)\times e^{-1/2l^2q_\rho^2}e^{iq_zz}d^2q_\rho dq_z$$

where

$$P_{nn'}(q_\rho)e^{-1/2q_\rho^2l^2}=\int \chi_{n0}e^{i\vec{q}_\rho\cdot\vec{\rho}}\chi_{n'0}d^2\rho.$$

In the high-field limit, $v(q)$ has the form $A/(q_z^2+\Lambda^2)$ where A and Λ depend only on q_ρ. Thus the q_z integral can be done immediately to yield Eq. (28).