PHYSICAL REVIEW A VOLUME 16, NUMBER 2 AUGUST 1977

Phenomena exhibiting strong field mixing

A. R. P. Rau*
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803
(Received 7 February 1977)

Novel phenomena in which two fields are of equal importance in determining electronic properties are considered through simple, semiclassical arguments. Both the range of field strengths where such "strong mixing" of fields sets in and the nature of the subsequent spectrum are established. Since this feature has not always been appreciated, implications for recent experiments in diverse situations in atomic and solid-state physics are pointed out and further experiments to explore such phenomena suggested.

INTRODUCTION

In recent years, several interesting experiments have dealt with the motion of electrons under the simultaneous influence of two (or, sometimes, more) fields which may be various combinations of a Coulomb, an electric, and a magnetic field. It has not always been appreciated that some of these experiments are dealing with the particularly interesting situation where both the fields involved are of equal importance in determining the electronic properties. Since neither field can be treated in perturbation theory, the theoretical treatment seems complicated at first sight, but simple, semiclassical arguments can in fact provide considerable insight into the phenomena.

As a first step in handling such situations, we will present a unified way of estimating when such "strong mixing" of the two fields is to be expected and what the nature of the resulting spectrum will be. It is pointed out that some of the novel phenomena seen in the experiments correlate with the onset of this strong mixing. Such considerations and more sophisticated treatments of it will, therefore, be important for analyzing these phenomena and for the planning of future experiments. We consider, in particular, three classes of experiments which deal with rather diverse physical systems, but have close similarities with regard to the basic physics involved. They are

(1) the quadratic Zeeman effect and the so-called "diamagnetic shifts" seen[1] near the continuum edge of a Rydberg series of an atom such as Ba or Sr in a 10^4-G field;

(2) the spectra of image-potential-induced surface states outside liquid helium in the presence of electric and magnetic fields,[2] and

(3) infra-red spectra from the inversion layer in a Si-MOS (metal-oxide-semiconductor) system and the effect of high magnetic fields (10^5 G) on the absorption linewidths.[3-5]

We will analyze each of these in turn from a simple, unified point of view. The close similarities in the basic phenomena should, as one by-product, suggest further interesting experiments in each system.

DIAMAGNETIC SHIFTS NEAR THE CONTINUUM EDGE OF A RYDBERG SERIES

Garton and Tomkins[1] measured under high resolution and in the presence of fields of roughly 10^4 G the spectra of the transition $s^2\ {}^1S \rightarrow snp\ {}^1P$ in Ba and Sr. Rydberg states up to $n = 75$ could be clearly seen in the absence of the magnetic field. In the presence of the field, a normal Zeeman triplet is seen at low n for each n, with the $\Delta m = \pm 1$ lines symmetrically placed on either side of the unshifted $B = 0$ line. As n increases, these lines shift towards higher energies as the quadratic term becomes more important. With l and then, even n, ceasing to be a good quantum number as n gets large, the spectra become more complicated beyond $n \simeq 30$. Most strikingly of all, one observes that a pattern of broadened lines appears *beyond* the continuum edge ($6s\ {}^2S_{1/2}$ of Ba^+). This pattern consists of equally spaced lines with a separation which is roughly $\frac{3}{2}\hbar\omega$ where ω is the cyclotron frequency ($= eB/mc$). This pattern extends on *either* side of the continuum edge at $B = 0$ so that the edge essentially disappears. On the low-energy side this equally spaced pattern, which is drastically different from a Rydberg pattern, begins to set in at roughly $n = 60$ or 70. Explanations for this peculiar spacing of $\frac{3}{2}\hbar\omega$ in the observed pattern were given in a WKB picture by Edmonds[6] and Starace[7] and by O'Connell[8] through a semiclassical argument. The following semiclassical argument which gives both the spacing and the onset of this pattern is complementary to O'Connell's.

At low n, the Coulomb field is dominant and the magnetic field can be considered a perturbation. For electrons high in the continuum it will be the magnetic field that will be dominant and, in fact at sufficiently high energies, where the Coulomb field may be neglected at the first step and the electron considered as essentially free, one would have the usual Landau spectrum of equally spaced levels, $\hbar\omega$ apart. But the region around the edge, $E=0$, is precisely the one where both fields are equally important with the total energy resulting from equal and opposite contributions: the negative Coulomb energy E_C and the positive magnetic ener- E_m. Using the Rydberg quantum number n, we have

$$E_C = -Z^2e^2/(2a_0n^2)\,, \tag{1}$$

where a_0 is the Bohr radius. $Z=1$ for neutral atoms as in the experiment being considered, but we leave it open in Eq. (1) as an effective charge for other applications to be discussed later. Since we are considering large values of n, the quantum defect which should be subtracted from n in Eq. (1) is negligible and can be dropped. The magnetic energy can be written as[9]

$$E_m = \tfrac{1}{8}m\omega^2\langle x^2+y^2\rangle \simeq \tfrac{1}{10}m\omega^2\langle r^2\rangle \simeq \tfrac{1}{4}m\omega^2n^4a_0^2/Z^2\,, \tag{2}$$

where, for concreteness, numerical coefficients obtained with hydrogenic functions have been displayed, though not much significance should be attached to them. It is the dependences on ω and n that are of interest. Equation (2) has been written down as the expectation value of the magnetic energy evaluated in the Coulomb basis. We have in mind, however, that the magnetic field is far from being a perturbation and that, in fact, the two contributions, E_C and E_m, to the total energy are numerically comparable near the edge, $E\simeq 0$. Equating these values from Eqs. (1) and (2), we have

$$n = (\sqrt{2}B_0/B)^{1/3}, \tag{3}$$

where $B_0 \equiv Z^2me^3c/\hbar = 2.35\times 10^9 Z^2$. For self-consistency of the argument, we should equally well be able to follow an alternative procedure which starts with the magnetic field with its Landau spectrum,

$$E_m = n_m\hbar\omega\,. \tag{4a}$$

We use n_m to characterize the magnetic quantum number and, once again, drop an additive term of $\frac{1}{2}$ as negligible compared to the large quantum numbers involved. This alternative procedure is, in fact, the one followed in Ref. 8 where one adds on to Eq. (4a) the Coulomb energy $\langle -Ze^2/r\rangle$ evaluated on semiclassical grounds in terms of the magnetic field[8]:

$$E_C = -(Ze^2a_0)(B/2n_mB_0)^{1/2}\,. \tag{4b}$$

Once again, near the edge, if the expressions in (4a) and (4b) are to be numerically comparable, we get

$$n_m = (B_0/2B)^{1/3}\,. \tag{4c}$$

Apart from unimportant numerical constants, which cannot in any case be fixed uniquely through semiclassical arguments, the values of n and n_m in Eqs. (3) and (4c) are the same. This is what one would expect because in the strongly mixed situation, there is one combined motion of the electron under the equal influence of two fields, and there should be one characteristic quantum number to express this. The WKB argument of Ref. 7 also illustrated this point and worked with a one-dimensional WKB formula involving one quantum number. Further, Ref. 7 estimated this number to be in the energy 40–70 for field strengths of 10–50 kG, and the expressions in Eqs. (3) and (4c) conform to this estimate.

Both of the above chains of arguments—one of which starts with the magnetic energy and then adds the Coulomb energy whereas the other does just the opposite—and the demonstration that they lead to the same result, are necessary to establish the self-consistency of the handling of strong-field mixing by writing down a perturbation-like expression for the energy of one field and equating it to the zeroth-order energy of the other field. A further tightening of the self-consistency and, at the same time, a useful alternative statement of strong mixing, is provided by equating the two different expressions for E_m in Eqs. (2) and (4a) [or, for that matter, the two expressions for E_C in Eqs. (1) and (4b)]. This connects n_m and n according to

$$n_m = \tfrac{1}{4}(B/B_0)n^4\,. \tag{5a}$$

The case of strong mixing corresponds to a removal of the distinction between n_m and n so that solving Eq. (5a) with $n_m = n$ gives

$$n_m = n = (4B_0/B)^{1/3}\,. \tag{5b}$$

For $Z=1$ and $B=25$ kG, this yields $n\simeq 70$, which is indeed roughly the kind of value at which the pattern of equally spaced levels around the continuum edge sets in the experiments of Ref. 1. It would be of interest to verify experimentally the B dependence of n that is given by Eq. (5b).

The view of strong mixing that has been presented in the previous paragraph affords a convenient way of handling such phenomena in general and will be adopted for the other cases that we consider later in this paper. The prescription is to start with one field, say the Coulomb field as in Eq. (1). With this starting point, we write down the contribution due to the second field as in Eq. (2) and set this equal to the alternative expression for the same energy which we would have, had we started with the second field. This step links the two quantum numbers, and a solution with the quantum numbers equal gives the regime of strong mixing. Not only do we determine in this way the region of strong mixing but the nature of the spectrum also follows immediately. From Eqs. (1) and (2),

$$E = E_C + E_m = -\frac{Z^2e^2}{2a_0n^2} + \frac{m\omega^2a_0^2n^4}{4Z^2}. \quad (6)$$

Therefore,

$$\frac{\delta E}{\delta n} = -\frac{2E_C}{n} + \frac{4E_m}{n} = -\frac{2E}{n} + \frac{6E_m}{n}. \quad (7)$$

However, from Eq. (5a), we have $\delta n_m = 4(n_m/n)\delta n$, so that

$$\frac{\delta E}{\delta n_m} = -\frac{1}{2}\frac{E}{n_m} + \frac{3}{2}\frac{E_m}{n_m}. \quad (8)$$

Near the continuum edge, $E_m \simeq 0$, the separation between the energy levels is, therefore, $\frac{3}{2}\hbar\omega$. The same result would follow had we used for E_C and E_m in Eq. (6) the values from Eqs, (4a) and (4b) and, in fact, it was in this manner that Eq. (8) was derived in Ref. 8. Far from the edge, when either the Coulomb or the magnetic field is dominant, the spectrum is characteristic of the corresponding field as demonstrated by the first equality in Eq. (7).

IMAGE-POTENTIAL-INDUCED SURFACE STATES OUTSIDE LIQUID HELIUM

A series of experiments[2,10] have established that a layer of electrons can be created outside the surface of liquid helium. The motion of the electrons perpendicular to the surface (z direction) is bounded on one side by a high barrier presented by the liquid surface (which can be well approximated by an infinite barrier at $z=0$) and on the other by the Coulomb potential due to the induced image charge so that

$$V(z) = \infty \quad z \le 0,$$
$$= -Ze^2/z, \quad z > 0. \quad (9)$$

The effective charge Z depends[2] on the dielectric constant of liquid helium and is equal to 6.96×10^{-3}. The one-dimensional Schrödinger equation for the potential in Eq. (9) is formally identical to the radial equation for s waves for the ordinary Coulomb potential, $-Ze^2/r$, with the usual convention for the radial wave functions that they include a multiplicative factor r so that they are normalized with respect to $\int_0^\infty dr$ and have an r^{l+1} structure near the origin. Therefore, the spectrum of Eq. (9) consists of a Rydberg series given by Eq. (1). The levels are not eigenstates of parity and, therefore, with an applied electric field (potential $e\mathcal{E}z$) they exhibit a linear Stark effect, which has been studied in recent experiments.[2(a)] The experiments measured transitions between the various excited states and the ground state for fields ranging from about 10 to 300 V/cm. Linear extrapolation down to zero field gave energy separations differing somewhat from the simple Rydberg values, and modifications of Eq. (9) to account for these differences have been suggested.[2(a)] However, because of the smallness of Z, even at fields of 10 V/cm, there is a strong mixing of the Coulomb and electric fields down to small values of n so that there could be radical departures from a linear dependence with $\mathcal{E}$ for even the $1\to2$ transition which would have to be taken into account. The argument is very similar to the one in the previous section.

States of near zero energy E result from roughly equal and opposite contributions E_C due to the Coulomb and E_e due to the electric field. To E_C in Eq. (1) has to be added

$$E_e = e\mathcal{E}\langle z\rangle = \tfrac{3}{2}e\mathcal{E}n^2a_0/Z. \quad (10)$$

On the other hand, one can start with the electric field and the known[11] spectrum of such a "triangular" potential well,

$$E_e = (\hbar^2/2m)^{1/3}(e\mathcal{E})^{2/3}[\tfrac{3}{2}\pi(n_e+\tfrac{3}{4})]^{2/3}. \quad (11)$$

Equating the two expressions for E_e in Eqs. (10) and (11) provides the relation

$$n_e + \tfrac{3}{4} = 7.7\times10^{-6}(\mathcal{E}/Z^3)^{1/2}n^3, \quad (12)$$

where $\mathcal{E}$ is in V/cm. For the smallest fields in Ref. 2, with $\mathcal{E}=10$ V/cm, Eq. (12) has solutions with $n_e = n$ for values of about 5, whereas for fields of 250 V/cm, this comes down to $n=2$. Thus, over the range of fields studied the spectrum down to small values of n is not simply a Rydberg spectrum with slight perturbative contributions from the electric field, but rather a strongly mixed spectrum with its own distinct characteristics. From Eqs. (1) and (10), we get

$$\frac{\delta E}{\delta n} = -\frac{2E_C}{n} + \frac{2E_e}{n} = -\frac{2E}{n} + \frac{4E_e}{n}. \quad (13)$$

Using Eq. (12) to connect δn and δn_e, we have

$$\frac{\delta E}{\delta n_e} = -\frac{2E}{3n_e} + \frac{4}{3}\frac{E_e}{n_e}. \quad (14)$$

Near $E=0$, therefore, the separation between energy levels is $4E_e/3n_e$ and quite different from the separation in a pure Coulomb or pure electric field (which would be $2E_e/3n_e$).[12] A WKB argument which goes further and gives the positions and widths of the energy levels will be considered elsewhere.

Very recent experiments[2(b)] in this system have gone further in having in addition to the electric field in the z direction a magnetic field (up to 2 kG) in the y direction. Once again, strong-mixing phenomena of these fields can set in already at this level and may account for some of the observations. An estimate of the expected regime for such strong mixing is also of interest for what follows in the next section. For the z motion, the magnetic field contributes the energy $\frac{1}{8}m\omega^2\langle z^2\rangle$. With the Airy functions that are the solutions for the electric field and which give the energy values in Eq. (11), one can write

$$E_m = \tfrac{1}{8}m\omega^2\langle z^2\rangle = \tfrac{1}{15}m\omega^2(E_e/e\mathcal{E})^2 . \qquad (15)$$

Equating this to the energy characteristic of the magnetic field $E_m = 2(n_m + \frac{3}{4})\hbar\omega$, and using Eq. (11), we get

$$\left(n_m + \frac{3}{4}\right)\left[\frac{\mathcal{E}}{1\ \mathrm{V/cm}}\right]^{2/3} = \left(n_e + \frac{3}{4}\right)^{4/3}\left[\frac{B}{4700\ \mathrm{G}}\right] . \qquad (16)$$

The experiments[2(b)] include values of $\mathcal{E}$ and B for which both expressions in square brackets in Eq. (16) are about unity. For the lowest number densities in the surface layer in Ref 2(b), the corresponding value of $\mathcal{E}$ is 10 V/cm and the magnetic field used was 2 kG. This is already close to the regime of strong mixing for even the low-lying levels. A further increase in B by a factor of 10 would allow a clearer study of strong-mixing phenomena in which, in fact, all three fields (Coulomb, electric, and magnetic) are equally significant in determining the nature of the spectrum.

Yet another interesting aspect of the image-potential-induced states is worthy of study. With no $\mathcal{E}$ field and only a magnetic field along the surface, the z motion is an example of combined Coulomb and magnetic fields, the case studied in the previous section. Since $Z = 7\times10^{-3}$, the value of B_0 in Eqs. (3) and (5b) is now about 10^5 G and, therefore, with fields of 10^4 or 10^5 G, which are easily accessible in the laboratory, effects (such as the $\frac{3}{2}\hbar\omega$ levels) analogous to those studied[1] in the spectra of Ba and Sr can be seen at small values of n. This is, therefore, another attractive experimental system in which to study the phenomenon of diamagnetic shifts seen in the spectra of atoms.

INVERSION LAYER IN A Si-MOS

The study of the inversion layer[3-5] in such assemblies is a close counterpart to the study of the image-induced states outside of liquid helium. The inversion layer also represents an effectively two-dimensional electron gas which is held in the z direction by an infinite barrier (at $z=0$) due to the oxide layer on the one hand and an electric field, $e\mathcal{E}z$, on the other. The strength of the field is related to the number density in the inversion layer, N_i, and the density in the depletion layer, N_d, by[13]

$$\mathcal{E} = e(N_i + N_d)/k\epsilon_0 , \qquad (17)$$

where k is the dielectric constant of Si. The energy levels due to the quantized z motion are given by Eq. (11) with the appropriate effective mass m_z. There are two sets of energy levels because of motion corresponding to four degenerate valleys with $m_z = 0.19m$ and motion in two degenerate valleys with $m_z = 0.916m$.[13] The ground state E_0 of the latter will lie below the ground state E_0' of the former and, for the particular experiment wherein this difference is 46 meV, this value enables us to fix the value of $\mathcal{E}$ in Eq. (11). The result is consistent with $N_d = 1.2\times10^{11}$ cm^{-2} and $N_i = 8.3\times10^{11}$ cm^{-2} in Eq. (17), which are the values in Ref. 13. In turn, we get $E_0 = 66.7$ meV and $E_1 - E_0 = 50$ meV, where E_1 is the first excited state in the two-valley motion. This places E_1 slightly above E_0' in agreement with the conclusions in Ref. 3.[14]

The experiments[5] measured infrared absorption in the system with a magnetic field in the z direction, which leads to additional quantization of the motion of the electrons, this time in the plane of the inversion layer. An interesting phenomenon observed was a sudden narrowing of the line at the highest fields studied, 1.5×10^5 G, for $N_i < 2.5\times10^{11}$ cm^{-2}. There was also a shift in the position of the line as a function of B (for fixed absorption frequency) as N_i was lowered and finally a leveling-off, with no further change with N_i.

A mechanism involving two-electron correlations in the inversion layer has been invoked[15] to account for this, but it is our purpose here to point out that the phenomenon may also be an indication of strong-mixing effects leading to a substantial distortion of the equally spaced magnetic levels and, therefore, both a shift and a change in width of the transition between these levels. For the fields involved, Eq. (16) does suggest that one is close to the strong-mixing regime. An alternative indication of this is to set $\hbar\omega$ equal to $E_1 - E_0$, which is a measure of the strength of the electric field. We obtain

$$\frac{\hbar eB}{0.19mc} = (50\ \mathrm{meV})\left(\frac{N_i + N_d}{9.5\times10^{11}}\right)^{2/3} . \qquad (18)$$

For $N_i = 2\times10^{11}$ cm^{-2}, this gives $B = 4\times10^5$ G. Though the strongest fields in the experiment fall short of this value by a factor of 2, there could still be sufficient alteration in the spectrum already to account for the observations. In support of this, the correlation between the B value at resonance and $(N_i + N_d)^{2/3}$ that is given by Eq. (18) seems compatible with the observed[5] shift to lower B as N_i decreases. Equation (18) also accounts naturally for a final leveling-off because once N_i drops below $N_d = 1.2\times10^{11}$ cm^{-2}, there will be no further shift in the position of the absorption line. The many-body implications that follow as a corollary of Eq. (18) are that once the magnetic field gets strong enough that the energies associated with motion in the inversion layer are larger than the excitation energies for the motion in the electric field normal to the plane (or, correspondingly, the distances associated with the motion in the layer become smaller than the excursions the electrons make in the layer in the z direction), the system can no longer be treated as a two-dimensional electron gas. It will be energetically favorable to excite states associated with the z motion and, in the limit of very large B, the main motion of the electrons will be a one-dimensional z motion. A collection of such one-dimensional "beads on strings (B field)" will then replace the two-dimensional electron gas that one has at $B = 0$.

ACKNOWLEDGMENTS

Several conversations with Dr. A. K. Rajagopal and Dr. R. G. Goodrich are gratefully acknowledged.

*Work supported by the National Science Foundation under Grant No. PHY76-05721.

[1]W. R. S. Garton and F. S. Tomkins, Astrophys. J. 158, 839 (1969); F. S. Tomkins (private communcation).

[2](a) C. C. Grimes, T. R. Brown, M. L. Burns, and C. L. Zipfel, Phys. Rev. B 13, 140 (1976). (b) C. L. Zipfel, T. R. Brown, and C. C. Grimes, Phys. Rev. Lett. 37, 1760 (1976).

[3]D. C. Tsui and G. Kaminsky, Phys. Rev. Lett. 35, 1468 (1975); E. Gornik and D. C. Tsui, Phys. Rev. Lett. 37, 1425 (1976).

[4]G. Abstreiter, P. Kneschaurak, J. P. Kotthaus, and J. F. Koch, Phys. Rev. Lett. 32, 104 (1975).

[5]T. A. Kennedy, R. J. Wagner, B. D. McCombe, and D. C. Tsui (unpublished).

[6]A. R. Edmonds, J. Phys. (Paris) Colloq. 31, C4-71.

[7]A. F. Starace, J. Phys. B 6, 585 (1973).

[8]R. F. O'Connell, Astrophys. J. 187, 275 (1974).

[9]L. I. Schiff and H. Snyder, Phys. Rev. 55, 59 (1939). This was the first paper to consider the influence of a magnetic field on high-lying levels of a Rydberg spectrum.

[10]See, for instance, the review: M. W. Cole, Rev. Mod. Phys. 46, 451 (1974).

[11]*Selected Problems in Quantum Mechanics*, edited by D. ter Haar (Academic, New York, 1964), p. 82–86. The result in Eq. (11) is the semiclassical one that follows from the Bohr-Sommerfeld quantization rule, and it differs only very slightly from the exact expression which has in lieu of the sequence $(n_e + \frac{3}{4})$ the numbers 0.7587, 1.754, 2.7525, ... See also Ref. 13.

[12]Once again, a complementary argument would begin with Eq. (11) and add on $E_c = -Ze^2\langle 1/z\rangle \propto (n_e + \frac{3}{4})^{-2/3}$, and we would again recover Eq. (14). We also note that as remarked earlier, the one-dimensional problem considered here with $V(z) = e\mathcal{E}z - Ze^2/z$, $z > 0$, is identical to the radial problem for motion in the corresponding three-dimensional potential with r in place of z. Such a potential has been considered as a model for quark confinement, and the regime of strong mixing may again be the one of particular interest.

[13]F. Stern, Phys. Rev. B 5, 4891 (1972).

[14]The simple model for the z motion in the inversion layer in terms of a triangular potential well given by the field in Eq. (17) is supposed to hold only for $N_i \lesssim N_d$. Several papers have considered the modifications due to the image potential and the self-consistent interactions of the electrons in the layer [see T. Ando, Phys. Rev. B 13, 3468 (1976) and references therein]. In the present paper, we have restricted ourselves to the simple model, treating Eq. (11) as a model for the inversion layer and fitting it to the experimental value for $E'_0 = E_0$ in Ref. 3 to extract the parameter $\mathcal{E}$. The further results that follow for $E_1 - E_0$ and N_i are compatible with values in Refs. 3 and 13. Together with the feature that E_0 in Ref. 13 does exhibit the $(N_i + N_d)^{2/3}$ dependence that follows from Eqs. (11) and (17) at least up to $N = 10^{12}$ cm^{-2}, this compatibility lends confidence to our use of the simple picture to estimate when strong mixing with the magnetic field is to be expected and to understand the results of Ref. 5 in terms of this condition as given in Eq. (18).

[15]K. L. Ngai and T. L. Reinecke, Phys. Rev. Lett. 37, 1418 (1976).