Some problems connected with the spectra of atoms in solids

being

A study of the theory of the absorption edge in semiconductors

by

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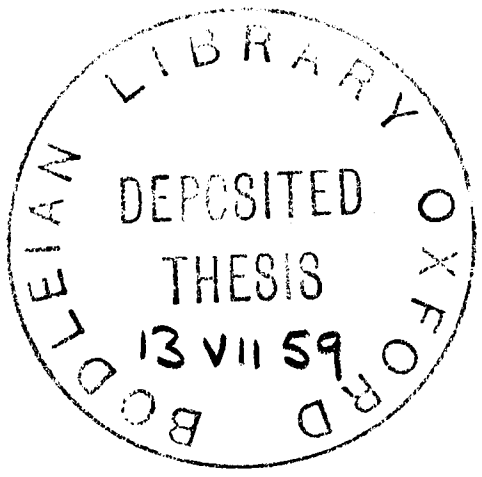

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Abstract

The thesis is concerned with optical absorption by a semiconductor due to the excitation of electrons from the valence band to the conduction band giving rise to the phenomenon of the absorption edge. In treating the final state of the semiconductor in such an absorption process it is shewn that the system may be considered as a two particle one in which the excited electron in the conduction band is bound to the hole left behind in the valence band, which behaves in many ways like a positively charged particle. A bound system of this type is called an exciton. The theory of the exciton is developed in some detail in the effective mass approximation for the case of a semiconductor with spherical energy bands. The effect of an externally applied uniform magnetic field is calculated.

Using the exciton wave-function derived in this way, a general expression for the absorption coefficient due to exciton creation in a magnetic field is obtained. The evaluation of this formula requires a knowledge of the wave-functions of the hydrogen atom in a magnetic field. For special cases, e.g. zero magnetic

field, it is shewn how the general absorption coefficient formula leads to expressions previously derived by other authors.

The wave-equation for the hydrogen atom in a magnetic field is solved by a perturbation theory approach for the case where the magnetic field energy is larger than the Coulomb energy, a case of some importance in semiconductors since the Coulomb interaction is reduced by the dielectric constant and the electron or hole effective masses are usually small. Both bound and free states of the exciton are considered, and formal expressions for f-values and absorption coefficients are presented.

These formal expressions are evaluated numerically for some important cases. The positions and intensities of the lowest observable absorption lines are calculated when the electronic transition from the valence band to the conduction band is either allowed or forbidden, and the values of the absorption coefficients close to the absorption edge are determined.

Finally the accuracy of the perturbation theory method used is assessed and recent experimental work on the absorption edge is discussed.

Contents

Chapter 1. INTRODUCTION.

1. The Absorption Edge. The infra-red absorption spectrum of a semiconductor provides important information about the electronic energy band structure of the crystal. To understand the qualitative features of the spectrum, only a simple discussion of the form of the energy bands of a semiconductor is required. The wave-function of an electron in the periodic potential field of a crystal may be taken in the Bloch form, which will be written $\psi_{n\underline{k}}(\underline{r})$. Here $\underline{r}$ is the position vector of the electron and $\underline{k}$ is its wave-vector. The energy of an electron in this state will be denoted by $E_n(\underline{k})$. For a given wave-vector $\underline{k}$ the electron may have many different wave-functions and these are enumerated by the subscript n. The states having a fixed value of n but different values of $\underline{k}$ are said to form the nth electronic energy band. These energy bands may be regarded as pseudo-surfaces in a four-dimensional space in which the four Cartesian axes are the energy $E_n(\underline{k})$ and the three components of the wave-vector $\underline{k}$. All distinct solutions of the wave-equation for an electron in the crystal are obtained by restricting $\underline{k}$ to lie in the first Brillouin zone corresponding to the crystal lattice under consideration. For a finite crystal containing N unit cells $\underline{k}$ has discrete eigenvalues, there being N of these within the first Brillouin zone. Neglecting electron

spin, as we shall do throughout, the maximum number of electrons which can occupy an energy band is therefore N.

A semiconducting crystal in its ground state has an energy band system in which a certain number of bands is filled and the remaining bands are empty. The filled bands of highest energy are the valence bands while the lowest empty bands are the conduction bands, and the points in E - $\underline{k}$ space where a valence band has its maximum energy and a conduction band has its minimum energy are called band edges. The energy separation between the highest valence band edge and the lowest conduction band edge is called the forbidden energy gap, and has values in the range nought to five electron volts. If radiation of a certain frequency is allowed to fall on a semi-conductor, absorption may take place if the photon energy is sufficiently large to excite valence electrons across the forbidden energy gap into the conduction bands. As the photon energy is lowered the absorption falls rapidly to zero at about the energy of the forbidden gap, giving rise to an absorption edge at a frequency which is usually in the infra-red or optical regions. Below this frequency the semiconductor is transparent.

In recent years there has been a great deal of experimental and theoretical study of the shape of the absorption edge in various semiconductors. High resolution experiments have shewn that the absorption edge may have a complicated shape and in some substances series of lines have been resolved. For example in cuprous oxide series of lines with spacings proportional to the

hydrogen atom level spacings have been observed at the absorption edge[1,2], while in germanium only one or two lines have been observed at the present time[3,4].

The band structures of some important semiconductors are known to be exceedingly complex. Several bands may be degenerate at the band edges, and the conduction (valence) band may have several energy minima (maxima) disposed about the Brillouin zone in a symmetrical array. By electronic standards the momentum carried by a photon is negligible, so that if momentum is to be conserved in the absorption process, the momentum of the excited electron must be unchanged as it moves from the valence band to the conduction band. Such a transition which conserves the total electronic momentum is called a vertical or a direct transition. However higher order processes are possible in which a phonon is created or annihilated at the same time as the photon is absorbed. In this case the excited electron, or the hole left behind in the valence band, must change its momentum during the absorption process in such a way as to compensate for the momentum carried away or given up by the phonon. Such an absorption process is called a non-vertical or indirect transition. It is clear that an electron can be transferred from any point in the valence band to any point in the conduction band by interaction with a suitable phonon in an absorption process of this kind. It follows that a semiconductor with several conduction band minima or valence band maxima may display several absorption edges.

These complications render detailed calculations of the

form of the absorption spectrum, using the known structure of the energy bands, impracticable for many semiconductors. Quantitative calculations have therefore in the main been carried out for an ideal semiconductor having spherical non-degenerate energy bands. This simplification will be adopted in the present discussion which will also be restricted to the case where both band edges occur at the centre of the Brillouin zone, i.e. at $\underline{k} = 0$. The theories considered below will therefore apply only to vertical transitions.

A theory based on the above approximations would be expected to yield only qualitative information about the form of the direct absorption edge in a semiconductor like germanium, which has a band structure of the complicated type described above, but the calculations should have some quantitative significance for a semiconductor such as cuprous oxide in which the energy bands seem to be approximately spherical.

2. Previous Calculations. Using the basic approximation of a simple energy band model, the photon absorption process may be treated theoretically in either of two degrees of refinement. In the less refined calculation the electron which has been excited into the conduction band is regarded as a free conduction electron whose wave-function is just the Bloch function corresponding to its momentum state. A calculation of this type leads to simple formulae for the shape of the absorption edge and line spectra of the form observed experimentally are not predicted[5]. To account for these line spectra

at the absorption edge the theory must be improved by inclusion of the effect due to the hole which is left behind in the valence band when an electron is excited into the conduction band. The hole behaves in many ways like a positively charged particle and in particular it exerts a Coulomb attraction on the excited electron. Because of this attraction the electron-hole pair may form bound hydrogen-like states in which case the pair is called an 'exciton'[6]. These bound states are formed by photons of energies smaller than the forbidden energy gap by an amount equal to the exciton binding energy and they give rise to a series of lines just below the absorption edge.

The semiconductors of interest have large dielectric constants as a result of which the electron-hole Coulomb interaction is weak and the electron-hole separation is correspondingly large compared to the lattice constant, so that the exciton can be treated in the effective mass approximation using methods similar to those developed by Luttinger and Kohn[7] for the treatment of impurity states in semiconductors. Dresselhaus[8] has demonstrated the way in which effective mass methods can be used for excitons and Elliott[9] has calculated line strengths and absorption coefficients taking excitonic effects into account. The main effect of including the electron-hole Coulomb interaction in the theory is that the wave-function of the system involves a sum of products of pairs of conduction and valence band Bloch functions corresponding to moments close to the conduction and valence band edges, instead of the single such product which is obtained when the Coulomb interaction is neglected. A study of the

absorption edge therefore gives information about the Bloch states just above and just below the forbidden energy gap. In particular information about the valence and conduction band effective masses is obtained.

This information may be supplemented by a study of the effects of magnetic fields on the absorption spectrum of the semiconductor. Experiments of this type are analogous to Zeeman effect experiments in atomic spectroscopy and similarly yield information about the nature of the energy levels responsible for the observed spectrum. Although the Zeeman effect has long been a powerful tool in elucidating the details of atomic spectra, the corresponding experiments in semiconductor spectroscopy have only recently been carried out successfully. It is observed that in the presence of a magnetic field the spectrum of the continuous absorption region above the edge changes shape and may form a series of peaks, while the discrete excitonic absorption lines change in position and intensity.

As in the zero field case the theory of optical absorption in a magnetic field may be worked out either with or without the inclusion of the Coulomb interaction between the electron and hole. The problem without the Coulomb interaction has already been treated[10], and the main result of this work is that in certain cases the continuous absorption above the edge should break up into a series of peaks whose distance from the absorption edge varies linearly with the magnetic field. The width of the forbidden

energy gap should therefore be determined very accurately by extrapolating the positions of the observed peaks back to zero magnetic field: a direct measurement of the energy gap is hampered by the clutter of lines due to bound exciton states which obscures the low frequency side of the absorption edge.

However a theory which does not take account of the electron-hole Coulomb interaction can make no predictions about the effect of a magnetic field on the bound exciton states and their associated line spectrum. Also the Coulomb interaction can make a radical change in the nature of the continuous absorption close to the edge as is shewn by the zero field case where the absorption coefficient at the edge is increased from zero to a finite value by the inclusion of Coulomb effects[9].

For these reasons it is important that a theory of optical absorption in the presence of a magnetic field should be developed which takes into account the excitonic nature of the final state produced in the semiconductor. It is the main purpose of this thesis to present such a theory. The arrangement of the work will be described in the following section.

3. The Present Calculation. In chapter 2 the general theory of the exciton in a magnetic field is derived in the effective mass approximation. It is shewn that the exciton wave-function consists of a product of three functions. The first two functions are linear combinations of Bloch functions corresponding to zero wave-vector,

i.e. $\underline{k} = 0$, one of these linear combinations representing the hole and the other the electron. The third component is a function denoted by F which will be called the envelope function of the exciton. The effect of the periodic lattice of the crystal on the exciton wave-function is entirely accounted for by its Bloch function components, and the envelope function F satisfies a Schrödinger equation which is independent of the lattice, being just that of a hydrogen atom in a magnetic field but with the Coulomb interaction reduced by the dielectric constant of the semiconductor.

Using this exciton wave-function, f-values and absorption coefficients for electric dipole absorption by excitons can be derived and a general formula for these quantities is presented at the beginning of chapter 3. In deriving this formula use is made of the results of appendix 1 where the effect of the refractive index of the semiconductor on the absorption coefficient is investigated. It is found that the absorption coefficient depends on the properties of the envelope function F at the points where its arguments, i.e. the position vectors of the electron and hole, are equal. With the aid of the general formula the absorption coefficients given by previous authors for less general cases may be easily derived. For example, the results of Elliott et al.[10] are obtained if the Coulomb term is removed from the Schrödinger equation for F. All the previously given absorption coefficients for direct optical transitions are derived in chapter 3 to demonstrate the ease with which the new general formula can be used. The wave-functions necessary for dealing

with the magnetic field case are obtained in appendix 2.

Chapter 4 contains the main contribution of the present calculation, a consideration of the theory of optical absorption in a magnetic field taking excitons into account. We have stated above, and will prove in chapter 2, that the envelope function F for this case satisfies the same wave-equation as the hydrogen atom in a magnetic field. Conservation of momentum requires that the centre of mass of the exciton shall be at rest and as a result of this we are concerned only with the familiar equation for the relative motion of the two particles constituting the exciton or hydrogen atom. In discussing the methods of solution of this equation it is convenient to characterize the strength of the magnetic field by its zero point energy $\frac{1}{2}\hbar\omega_c$, where ω_c is the cyclotron frequency, and to characterize the strength of the Coulomb interaction by the binding energy, R say, of the ground state of the exciton in zero magnetic field:

For $\frac{1}{2}\hbar\omega_c \ll R$ the magnetic field is weak and the magnetic field terms in the hydrogen atom Schrödinger equation can be treated by perturbation theory. The bound exciton states exhibit the usual Zeeman and quadratic Zeeman effects.

For $\frac{1}{2}\hbar\omega_c \sim R$ the Coulomb and magnetic field terms are equally important and there is no simple way of solving the Schrödinger equation.

For $\frac{1}{2}\hbar\omega_c \gg R$ a perturbation theory approach again becomes possible, for the Coulomb energy is now small in

comparison with the magnetic field energy and the Coulomb term can be treated as a perturbation.

To give some idea of the type of approximation suitable for dealing with experimentally obtainable fields we list the magnetic field strengths required to attain the condition $\frac{1}{2}\hbar\omega_c = R$ for several semiconductors and also for the hydrogen atom:

Hydrogen atom	:	2,400,000,000 gauss
Germanium	:	8,900 gauss
Cuprous oxide	:	6,500,000 gauss
Indium antimonide	:	1,900 gauss

In the cases of Ge and particularly of InSb experiments for which the condition $\frac{1}{2}\hbar\omega_c \gg R$ holds can easily be carried out. However for Cu_2O the condition $\frac{1}{2}\hbar\omega_c \ll R$ will always hold since the steady magnetic fields normally available are of the order of tens of thousands of gauss. The critical field for an exciton in Cu_2O is lower than that for the hydrogen atom by a factor of about 370 and this difference results in the quadratic Zeeman effect being easily observable in a Cu_2O exciton whereas it is not in hydrogen.

It is seen that excitons may be expected to display a great diversity of Zeeman effects. The case considered in chapter 4 is that of a high magnetic field, $\frac{1}{2}\hbar\omega_c \gg R$, though the low magnetic field Zeeman effects will be briefly mentioned in the following chapter in connection with a discussion of experimental work on Cu_2O. Previous work on the high magnetic field case has been restricted to bound impurity states for which the Schrödinger equation to be solved is very

similar to that for the exciton. The variation in the energy of the ground state with magnetic field has been calculated by numerical integration of an approximate Schrödinger equation using an electronic computor[11] and calculations on the lowest few bound levels have been carried out using variational wave-functions[12,13]. The approximate method of calculation presented in chapter 4 applies to both bound and continuum states of the exciton in a magnetic field. Further, the energies of excited states are as easily calculated as the energy of the ground state in various magnetic fields, which is not the case with the variational calculations where the numerical complexity of the computations increases as one goes to higher states.

Formal expressions for line strengths and absorption coefficients are also presented in chapter 4. In deriving these much use is made of the properties of Whittaker's confluent hypergeometric functions and these are briefly treated in appendix 3. In the limit of an infinite magnetic field the component of the wave-function corresponding to motion along the field separates and satisfies the one-dimensional hydrogen atom wave-equation. It is useful to know the solution of the problem in the infinite field limit, and the final appendix is therefore devoted to the one-dimensional hydrogen atom.

In chapter 5 the results of numerical calculations based on the preceding theory are given. The variations in the energies and intensities of the most important bound state exciton lines with magnetic field are plotted and the shape of the absorption edge at several magnetic field strengths is given. A discussion of these results

will be deferred until chapter 5. Finally the range of validity of the approximate method of chapter 4 will be considered and experimental work on the absorption edge will be commented upon.

Chapter 2. EFFECTIVE MASS THEORY FOR THE EXCITON.

1. Introduction. Consider a solid having simple valence and conduction bands, both with their edges at the centre of the Brillouin zone. Let the volume of the unit cell be Ω and let N be the number of unit cells in the crystal. Let $H_o(\underline{r})$ be the Hamiltonian of an electron in the periodic potential of the crystal. We denote the eigenfunctions of H_o, the Bloch functions, by:

$$\psi_{n\underline{k}}(\underline{r}) = e^{i\underline{k}.\underline{r}}\, u_{n\underline{k}}(\underline{r}) \qquad (2.1)$$

where n specifies the band and $\underline{k}$ the wave-vector. The eigenvalues of H_o we denote by $E_n(\underline{k})$ so that:

$$H_o(\underline{r})\,\psi_{n\underline{k}}(\underline{r}) = E_n(\underline{k})\,\psi_{n\underline{k}}(\underline{r}) \qquad (2.2)$$

The Bloch functions are defined only at discrete values of $\underline{k}$, there being N of these allowed values in each energy band, say $\underline{k}_1, \underline{k}_2, \ldots\ldots \underline{k}_N$ (we are neglecting spin). In the ground state, when the valence band is full, the zero order wave-function is given by a Slater determinant:

$$\Psi_o = \frac{1}{\sqrt{N!}}\,\mathcal{A}\,\psi_{v\underline{k}_1}(\underline{r}_1)\,\psi_{v\underline{k}_2}(\underline{r}_2)\ldots\ldots\ldots\,\psi_{v\underline{k}_N}(\underline{r}_N) \qquad (2.3)$$

where $\mathcal{A}$ is an antisymmetrization operator, operating on the electron co-ordinates. Consider now a state of the crystal in which a

single electron has been excited from state $\psi_{v,-\underline{k}_h}(\underline{r}_h)$ in the valence band to a state $\psi_{c\underline{k}_e}(\underline{r}_e)$ in the conduction band to form an exciton. The wave-function is given in zero order by:

$$\Psi_{\underline{k}_e,-\underline{k}_h} = \frac{1}{\sqrt{N}} \mathcal{A}\, \psi_{v\underline{k}_1}(\underline{r}_1) \cdots \psi_{c\underline{k}_e}(\underline{r}_e) \cdots \psi_{v\underline{k}_N}(\underline{r}_N) \qquad (2.4)$$

where $\psi_{c\underline{k}_e}(\underline{r}_e)$ has replaced the valence band Bloch function $\psi_{v,-\underline{k}_h}(\underline{r}_h)$. There are N^2 wave-functions of this type corresponding to the N possible choices each for $\underline{k}_e$ and $\underline{k}_h$. The Hamiltonian of the system is:

$$H = \sum_i H_o(\underline{r}_i) + \sum_{i<j} \frac{e^2}{r_{ij}} \qquad (2.5)$$

Using this Hamiltonian and the basic set of wave-functions (2.4) it is possible to calculate the energy matrix for the system, the calculation being very similar to that used to set up the electrostatic energy matrix of a many electron atom (Corson[14] treats this problem very fully). A general matrix element of the Hamiltonian has the form:

$$\begin{aligned}\left(\Psi_{\underline{k}_e,-\underline{k}_h} \middle| H \middle| \Psi_{\underline{k}'_e,-\underline{k}'_h}\right) = {} & \left[E_o + E'_c(\underline{k}_e) - E'_v(\underline{k}_h)\right] \delta_{\underline{k}_e\underline{k}'_e}\, \delta_{\underline{k}_h\underline{k}'_h} \\ & + \left\{ -\iint \psi^*_{v,-\underline{k}'_h}(\underline{r}_h)\, \psi^*_{c\underline{k}_e}(\underline{r}_e) \frac{e^2}{|\underline{r}_e - \underline{r}_h|} \psi_{v,-\underline{k}_h}(\underline{r}_h)\, \psi_{c\underline{k}'_e}(\underline{r}_e)\, d\underline{r}_e d\underline{r}_h \right. \\ & \left. + \iint \psi^*_{v,-\underline{k}'_h}(\underline{r}_h)\, \psi^*_{c\underline{k}_e}(\underline{r}_e) \frac{e^2}{|\underline{r}_e - \underline{r}_h|} \psi_{v,-\underline{k}_h}(\underline{r}_e)\, \psi_{c\underline{k}'_e}(\underline{r}_h)\, d\underline{r}_e d\underline{r}_h \right\} \\ & \times \delta_{\underline{k}_e+\underline{k}_h,\, \underline{k}'_e+\underline{k}'_h}\end{aligned} \qquad (2.6)$$

where E_0 is the ground state energy, $E'_c(\underline{k}_e)$ is the conduction band energy $E_c(\underline{k}_e)$ renormalised to take into account the interaction of the excited electron with all the electrons in the valence band, and $E'_v(\underline{k}_h)$ is similarly defined.

The most striking feature of the matrix element (2.6) is that, apart from the renormalisation of the energy bands, only the Bloch functions corresponding to the excited electron and the electron missing from the valence band are involved. In fact the matrix elements of $e^2/|\underline{r}_e - \underline{r}_h|$ which occur are the same as we should have if there were only two electrons in the system, except that their signs are reversed. This reversal of sign indicates that the system can be regarded as a two particle one involving a 'hole' with effective positive charge in the valence band and an electron in the conduction band. The form of (2.6) shows that if we are prepared to neglect the contribution to the energy matrix arising from the exchange integrals (third line) while retaining integrals of the Coulomb type (second line), then the wave-functions of the exciton may be expanded in a series of products of pairs of Bloch functions instead of a series of products of N Bloch functions, provided that their renormalized energy eigenvalues are used.

An analogous state of affairs to the above occurs in atomic physics for a configuration of the type $l_1^{n-1} l_2$ where n is the number of electrons in a closed shell for orbital angular momentum l_1. In the expressions for the energy level spacings due to the electrostatic interaction between the l_2 electron and the nearly closed shell, the

terms resulting from Coulomb integrals are the same, except for a change of sign, as for the configuration $l_1 l_2$ obtained by replacing the 'hole' in the almost closed shell by an electron. The two configurations have of course the same allowed states.

If we consider a diagonal matrix element of the type (2.6) then the first integral represents the energy due to the Coulomb interaction between two charge distributions $|\psi_{v,-k_h}(\underline{r}_h)|^2$ and $|\psi_{c k_e}(\underline{r}_e)|^2$ and this term is appreciable even when the electron-hole separation is large compared to the lattice constant. For a discussion of the second integral in (2.6) it is more convenient to transform from the Bloch functions to a set of localised functions, the Wannier functions,[6] defined by:

$$a_n(\underline{r} - \underline{R}) = \frac{1}{\sqrt{N}} \sum_{\underline{k}} e^{-i\underline{k}\cdot\underline{R}} \psi_{n\underline{k}}(\underline{r}) \qquad (2.7)$$

where $\underline{R}$ is a lattice point. For a given band n there are N Bloch functions corresponding to the N values of $\underline{k}$ and N Wannier functions corresponding to the N lattice points. Transforming to these localised functions the diagonal exchange integral may be reduced to[15]:

$$\iint a_v^*(\underline{r}_h - \underline{R}_1)\, a_c^*(\underline{r}_e - \underline{R}_2) \frac{e^2}{|\underline{r}_e - \underline{r}_h|}\, a_v(\underline{r}_e - \underline{R}_1)\, a_c(\underline{r}_h - \underline{R}_2)\, d\underline{r}_e\, d\underline{r}_h$$

Since the Wannier functions are localised this integral is negligible unless $\underline{R}_1 = \underline{R}_2$, in which case its value has the order of magnitude of an atomic exchange integral. Hence in (2.6) the diagonal exchange integral is approximately equal to the probability that the electron

and hole are centred on the same lattice point times the appropriate atomic exchange integral. The off-diagonal matrix elements of the type (2.6) are less important than the diagonal ones. Numerical estimates of the order of magnitude of the exchange integral for the semiconductors of interest shew that it is negligible in comparison with the Coulomb integral. The approximation of neglecting it is therefore a good one and will be adopted here.

Regarding then the exciton as a two particle problem, we can write down the exciton Hamiltonian as:

$$H_{Ex}(\underline{r}_e, \underline{r}_h) = H_o(\underline{r}_e) + H_o(\underline{r}_h) + V(\underline{r}_e - \underline{r}_h) \tag{2.8}$$

where $V(\underline{r}_e - \underline{r}_h)$, the interaction between the electron and hole, will not be completely specified at the moment. In determining the eigenfunctions and eigenvalues of this Hamiltonian we follow closely the methods used by Luttinger and Kohn[7] in their treatment of impurity states in semiconductors. Instead of expanding the exciton wave-function in a series of products of pairs of Bloch functions, we use the set of functions:

$$\chi^{st}_{\underline{k}_e \underline{k}_h} = e^{i\underline{k}_e \cdot \underline{r}_e} u_{so}(\underline{r}_e)\, e^{i\underline{k}_h \cdot \underline{r}_h} u_{to}(\underline{r}_h) \tag{2.9}$$

These functions form a complete set since any product of two Bloch functions can be expanded in them and the Bloch functions themselves form a complete set.

Although the Bloch functions are strictly defined only at discrete values of $\underline{k}$, it is convenient to take the range of $\underline{k}$ to be

continuous so that integrals can be used instead of summations. We accordingly assume the following normalisation:

$$\int_{\text{crystal}} \psi^{*}_{n\underline{k}}(\underline{r})\,\psi_{n'\underline{k}'}(\underline{r})\,d\underline{r} = \delta_{nn'}\,\delta(\underline{k}-\underline{k}') \qquad (2.10)$$

With this assumption it may be shown that the functions (2.9) form an orthonormal set if we make use of the theorem that if $f(\underline{r})$ is any function which is periodic with the periodicity of the lattice then:

$$\int_{\text{crystal}} e^{i(\underline{k}'-\underline{k})\cdot\underline{r}}\,f(\underline{r})\,d\underline{r} = \frac{(2\pi)^3}{\Omega}\,\delta(\underline{k}'-\underline{k})\int_{\text{unit cell}} f(\underline{r})\,d\underline{r} \qquad (2.11)$$

This theorem is proved as follows. $f(\underline{r})$ can be expanded in a Fourier series involving only the reciprocal lattice vectors $\underline{K}_m$:

$$f(\underline{r}) = \sum_m B_m\,e^{-i\underline{K}_m\cdot\underline{r}} \qquad (2.12)$$

Hence:

$$\int_{\text{all space}} e^{i(\underline{k}'-\underline{k})\cdot\underline{r}}\,f(\underline{r})\,d\underline{r} = \sum_m B_m \int_{\text{all space}} e^{i(\underline{k}'-\underline{k}-\underline{K}_m)\cdot\underline{r}}\,d\underline{r}$$

$$= (2\pi)^3 \sum_m B_m\,\delta(\underline{k}'-\underline{k}-\underline{K}_m) \qquad (2.13)$$

The only possible $\underline{K}_m$ which $\underline{k}' - \underline{k}$ can be equal to is $\underline{K}_0 = 0$ since $\underline{k}'$ and $\underline{k}$ both lie within the first Brillouin zone. Hence the right hand side of (2.13) reduces to just one term:

$$\int_{\text{all space}} e^{i(\underline{k}'-\underline{k}).\underline{r}}\, f(\underline{r})\, d\underline{r} = (2\pi)^3 B_0\, \delta(\underline{k}'-\underline{k}) \qquad (2.14)$$

Multiply both sides of (2.12) by $e^{i\underline{K}_m.\underline{r}}$ and integrate over the unit cell:

$$\int_{\text{unit cell}} e^{i\underline{K}_m.\underline{r}}\, f(\underline{r})\, d\underline{r} = B_m \Omega \qquad (2.15)$$

Combination of (2.14) and (2.15) now leads to (2.11), which we observe holds strictly only for an infinite crystal.

Applying this theorem to the $u_{n\underline{k}}(\underline{r})$ which are lattice periodic, we may carry out the normalisation integral for the expansion functions (2.9):

$$\iint_{\text{crystal}} \chi^{s't'*}_{\underline{k}'_e\underline{k}'_h}\, \chi^{st}_{\underline{k}_e\underline{k}_h}\, d\underline{r}_e\, d\underline{r}_h = \frac{(2\pi)^6}{\Omega^2} \iint_{\text{unit cell}} v^*_{s'0}(\underline{r}_e)\, v_{s0}(\underline{r}_e)\, v^*_{t'0}(\underline{r}_h)\, v_{t0}(\underline{r}_h)\, d\underline{r}_e\, d\underline{r}_h \times \delta(\underline{k}'_e-\underline{k}_e)\,\delta(\underline{k}'_h-\underline{k}_h)$$

But by (2.10):

$$\frac{(2\pi)^3}{\Omega} \int_{\text{unit cell}} v^*_{n\underline{k}}(\underline{r})\, v_{n'\underline{k}}(\underline{r})\, d\underline{r} = \delta_{nn'} \qquad (2.16)$$

Hence:

$$\iint_{\text{crystal}} \chi^{s't'*}_{\underline{k}'_e\underline{k}'_h}\, \chi^{st}_{\underline{k}_e\underline{k}_h}\, d\underline{r}_e\, d\underline{r}_h = \delta(\underline{k}'_e-\underline{k}_e)\,\delta(\underline{k}'_h-\underline{k}_h)\,\delta_{s's}\,\delta_{t't} \qquad (2.17)$$

and we have proved the orthonormality of our set of expansion functions.

2. Derivation of the Effective Mass Equation. We expand an exciton wave-function in the χ as follows:

$$\Psi_n^{Ex}(\underline{r}_e, \underline{r}_h) = \sum_{s',t'} \iint_{B.Z.} A_n^{s't'}(\underline{k}_e', \underline{k}_h') \chi_{\underline{k}_e' \underline{k}_h'}^{s't'} \, d\underline{k}_e' \, d\underline{k}_h' \qquad (2.18)$$

where $\underline{k}_e'$ and $\underline{k}_h'$ are integrated over the Brillouin zone and s', t' are summed over all the bands. The $A_n^{s't'}$ are expansion coefficients, n enumerating the different states of the system. Using (2.17) the normalization condition for the exciton wave-function is:

$$\sum_{s't'} \iint_{B.Z.} \left| A_n^{s't'}(\underline{k}_e', \underline{k}_h') \right|^2 d\underline{k}_e' \, d\underline{k}_h' = 1 \qquad (2.19)$$

To find the energy levels E_n^{Ex} of the exciton we require to solve:

$$H_{Ex}(\underline{r}_e, \underline{r}_h) \Psi_n^{Ex}(\underline{r}_e, \underline{r}_h) = E_n^{Ex} \Psi_n^{Ex}(\underline{r}_e, \underline{r}_h) \qquad (2.20)$$

Substitute for Ψ from (2.18), multiply both sides by $\chi_{\underline{k}_e \underline{k}_h}^{st\,*}$ and integrate over $\underline{r}_e$ and $\underline{r}_h$:

$$\sum_{s't'} \iint_{B.Z.} A_n^{s't'}(\underline{k}_e', \underline{k}_h') \iint_{crystal} \chi_{\underline{k}_e \underline{k}_h}^{st\,*} H_{Ex} \chi_{\underline{k}_e' \underline{k}_h'}^{s't'} \, d\underline{r}_e \, d\underline{r}_h \, d\underline{k}_e' \, d\underline{k}_h' = E_n^{Ex} A_n^{st}(\underline{k}_e, \underline{k}_h) \qquad (2.21)$$

We evaluate the integral on the left separately for each of the three terms in H_{Ex} given by (2.8), i.e. the electron and hole kinetic energies and the interaction term:

$$\iint_{\text{crystal}} \chi^{st\,*}_{\underline{k}_e \underline{k}_h} H_0(\underline{r}_e)\, \chi^{s't'}_{\underline{k}_e' \underline{k}_h'}\, d\underline{r}_e\, d\underline{r}_h \tag{2.22}$$

$$= \delta_{tt'}\, \delta(\underline{k}_h' - \underline{k}_h) \left\{ \left[E_s(0) + \frac{\hbar^2 k_e^2}{2m} \right] \delta_{ss'} + \frac{\hbar \underline{k}_e \cdot \underline{p}_{ss'}}{m} \right\} \delta(\underline{k}_e' - \underline{k}_h)$$

where we have again used the theorem (2.11) and the normalization (2.10). By definition:

$$\underline{p}_{ss'} = \frac{(2\pi)^3}{\Omega} \int_{\text{unit cell}} u^*_{s0}(\underline{r}) \left(-i\hbar\nabla\right) u_{s'0}(\underline{r})\, d\underline{r} \tag{2.23}$$

m being the free electron mass. Similarly:

$$\iint_{\text{crystal}} \chi^{st\,*}_{\underline{k}_e \underline{k}_h} H_0(\underline{r}_h)\, \chi^{s't'}_{\underline{k}_e' \underline{k}_h'}\, d\underline{r}_e\, d\underline{r}_h \tag{2.24}$$

$$= \delta_{ss'}\, \delta(\underline{k}_e' - \underline{k}_e) \left\{ \left[E_t(0) + \frac{\hbar^2 k_h^2}{2m} \right] \delta_{tt'} + \frac{\hbar \underline{k}_h \cdot \underline{p}_{tt'}}{m} \right\} \delta(\underline{k}_h' - \underline{k}_h)$$

Finally the interaction term gives:

$$\iint_{\text{crystal}} \chi^{st\,*}_{\underline{k}_e \underline{k}_h} V(\underline{r}_e - \underline{r}_h)\, \chi^{s't'}_{\underline{k}_e' \underline{k}_h'}\, d\underline{r}_e\, d\underline{r}_h \tag{2.25}$$

$$= \iint_{\text{crystal}} e^{-i\underline{k}_e \cdot \underline{r}_e} u^*_{s0}(\underline{r}_e)\, e^{-i\underline{k}_h \cdot \underline{r}_h} u^*_{t0}(\underline{r}_h)\, V(\underline{r}_e - \underline{r}_h)\, e^{i\underline{k}_e' \cdot \underline{r}_e} u_{s'0}(\underline{r}_e)\, e^{i\underline{k}_h' \cdot \underline{r}_h} u_{t'0}(\underline{r}_h)\, d\underline{r}_e\, d\underline{r}_h$$

We can expand $u^*_{s0}(\underline{r}_e)\, u_{s'0}(\underline{r}_e)$ and $u^*_{t0}(\underline{r}_h)\, u_{t'0}(\underline{r}_h)$ in Fourier series involving only the reciprocal lattice vectors, as in (2.12), since both expressions are periodic functions. We now assume that $V(\underline{r}_e - \underline{r}_h)$ is

sufficiently slowly varying for its Fourier transform to be negligible at all reciprocal lattice points except the centre of the Brillouin zone. In this case we need keep only the first terms in the two Fourier series, and using (2.15) and (2.16) these are:

$$\frac{1}{\Omega}\int_{\text{unit cell}} u^*_{s0}(\underline{r}_e)\, u_{s'0}(\underline{r}_e)\, d\underline{r}_e = \frac{1}{(2\pi)^3}\delta_{ss'} \qquad \frac{1}{\Omega}\int_{\text{unit cell}} u^*_{t0}(\underline{r}_h)\, u_{t'0}(\underline{r}_h)\, d\underline{r}_h = \frac{1}{(2\pi)^3}\delta_{t't} \tag{2.26}$$

The matrix element (2.25) therefore becomes:

$$\iint_{\text{crystal}} \chi^{st\,*}_{\underline{k}_e\underline{k}_h} V(\underline{r}_e - \underline{r}_h)\, \chi^{s't'}_{\underline{k}'_e\underline{k}'_h}\, d\underline{r}_e\, d\underline{r}_h$$

$$= \frac{1}{(2\pi)^6}\delta_{s's}\,\delta_{t't}\iint_{\text{crystal}} e^{-i\underline{k}_e\cdot\underline{r}_e}\, e^{-i\underline{k}_h\cdot\underline{r}_h}\, V(\underline{r}_e-\underline{r}_h)\, e^{i\underline{k}'_e\cdot\underline{r}_e}\, e^{i\underline{k}'_h\cdot\underline{r}_h}\, d\underline{r}_e\, d\underline{r}_h$$

$$= \frac{1}{(2\pi)^6}\delta_{s's}\,\delta_{t't}\iint_{\text{crystal}} e^{i(\underline{K}'-\underline{K})\cdot\underline{R}}\, e^{i(\underline{k}'-\underline{k})\cdot\underline{r}}\, V(\underline{r})\, d\underline{r}\, d\underline{R}$$

$$= \frac{1}{(2\pi)^3}\delta_{s's}\,\delta_{t't}\,\delta(\underline{K}'-\underline{K})\int_{\text{crystal}} e^{i(\underline{k}'-\underline{k})\cdot\underline{r}}\, V(\underline{r})\, d\underline{r} \tag{2.27}$$

$$= \delta_{s's}\,\delta_{t't}\,\delta(\underline{K}'-\underline{K})\,\mathcal{V}(\underline{k}'-\underline{k})$$

where this is to be taken as the definition of the function $\mathcal{V}(\underline{k}'-\underline{k})$. In deriving the above we have assumed periodic boundary conditions and have introduced the conjugate pairs of co-ordinates:

$$\left.\begin{aligned} \underline{r} &= \underline{r}_e - \underline{r}_h \\ \underline{k} &= \tfrac{1}{2}(\underline{k}_e - \underline{k}_h) \end{aligned}\right\} \qquad \left.\begin{aligned} \underline{R} &= \tfrac{1}{2}(\underline{r}_e + \underline{r}_h) \\ \underline{K} &= \underline{k}_e + \underline{k}_h \end{aligned}\right\} \tag{2.28}$$

We now collect together the various terms in (2.21) to obtain the following equation:

$$\left\{E_s(0) + E_t(0) + \frac{\hbar^2}{2m}(\underline{k}_e^2 + \underline{k}_h^2)\right\} A_n^{st}(\underline{k}_e, \underline{k}_h) + \sum_{s'} \frac{\hbar \underline{k}_e \cdot \underline{p}_{ss'}}{m} A_n^{s't}(\underline{k}_e, \underline{k}_h)$$

$$+ \sum_{t'} \frac{\hbar \underline{k}_h \cdot \underline{p}_{tt'}}{m} A_n^{st'}(\underline{k}_e, \underline{k}_h) + \iint_{B.Z.} \delta(\underline{K}' - \underline{K})\, v(\underline{k}' - \underline{k})\, A_n^{st}(\underline{k}_e', \underline{k}_h')\, d\underline{k}_e'\, d\underline{k}_h' \tag{2.29}$$

$$= E_n^{Ex} A_n^{st}(\underline{k}_e, \underline{k}_h)$$

This then is the equation satisfied by the expansion coefficients of the exciton wave-function (2.18). It is not in a very convenient form as it stands because it contains interband coupling terms, i.e. the terms involving $\underline{p}_{ss'}$ and $\underline{p}_{tt'}$. These terms are linear in $\underline{k}_e$ and $\underline{k}_h$. Now effective mass theory applies only to perturbations of the electronic system of the crystal in which the important wave-vectors involved are small in comparison with the dimensions of the Brillouin zone. $\underline{k}_e$ and $\underline{k}_h$ must therefore be small for the theory to apply, and the interband coupling terms are small quantities of the first order in $\underline{k}$. They can be reduced to a lower order by means of a canonical transformation T. We put:

$$A_n^{st}(\underline{k}_e,\underline{k}_h) = \sum_{s't'} \iint_{\text{B.Z. crystal}} \iint \chi^{st\,*}_{\underline{k}_e\underline{k}_h}\, T\, \chi^{s't'}_{\underline{k}_e'\underline{k}_h'}\, d\underline{r}_e\, d\underline{r}_h\, B_n^{s't'}(\underline{k}_e',\underline{k}_h')\, d\underline{k}_e'\, d\underline{k}_h' \tag{2.30}$$

This can be written symbolically:

$$A = TB = e^{S} B \tag{2.31}$$

We also write (2.29) in the symbolic form:

$$HA = EA$$

Then under the transformation T the momentum space Hamiltonian becomes:

$$\tilde{H} = e^{-S} H e^{S} = H + [H,S] + \tfrac{1}{2}[[H,S],S] + \ldots \tag{2.32}$$

We write the original Hamiltonian as $H^0 + H' + U$ where:

$$\iint \chi^{st\,*}_{\underline{k}_e\underline{k}_h}\, H^0\, \chi^{s't'}_{\underline{k}_e'\underline{k}_h'}\, d\underline{r}_e\, d\underline{r}_h = \left\{E_s(0) + E_t(0) + \frac{\hbar^2}{2m}(k_e^2 + k_h^2)\right\}\delta_{s's}\,\delta_{t't}\,\delta(\underline{k}_e'-\underline{k}_e)\,\delta(\underline{k}_h'-\underline{k}_h)$$

$$\iint \chi^{st\,*}_{\underline{k}_e\underline{k}_h}\, H'\, \chi^{s't'}_{\underline{k}_e'\underline{k}_h'}\, d\underline{r}_e\, d\underline{r}_h = \left\{\frac{\hbar\underline{k}_e\cdot\underline{p}_{ss'}}{m}\delta_{tt'} + \frac{\hbar\underline{k}_h\cdot\underline{p}_{tt'}}{m}\delta_{ss'}\right\}\delta(\underline{k}_e'-\underline{k}_e)\,\delta(\underline{k}_h'-\underline{k}_h)$$

$$\iint \chi^{st\,*}_{\underline{k}_e\underline{k}_h}\, U\, \chi^{s't'}_{\underline{k}_e'\underline{k}_h'}\, d\underline{r}_e\, d\underline{r}_h = V(\underline{k}'-\underline{k})\,\delta_{s's}\,\delta_{t't}\,\delta(\underline{K}'-\underline{K}) \tag{2.33}$$

Then the transformation which removes H', the part of the Hamiltonian containing interband matrix elements, to first order satisfies:

$$H' + [H^0, S] = 0 \tag{2.34}$$

using (2.32). Hence:

$$\iint_{\text{crystal}} \chi^{st\,*}_{\underline{k}_e \underline{k}_h} \, S \, \chi^{s't'}_{\underline{k}_e' \underline{k}_h'} \, d\underline{r}_e \, d\underline{r}_h = - \frac{\frac{\hbar}{m}\left[\underline{k}_e \cdot \underline{p}_{ss'} \delta_{tt'} + \underline{k}_h \cdot \underline{p}_{tt'} \delta_{ss'} \right]}{E_{s'}(0) + E_{t'}(0) - E_s(0) - E_t(0)} \delta(\underline{k}_e' - \underline{k}_e) \delta(\underline{k}_h' - \underline{k}_h)$$

$$\text{for } s \neq s' \text{ or } t \neq t'$$

$$= 0 \qquad \text{for } s = s' \text{ and } t = t' \tag{2.35}$$

In the transformed Hamiltonian $\tilde{H}$ the most important term involving the interband matrix elements is the second order term:

$$\tfrac{1}{2} \iint_{\text{crystal}} \chi^{st\,*}_{\underline{k}_e \underline{k}_h} \left[H', S \right] \chi^{s't'}_{\underline{k}_e' \underline{k}_h'} \, d\underline{r}_e \, d\underline{r}_h$$

$$= \frac{\hbar^2}{2m^2} \sum_{\substack{s'' \neq s, s' \\ t'' \neq t, t'}} \left\{ \left[\underline{k}_e \cdot \underline{p}_{s's''} \delta_{t't''} + \underline{k}_h \cdot \underline{p}_{t't''} \delta_{s's''} \right] \frac{\left[\underline{k}_e \cdot \underline{p}_{s''s} \delta_{t''t} + \underline{k}_h \cdot \underline{p}_{t''t} \delta_{s''s} \right]}{E_s(0) + E_t(0) - E_{s''}(0) - E_{t''}(0)} \right.$$

$$\left. + \frac{\left[\underline{k}_e \cdot \underline{p}_{s's''} \delta_{t't''} + \underline{k}_h \cdot \underline{p}_{t't''} \delta_{s's''} \right]}{E_{s'}(0) + E_{t'}(0) - E_{s''}(0) - E_{t''}(0)} \left[\underline{k}_e \cdot \underline{p}_{s''s} \delta_{t''t} + \underline{k}_h \cdot \underline{p}_{t''t} \delta_{s''s} \right] \right\} \tag{2.36}$$

$$\times \delta(\underline{k}_e' - \underline{k}_e) \delta(\underline{k}_h' - \underline{k}_h)$$

For the diagonal case this matrix element reduces to:

$$\frac{\hbar^2}{m^2} \sum_{s'' \neq s} \frac{\underline{k}_e \cdot \underline{p}_{ss''} \; \underline{k}_e \cdot \underline{p}_{s''s}}{E_s(0) - E_{s''}(0)} + \frac{\hbar^2}{m^2} \sum_{t'' \neq t} \frac{\underline{k}_h \cdot \underline{p}_{tt''} \; \underline{k}_h \cdot \underline{p}_{t''t}}{E_t(0) - E_{t''}(0)} \tag{2.37}$$

The off-diagonal matrix elements of the type (2.36) can be removed to

lower order than second in the wave-vector by a further transformation, so we need not consider them. All further contributions to the Hamiltonian introduced by the canonical transformation (2.30) are already of lower order than second provided that the extension of the exciton state is large compared to the lattice constant. Correct to second order in the wave-vector equation (2.29) has now been transformed to:

$$\left\{E_s(0)+E_t(0)+\frac{\hbar^2}{2m}\left(k_e^2+k_h^2\right)+\frac{\hbar^2}{m^2}\sum_{s''\neq s}\frac{\underline{k}_e\cdot\underline{p}_{ss''}\;\underline{k}_e\cdot\underline{p}_{s''s}}{\omega_{ss''}}+\frac{\hbar^2}{m^2}\sum_{t''\neq t}\frac{\underline{k}_h\cdot\underline{p}_{tt''}\;\underline{k}_h\cdot\underline{p}_{t''t}}{\omega_{tt''}}\right\}B_n^{st}(\underline{k}_e,\underline{k}_h)$$

$$+\iint_{B.Z.}\delta(\underline{k}'-\underline{k})\,v(\underline{k}'-\underline{k})\,B_n^{st}(\underline{k}_e',\underline{k}_h')\,d\underline{k}_e'\,d\underline{k}_h' \;=\; E_n^{Ex}\,B_n^{st}(\underline{k}_e,\underline{k}_h) \qquad (2.38)$$

where $\omega_{nm}=E_n(0)-E_m(0)$ is the energy difference between the nth and mth bands at the centre of the Brillouin zone. Using the f-sum rule:

$$\frac{2}{m}\sum_{n''\neq n}\frac{p_{nn''}^{\alpha}\;p_{n''n}^{\beta}}{\omega_{n''n}}=\delta_{\alpha\beta}-m\frac{\partial^2E_n(\underline{k})}{\partial k_\alpha\,\partial k_\beta}_{\underline{k}=0} \qquad (2.39)$$

where α and β denote components of $\underline{k}$, it is easily verified that the large bracket on the left hand side of (2.38) is just $E_s(\underline{k}_e)+E_t(\underline{k}_h)$ expanded to second order in $\underline{k}$. The equation for B_n^{st} correct to second order is therefore:

$$\left\{E_s(\underline{k}_e)+E_t(\underline{k}_h)\right\}B_n^{st}(\underline{k}_e,\underline{k}_h)+\iint_{B.Z.}\delta(\underline{k}'-\underline{k})\,v(\underline{k}'-\underline{k})\,B_n^{st}(\underline{k}_e',\underline{k}_h')\,d\underline{k}_e'\,d\underline{k}_h'=E_n^{Ex}\,B_n^{st}(\underline{k}_e,\underline{k}_h) \qquad (2.40)$$

This is the effective mass equation written in momentum space. Note that

it is diagonal in $\underline{K}$ so that the total momentum of the exciton is a good quantum number. The exciton wave-function may now be simplified. To first order in S we have from (2.30) and (2.31):

$$A_n^{st}(\underline{k}_e,\underline{k}_h) = B_n^{st}(\underline{k}_e,\underline{k}_h) + \sum_{s',t'} \iint_{B.Z.} d\underline{k}_e' d\underline{k}_h' \, B_n^{s't'}(\underline{k}_e',\underline{k}_h') \iint_{crystal} \chi^{st\,*}_{\underline{k}_e\underline{k}_h} \, S \, \chi^{s't'}_{\underline{k}_e'\underline{k}_h'} \, d\underline{r}_e d\underline{r}_h \tag{2.41}$$

$$= B_n^{st}(\underline{k}_e,\underline{k}_h) - \frac{\hbar}{m}\left\{\sum_{s'\neq s} \frac{\underline{k}_e\cdot\underline{p}_{ss'}}{\omega_{ss'}} B_n^{s't}(\underline{k}_e,\underline{k}_h) + \sum_{t'\neq t} \frac{\underline{k}_h\cdot\underline{p}_{tt'}}{\omega_{tt'}} B_n^{st'}(\underline{k}_e,\underline{k}_h)\right\}$$

where we have made use of (2.35). By (2.9) and (2.18):

$$\Psi_n^{Ex}(\underline{r}_e,\underline{r}_h) = \sum_{s,t} \iint_{B.Z.} A_n^{st}(\underline{k}_e,\underline{k}_h)\, \chi^{st}_{\underline{k}_e\underline{k}_h} \, d\underline{k}_e \, d\underline{k}_h \tag{2.42}$$

$$= \sum_{s,t} u_{s0}(\underline{r}_e)\, u_{t0}(\underline{r}_h) \iint_{B.Z.} e^{i\underline{k}_e\cdot\underline{r}_e} \, e^{i\underline{k}_h\cdot\underline{r}_h} \, A_n^{st}(\underline{k}_e,\underline{k}_h)\, d\underline{k}_e d\underline{k}_h$$

Substituting for A_n^{st} from (2.41), we have:

$$\Psi_n^{Ex} = \sum_{s,t} \iint_{B.Z.} \left\{B_n^{st} - \frac{\hbar}{m}\left[\sum_{s'\neq s} \frac{\underline{k}_e\cdot\underline{p}_{ss'}}{\omega_{ss'}} B_n^{s't} + \sum_{t'\neq t} \frac{\underline{k}_h\cdot\underline{p}_{tt'}}{\omega_{tt'}} B_n^{st'}\right]\right\} e^{i\underline{k}_e\cdot\underline{r}_e} \, e^{i\underline{k}_h\cdot\underline{r}_h} \tag{2.43}$$

$$\times\, u_{s0}(\underline{r}_e)\, u_{t0}(\underline{r}_h)\, d\underline{k}_e d\underline{k}_h$$

The right hand side consists of a sum of three terms. Consider the term involving the first part of the square bracket. Interchanging s and s' it is:

$$\sum_{s',t} \frac{\hbar}{m} \iint_{B.Z.} u_{s'0}(\underline{r}_e)\, u_{t0}(\underline{r}_h)\, e^{i\underline{k}_e\cdot\underline{r}_e} \, e^{i\underline{k}_h\cdot\underline{r}_h} \sum_{s\neq s'} \frac{\underline{k}_e\cdot\underline{p}_{s's}}{\omega_{ss'}} B_n^{st} \, d\underline{k}_e \, d\underline{k}_h$$

since $\omega_{nm} = -\omega_{mn}$. The second part of the square bracket may be similarly dealt with. Now equation (2.40) for $\mathcal{B}_n^{st}$ contains no interband coupling so we need retain for the exciton wave-function only those terms in the summations over s and t for which s is the conduction band and t is the valence band. Hence dropping the superscripts on $\mathcal{B}_n$ we have:

$$\Psi_n^{Ex}(\underline{r}_e, \underline{r}_h) = \iint_{B.Z.} \left\{ u_{c0}(\underline{r}_e)\, u_{v0}(\underline{r}_h) + \frac{\hbar}{m}\left[u_{v0}(\underline{r}_h) \sum_{s' \neq c} \frac{\underline{k}_e \cdot \underline{p}_{s'c}}{\omega_{cs'}} u_{s'0}(\underline{r}_e) \right.\right. \tag{2.44}$$

$$\left.\left. + u_{c0}(\underline{r}_e) \sum_{t' \neq v} \frac{\underline{k}_h \cdot \underline{p}_{t'v}}{\omega_{vt'}} u_{t'0}(\underline{r}_h) \right] \right\} \mathcal{B}_n(\underline{k}_e, \underline{k}_h)\, e^{i\underline{k}_e \cdot \underline{r}_e}\, e^{i\underline{k}_h \cdot \underline{r}_h}\, d\underline{k}_e\, d\underline{k}_h$$

Correct to first order in the interband matrix elements this may be written in the final form:

$$\Psi_n^{Ex}(\underline{r}_e, \underline{r}_h) = \iint_{B.Z.} \left\{ u_{c0}(\underline{r}_e) + \sum_{s \neq c} \frac{\underline{p}_{sc}}{m\omega_{cs}} \cdot \hbar \underline{k}_e\, u_{s0}(\underline{r}_e) \right\} \tag{2.45}$$

$$\times \left\{ u_{v0}(\underline{r}_h) + \sum_{t \neq v} \frac{\underline{p}_{tv}}{m\omega_{vt}} \cdot \hbar \underline{k}_h\, u_{t0}(\underline{r}_h) \right\} \mathcal{B}_n(\underline{k}_e, \underline{k}_h)\, e^{i\underline{k}_e \cdot \underline{r}_e}\, e^{i\underline{k}_h \cdot \underline{r}_h}$$

$$d\underline{k}_e\, d\underline{k}_h$$

3. Transformation to Co-ordinate Space. To transform the effective mass equations from momentum to co-ordinate space we note that since $\mathcal{B}_n(\underline{k}_e, \underline{k}_h)$ is periodic in $\underline{k}_e$ and $\underline{k}_h$ it may be expanded in a Fourier series as follows:

$$\mathcal{B}_n(\underline{k}_e, \underline{k}_h) = \frac{\Omega^2}{(2\pi)^3} \sum_{a,b} e^{-i\underline{k}_e \cdot \underline{R}_e^a}\, e^{-i\underline{k}_h \cdot \underline{R}_h^b}\, F_n(\underline{R}_e^a, \underline{R}_h^b) \tag{2.46}$$

where $\underline{R}^a$ and $\underline{R}^b$ are lattice vectors and the F_n are coefficients. The Fourier transform of this equation is:

$$F_n(\underline{R}^a_e, \underline{R}^b_h) = \frac{1}{(2\pi)^3} \iint_{B.Z.} e^{i\underline{k}_e \cdot \underline{R}^a_e} e^{i\underline{k}_h \cdot \underline{R}^b_h} B_n(\underline{k}_e, \underline{k}_h)\, d\underline{k}_e\, d\underline{k}_h \qquad (2.47)$$

The coefficient F_n is strictly defined only at the lattice points, and substitution of (2.46) into (2.40) would lead to a set of difference equations for these coefficients. The difference equations can be replaced by differential equations to a good approximation, provided again that the extension of the exciton wave-function is large compared to the lattice constant. This replacement is effected if we define a function F_n of continuous variables by:

$$F_n(\underline{r}_e, \underline{r}_h) = \frac{1}{(2\pi)^3} \iint_{B.Z.} e^{i\underline{k}_e \cdot \underline{r}_e} e^{i\underline{k}_h \cdot \underline{r}_h} B_n(\underline{k}_e, \underline{k}_h)\, d\underline{k}_e\, d\underline{k}_h \qquad (2.48)$$

and the inverse of this is:

$$B_n(\underline{k}_e, \underline{k}_h) = \frac{1}{(2\pi)^3} \iint_{crystal} e^{-i\underline{k}_e \cdot \underline{r}_e} e^{-i\underline{k}_h \cdot \underline{r}_h} F_n(\underline{r}_e, \underline{r}_h)\, d\underline{r}_e\, d\underline{r}_h \qquad (2.49)$$

We shall sometimes write these equations in terms of the co-ordinates defined in (2.28), e.g. (2.48) would become:

$$F_n(\underline{r}, \underline{R}) = \frac{1}{(2\pi)^3} \iint_{B.Z.} e^{i\underline{k} \cdot \underline{r}} e^{i\underline{K} \cdot \underline{R}} B_n(\underline{k}, \underline{K})\, d\underline{k}\, d\underline{K} \qquad (2.50)$$

Now using (2.48):

$$\iint_{\text{crystal}} |F_n(\underline{r}_e, \underline{r}_h)|^2 \, d\underline{r}_e \, d\underline{r}_h = \iint_{B.Z.} |B_n(\underline{k}_e, \underline{k}_h)|^2 \, d\underline{k}_e \, d\underline{k}_h \doteq \iint_{B.Z.} |A_n(\underline{k}_e, \underline{k}_h)|^2 \, d\underline{k}_e \, d\underline{k}_h \tag{2.51}$$

Hence by (2.19) Ψ_n^{Ex} is automatically normalized to the crystal volume if F_n is so normalized. Introducing the function F_n into (2.40) it takes the form:

$$\left[E_c(-i\nabla_e) + E_v(-i\nabla_h) + V(\underline{r}_e - \underline{r}_h)\right] F_{n\underline{K}}(\underline{r}_e, \underline{r}_h) = E_{n\underline{K}}^{Ex} F_{n\underline{K}}(\underline{r}_e, \underline{r}_h) \tag{2.52}$$

which is the effective mass equation in co-ordinate space. We have added a subscript $\underline{K}$ to F_n to denote the total exciton wave-vector which we have shewn to be a good quantum number. As before E_c and E_v are to be expanded to second order in their arguments. ∇_e and ∇_h are the gradient operators in the electron and hole co-ordinates respectively. In reducing the interaction term we have used (2.27) and have taken:

$$\int_{B.Z.} e^{i\underline{k}_e \cdot (\underline{r}_e' - \underline{r}_e)} \, d\underline{k}_e = (2\pi)^3 \delta'(\underline{r}_e' - \underline{r}_e)$$

$$\int_{B.Z.} e^{i\underline{k}_h \cdot (\underline{r}_h' - \underline{r}_h)} \, d\underline{k}_h = (2\pi)^3 \delta'(\underline{r}_h' - \underline{r}_h) \tag{2.53}$$

The prime on the deltas signifies that they are not sharp delta functions but extend over a region of space of the order of the unit

cell volume. Since V and F have been taken to be slowly varying functions, it is a good approximation to replace these spread out deltas by sharp delta functions.

The exciton wave-function (2.45) may also be transformed into co-ordinate space by the use of (2.48) giving:

$$\Psi^{Ex}_{n\underline{K}}(\underline{r}_e,\underline{r}_h) = (2\pi)^3\left[v_{co}(\underline{r}_e) - \frac{it}{m}\sum_{s\neq c}\frac{\underline{p}_{sc}\cdot\nabla^F_e}{\omega_{cs}}v_{so}(\underline{r}_e)\right]$$

$$\times\left[v_{vo}(\underline{r}_h) - \frac{it}{m}\sum_{t\neq v}\frac{\underline{p}_{tv}\cdot\nabla^F_h}{\omega_{vt}}v_{to}(\underline{r}_h)\right]F_{n\underline{K}}(\underline{r}_e,\underline{r}_h) \qquad (2.54)$$

where the superscript F on the gradient operators signifies that they operate only on the function $F_{n\underline{K}}$. The error introduced into this wave-function by the approximations made in its derivation is of order $\left(\frac{L}{a_0}\right)^2$ where L is the lattice constant and a_0 is the extension of the exciton state.

4. External Magnetic Field. The case where there is an external magnetic field acting on the exciton may also be treated by the method of Luttinger and Kohn, generalised as above to take account of the two interacting particles. This generalization is straightforward and we give here only the results. The exciton wave-function correct to first order in the interband matrix elements is:

$$\Psi^{Ex}_{n\underline{K}}(\underline{r}_e,\underline{r}_h) = \iint_{B.Z.}\left\{v_{c0}(\underline{r}_e)+\sum_{s\neq c}\frac{\underline{p}_{sc}}{m\omega_{cs}}\cdot\left[\hbar\underline{k}_e+\frac{e}{c}\underline{A}(i\nabla^B_{\underline{k}_e})\right]v_{s0}(\underline{r}_e)\right\}$$

$$\times\left\{v_{v0}(\underline{r}_h)+\sum_{t\neq v}\frac{\underline{p}_{tv}}{m\omega_{vt}}\cdot\left[\hbar\underline{k}_h-\frac{e}{c}\underline{A}(i\nabla^B_{\underline{k}_h})\right]v_{t0}(\underline{r}_h)\right\}B_n(\underline{k}_e,\underline{k}_h)$$

$$\times e^{i\underline{k}_e\cdot\underline{r}_e}e^{i\underline{k}_h\cdot\underline{r}_h}d\underline{k}_e\,d\underline{k}_h$$

$$=(2\pi)^3\left\{v_{c0}(\underline{r}_e)+\sum_{s\neq c}\frac{\underline{p}_{sc}}{m\omega_{cs}}\cdot\left[-i\hbar\nabla^F_e+\frac{e}{c}\underline{A}(\underline{r}_e)\right]v_{s0}(\underline{r}_e)\right\} \qquad (2.55)$$

$$\times\left\{v_{v0}(\underline{r}_h)+\sum_{t\neq v}\frac{\underline{p}_{tv}}{m\omega_{vt}}\cdot\left[-i\hbar\nabla^F_h-\frac{e}{c}\underline{A}(\underline{r}_h)\right]v_{t0}(\underline{r}_h)\right\}F_{n\underline{K}}(\underline{r}_e,\underline{r}_h)$$

where the $\nabla^B_{\underline{k}}$ in the argument of $\underline{A}$, the vector potential of the magnetic field, is the gradient operator in momentum space and acts only on the function B_n. The errors in this wave-function are of order $\left(\frac{L}{a_0}\right)^2$ and $\left(\frac{L}{\lambda}\right)^2$ where λ is a length characteristic of the magnetic field defined in (A2.16). For extended exciton states and normally attainable magnetic fields both these errors are small. F_n and B_n are still related by the transformation (2.48).

It is of interest to note that the presence of the magnetic field changes the contribution to the exciton wave-function from bands other than the conduction and valence bands [compare (2.54) with (2.55)] . On the other hand the electron-hole interaction $V(\underline{r}_e - \underline{r}_h)$ has no effect on the admixtures of other bands. This difference is due to the fact that the magnetic field extends over all

lattice points whereas $V(\underline{r}_e - \underline{r}_h)$ is a localized potential affecting only a few of the lattice points.

The wave-function B_n in momentum space satisfies the wave-equation:

$$\left\{E_c\left[\underline{k}_e + \frac{e}{\hbar c}\underline{A}(i\nabla_{\underline{k}_e})\right] + E_v\left[\underline{k}_h - \frac{e}{\hbar c}\underline{A}(i\nabla_{\underline{k}_h})\right]\right\} B_n(\underline{k}_e, \underline{k}_h) \tag{2.56}$$

$$+ \iint_{B.Z.} V(\underline{k}'-\underline{k})\,\delta(\underline{K}'-\underline{K})\,B_n(\underline{k}_e', \underline{k}_h')\,d\underline{k}_e'\,d\underline{k}_h' = E_n^{Ex} B_n(\underline{k}_e, \underline{k}_h)$$

while the co-ordinate space wave-function F_n satisfies:

$$\left\{E_c\left[-i\nabla_e + \frac{e}{\hbar c}\underline{A}(\underline{r}_e)\right] + E_v\left[-i\nabla_h - \frac{e}{\hbar c}\underline{A}(\underline{r}_h)\right] + V(\underline{r}_e - \underline{r}_h)\right\} F_{n\underline{K}}(\underline{r}_e, \underline{r}_h) \tag{2.57}$$

$$= E_{n\underline{K}}^{Ex}\, F_{n\underline{K}}(\underline{r}_e, \underline{r}_h)$$

In both these wave-equations the conduction and valence band energies are to be expanded as far as second order in their arguments.

We now consider the simplification of equation (2.57) in the case where the valence and conduction bands are both spherical with effective masses m_h and m_e. The valence band is assumed to be such that the energy of an electron in it decreases quadratically with increasing $\underline{k}$. The energy of a hole in the valence band will therefore increase quadratically with increasing $\underline{k}$ and the effective mass m_h must be a positive quantity. We take $E_v(0)$ as the zero for the energy and denote the forbidden energy gap by $E_0 = E_c(0) - E_v(0)$. The discussion of section 1 of this chapter suggests that a first approximation to the electron-hole interaction V would be a simple

Coulomb expression $-e^2/|r_e - r_h|$. We are only considering states of the semiconductor in which a single electron has been excited into the conduction band. However if states in which more than one electron has been excited are taken into account then it is found that the effective electron-hole interaction for a single pair excitation is reduced by the static dielectric constant $\varkappa$ of the material[16], and we adopt this approximation to $V(\underline{r}_e - \underline{r}_h)$. With these substitutions (2.57) becomes:

$$\left\{\frac{1}{2m_e}\left[-i\hbar\nabla_e + \frac{e}{c}\underline{A}(\underline{r}_e)\right]^2 + \frac{1}{2m_h}\left[-i\hbar\nabla_h - \frac{e}{c}\underline{A}(\underline{r}_h)\right]^2 - \frac{e^2}{\varkappa|\underline{r}_e - \underline{r}_h|}\right\}F_{n\underline{K}} \tag{2.58}$$

$$= \left(E^{Ex}_{n\underline{K}} - E_G\right)F_{n\underline{K}} = E_{n\underline{K}}F_{n\underline{K}}$$

say. We choose a particular gauge for the vector potential:

$$\underline{A}(\underline{r}) = \tfrac{1}{2}\underline{H}\times\underline{r} \tag{2.59}$$

so that the Hamiltonian of the wave-equation (2.58) is:

$$\mathcal{H} = \frac{1}{2m_e}\left[-i\hbar\nabla_e + \frac{e}{2c}\underline{H}\times\underline{r}_e\right]^2 + \frac{1}{2m_h}\left[-i\hbar\nabla_h - \frac{e}{2c}\underline{H}\times\underline{r}_h\right]^2 - \frac{e^2}{\varkappa|\underline{r}_e - \underline{r}_h|} \tag{2.60}$$

We now wish to transform the Hamiltonian to the co-ordinates $\underline{r}$ and $\underline{R}$ of (2.28). This transformation is facilitated however if we first make a canonical transformation of the Hamiltonian. We define a new wave-function $\tilde{F}_{n\underline{K}}$ by:

$$F_{n\underline{K}} = e^{S}\tilde{F}_{n\underline{K}} \tag{2.61}$$

The transformed Hamiltonian is:

$$\tilde{\mathcal{H}} = e^{-S}\mathcal{H}e^{S} \tag{2.62}$$

We choose:

$$S = \frac{ie}{2\hbar c}\, \underline{H} \cdot \underline{r}_e \times \underline{r}_h \tag{2.63}$$

and this gives a transformed Hamiltonian:

$$\tilde{\mathcal{H}} = \frac{1}{2m_e}\left[-i\hbar\nabla_e + \frac{e}{2c}\,\underline{H}\times(\underline{r}_e-\underline{r}_h)\right]^2 + \frac{1}{2m_h}\left[-i\hbar\nabla_h - \frac{e}{2c}\,\underline{H}\times(\underline{r}_h-\underline{r}_e)\right]^2 - \frac{e^2}{\varkappa|\underline{r}_e-\underline{r}_h|} \tag{2.64}$$

Making the co-ordinate transformation (2.28) then gives:

$$\tilde{\mathcal{H}} = -\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{1}{4}\frac{\hbar^2}{2\mu}\nabla_R^2 + \frac{\hbar^2}{2}\frac{(m_e-m_h)}{m_e m_h}\nabla_r\cdot\nabla_R - \frac{ie\hbar}{4\mu c}\,\underline{H}\cdot\underline{r}\times\nabla_R$$

$$+ \frac{ie\hbar}{2c}\frac{(m_e-m_h)}{m_e m_h}\,\underline{H}\cdot\underline{r}\times\nabla_r + \frac{e^2}{8\mu c^2}(\underline{H}\times\underline{r})^2 - \frac{e^2}{\varkappa r} \tag{2.65}$$

where: $\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h}$.

Note that the Hamiltonian depends on $\underline{R}$ only through terms in ∇_R and therefore ∇_R commutes with the Hamiltonian and $\underline{K}$ is a constant of the motion. The eigenfunctions of (2.65) can therefore be written:

$$\tilde{F}_{n\underline{K}}(\underline{r}_e,\underline{r}_h) = \tilde{F}_{n\underline{K}}(\underline{r},\underline{R}) = \frac{1}{\sqrt{N\Omega}}\, e^{i\underline{K}\cdot\underline{R}}\;\tilde{F}_{n\underline{K}}(\underline{r}) \tag{2.66}$$

where $\tilde{F}_{n\underline{K}}(\underline{r})$ is an eigenfunction of (2.65) but with $-i\nabla_R$ replaced by the constant $\underline{K}$. Noting that $\underline{r}_e\times\underline{r}_h = \underline{r}\times\underline{R}$ and using (2.61) and (2.63) we have finally that:

$$F_{n\underline{K}}(\underline{r}_e,\underline{r}_h) = e^{\frac{ie}{2\hbar c}\,\underline{H}\cdot\underline{r}\times\underline{R}}\,\frac{1}{\sqrt{N\Omega}}\, e^{i\underline{K}\cdot\underline{R}}\;\tilde{F}_{n\underline{K}}(\underline{r}) \tag{2.67}$$

Chapter 3. OPTICAL ABSORPTION COEFFICIENTS.

1. Derivation of General Formula. To determine optical electric dipole absorption coefficients we require matrix elements of $\underline{\epsilon}.\underline{p}$ between the initial and final states of the system, $\underline{\epsilon}$ being the polarisation vector for the incident radiation and $\underline{p}$ being the momentum operator. When the final state of the system is one in which an exciton of wave-function $\Psi^{Ex}_{n\underline{K}}$ has been formed in a crystal which was initially in its ground state, we shall write this matrix element $\langle n\underline{K}|\underline{\epsilon}.\underline{p}|0\rangle$. The exciton described by the wave-function (2.55) is formed by excitation of an electron from an initial state with wave-vector $-\underline{k}_h$ in the valence band to a final state with wave-vector $\underline{k}_e$ in the conduction band. The matrix element we require is therefore:

$$\langle n\underline{K}|\underline{\epsilon}.\underline{p}|0\rangle = -i\hbar \int_{\text{crystal}} \iint_{B.Z.} e^{-i\underline{k}_e.\underline{r}'} \left\{ u^*_{c0}(\underline{r}') + \sum_{s\neq c} \frac{\underline{p}_{sc}}{m\omega_{cs}} . \left[\hbar\underline{k}_e + \frac{e}{c}\underline{A}\left(i\nabla^B_{k_e}\right)\right] u^*_{s0}(\underline{r}') \right\} \tag{3.1}$$

$$\times (\epsilon.\nabla) e^{-i\underline{k}_h.\underline{r}'} \left\{ u_{v0}(\underline{r}') + \sum_{t\neq v} \frac{\underline{p}_{tv}}{m\omega_{vt}} . \left[-\hbar\underline{k}_h - \frac{e}{c}\underline{A}\left(i\nabla^B_{k_h}\right)\right] u_{t0}(\underline{r}') \right\}$$

$$\times B_n(\underline{k}_e, \underline{k}_h)\, d\underline{k}_e\, d\underline{k}_h\, d\underline{r}'$$

where we have set $\underline{r}_e = \underline{r}_h = \underline{r}'$. Using the theorem (2.11) this can be reduced to:

$$\langle n\underline{K}|\underline{\epsilon}.\underline{p}|0\rangle = -i\hbar\frac{(2\pi)^3}{\Omega}\delta(\underline{k}_e+\underline{k}_h)\int_{\substack{\text{unit}\\ \text{cell}}}\iint_{\text{B.Z.}}\left\{v_{co}^*(\underline{r}')+\sum_{s\neq c}\frac{p_{sc}}{m\omega_{cs}}\cdot\left[\hbar\underline{k}_e+\frac{e}{c}\underline{A}(i\nabla_{k_e}^B)\right]v_{so}^*(\underline{r}')\right\}$$

$$\times\ \underline{\epsilon}.(\nabla-i\underline{k}_h)\left\{v_{vo}(\underline{r}')+\sum_{t\neq v}\frac{p_{tv}}{m\omega_{vt}}\cdot\left[-\hbar\underline{k}_h-\frac{e}{c}\underline{A}(i\nabla_{k_h}^B)\right]v_{to}(\underline{r}')\right\} \qquad (3.2)$$

$$\times B_n(\underline{k}_e,\underline{k}_h)\,d\underline{k}_e\,d\underline{k}_h\,d\underline{r}'$$

Only excitons of zero total momentum can be formed in this type of absorption process. Specializing (3.2) to this case and introducing the co-ordinates of (2.28)

$$\langle n\mathbf{O}|\underline{\epsilon}.\underline{p}|0\rangle = -i\hbar\frac{(2\pi)^3}{\Omega}\int_{\substack{\text{unit}\\ \text{cell}}}\int_{\text{B.Z.}}\left\{v_{co}^*(\underline{r}')+\sum_{s\neq c}\frac{p_{sc}}{m\omega_{cs}}\cdot\left[\hbar\underline{k}+\frac{e}{c}\underline{A}(i\nabla_k^B)\right]v_{so}^*(\underline{r}')\right\} \qquad (3.3)$$

$$\times\ \underline{\epsilon}.(\nabla+i\underline{k})\left\{v_{vo}(\underline{r}')+\sum_{t\neq v}\frac{p_{tv}}{m\omega_{vt}}\cdot\left[\hbar\underline{k}+\frac{e}{c}\underline{A}(i\nabla_k^B)\right]v_{to}(\underline{r}')\right\}$$

$$\times B_n(\underline{k},0)\,d\underline{k}\,d\underline{r}'$$

These integrals may now be evaluated term by term. The integral over $\underline{r}'$ always gives a momentum matrix element of the type defined in (2.23). As for the integral over $\underline{k}$ we note that the inverse of (2.50) gives:

$$B_n(\underline{k},0) = \frac{1}{(2\pi)^3}\iint_{\text{crystal}} e^{-i\underline{k}.\underline{r}}\,F_{no}(\underline{r},\underline{R})\,d\underline{r}\,d\underline{R} \qquad (3.4)$$

Three types of integral over $\underline{k}$ are required:

$$\int_{B.Z.} B_n(\underline{k},0)\,d\underline{k} = \frac{1}{(2\pi)^3}\int_{B.Z.}\iiint_{crystal} e^{-i\underline{k}\cdot\underline{r}}\, F_{no}(\underline{r},\underline{R})\,d\underline{r}\,d\underline{R}\,d\underline{k}$$

$$= \int_{crystal} F_{no}(0,R)\,d\underline{R}$$

$$= \frac{1}{\sqrt{N\Omega}}\,\tilde{F}_{no}(0)\int_{crystal} d\underline{R} = \sqrt{N\Omega}\;\tilde{F}_{no}(0) \qquad (3.5)$$

where we have used (2.67). In a similar manner it follows that:

$$\int_{B.Z.} \underline{k}\,B_n(\underline{k},0)\,d\underline{k} = -i\sqrt{N\Omega}\left[\nabla_r\,\tilde{F}_{no}(\underline{r})\right]_{\underline{r}=0} \qquad (3.6)$$

$$\int_{B.Z.} \nabla_k\,B_n(\underline{k},0)\,d\underline{k} = -i\sqrt{N\Omega}\left[\underline{r}\;\tilde{F}_{no}(\underline{r})\right]_{\underline{r}=0} \qquad (3.7)$$

Collecting together the various terms and keeping contributions up to second order in the interband matrix elements, (3.3) reduces to:

$$\langle n0|\underline{\epsilon}\cdot\underline{p}|0\rangle = \sqrt{N\Omega}\left\{\underline{\epsilon}\cdot\underline{p}_{cv}\;\tilde{F}_{no}(0) + \left[\sum_{s\neq c}(\underline{\epsilon}\cdot\underline{p}_{sv})\,\frac{\underline{p}_{sc}}{m\omega_{cs}} + \sum_{t\neq v}(\underline{\epsilon}\cdot\underline{p}_{ct})\,\frac{\underline{p}_{tv}}{m\omega_{vt}}\right]\right.$$
$$\left.\cdot\left\{\left[-i\hbar\nabla_r + \frac{e}{c}\underline{A}(\underline{r})\right]\tilde{F}_{no}(\underline{r})\right\}_{\underline{r}=0}\right\} \qquad (3.8)$$

If we define:

$$\underline{\Pi} = -i\hbar\nabla_r + \frac{e}{c}\underline{A}(\underline{r}) \qquad (3.9)$$

and also:

$$\underline{M}_{cv} = \frac{1}{m}\sum_s \left[\frac{\underline{p}_{sc}}{\omega_{cs}}(\underline{\epsilon}\cdot\underline{p}_{vs}) - \frac{\underline{p}_{vs}}{\omega_{sv}}(\underline{\epsilon}\cdot\underline{p}_{sc})\right]$$

$$= \frac{1}{\hbar}\left[\nabla_k\left(\underline{\epsilon}\cdot\underline{p}_{cv}(\underline{k})\right)\right]_{\underline{k}=0} \qquad (3.10)$$

using the f-sum rule (2.39), then (3.8) can be written in the simple form:

$$\langle n0|\underline{\epsilon}\cdot\underline{p}|0\rangle = \sqrt{N\Omega}\left\{\underline{\epsilon}\cdot\underline{p}_{cv}\,\tilde{F}_{n0}(0) + \left[\underline{M}_{cv}\cdot\underline{\underline{\Pi}}\,\tilde{F}_{n0}(\underline{r})\right]_{\underline{r}=0}\right\} \qquad (3.11)$$

$\tilde{F}_{n0}(\underline{r})$ (we shall in future drop the subscript 0) satisfies a wave-equation whose Hamiltonian is (2.65) with $\underline{K} = -i\nabla_R$ set equal to zero:

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{ie\hbar}{2c}\frac{m_e - m_n}{m_e m_n}\underline{H}.\underline{r}\times\nabla + \frac{e^2}{8\mu c^2}(\underline{H}\times\underline{r})^2 - \frac{e^2}{\varkappa r}\right\}\tilde{F}_n(\underline{r}) = E_n\,\tilde{F}_n(\underline{r}) \qquad (3.12)$$

The absorption is said to be allowed if p_{cv} is non-zero, in which case the first term in (3.11) is of much greater importance than the second term. If on the other hand $p_{cv} = 0$ the absorption is said to be forbidden and the second term in (3.11) must be used.

The absorption coefficient is shewn in appendix 1 to be:

$$K = \frac{4\pi^2 e^2}{N\Omega m^2 c\,\omega\,\eta}\overline{|\langle n0|\underline{\epsilon}\cdot\underline{p}|0\rangle|^2}\,S(E) \qquad (3.13)$$

where ω is the angular frequency of the radiation, η is the low frequency refractive index and S(E) is the number of excited states per unit energy range. We shall require this density of states for the cases of plane waves in both one and three dimensions; they are:

$$S_1(E) = \frac{L_z}{4\pi\hbar}\sqrt{\frac{2\mu}{E}} = L_z \frac{\mu}{2\pi\hbar^2}\frac{1}{k} \tag{3.14}$$

$$S_3(E) = \frac{N\Omega}{4\pi^2}\left(\frac{2\mu}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E} = N\Omega \frac{\mu}{2\pi^2\hbar^2} k \tag{3.15}$$

taking account of only one spin orientation. L_z is the length of the crystal in the z-direction.

2. Particular Cases. In chapter 4 we shall solve equation (3.12) taking into account both the Coulomb and magnetic field terms in an approximation which is valid for sufficiently large magnetic fields. Before doing this however we consider here the solutions for the cases when one or both of these terms are neglected, for this shews how the new general formula (3.11) leads to results previously determined by other authors using different methods. In each case we indicate the authors originally responsible for the formulae concerned.

(i) Zero magnetic field, Coulomb interaction neglected. (Hall, Bardeen and Blatt[5])

The solutions of (3.12) are plane waves:

$$\tilde{F}(\underline{r}) = \frac{1}{\sqrt{N\Omega}} e^{i\underline{k}\cdot\underline{r}} \tag{3.16}$$

Hence in the allowed case:

$$\langle n\,0|\,\underline{\epsilon}\cdot\underline{p}\,|\,0\rangle = \underline{\epsilon}\cdot\underline{p}_{cv} \tag{3.17}$$

The absorption coefficient is therefore:

$$K = \frac{e^2}{m^2 c\,\omega\,\eta}\left(\frac{2\mu}{\hbar^2}\right)^{\frac{3}{2}} |p_{cv}|^2 (\hbar\omega - E_G)^{\frac{1}{2}} \qquad (3.18)$$

where we have used energy conservation to give: $\hbar\omega = E_G + \frac{\hbar^2 k^2}{2\mu}$

In the forbidden case:

$$\langle n0 | \underline{\epsilon}.\underline{p} | 0 \rangle = \hbar \underline{M}_{cv}.\underline{k} \qquad (3.19)$$

so that the absorption coefficient is:

$$K = \frac{e^2\hbar^2}{m^2 c\,\omega\,\eta}\overline{|\underline{M}_{cv}.\underline{k}|^2}\left(\frac{2\mu}{\hbar^2}\right)^{\frac{3}{2}}(\hbar\omega - E_G)^{\frac{1}{2}} = \frac{e^2\hbar^2}{3m^2 c\,\omega\,\eta}\left(\frac{2\mu}{\hbar^2}\right)^{\frac{3}{2}}|\underline{M}_{cv}|^2(\hbar\omega - E_G)^{\frac{1}{2}} \qquad (3.20)$$

Note that in both cases the absorption coefficient rises from zero at the absorption edge, $E_G = \hbar\omega$.

(ii) Zero magnetic field. (Elliott[9])

In this case (3.12) is the wave-equation for the hydrogen atom. The final state of the system now has discrete as well as continuous systems of energy levels. For these discrete levels we may calculate f-values defined by:

$$f_n = \frac{2}{\hbar m \omega}\,|\langle n0 | \underline{\epsilon}.\underline{p} | 0 \rangle|^2 \qquad (3.21)$$

For the hydrogen atom $\tilde{F}_n(0)$ is non-zero only for s-states in which case for discrete levels:

$$|\tilde{F}_n(0)|^2 = \frac{1}{\pi a_0^3 n^3} \qquad (3.22)$$

where $a_0 = \frac{\hbar^2 \varkappa}{\mu e^2}$ is the effective Bohr radius and n is the principal quantum number. There is therefore a series of lines at energies:

$$\hbar\omega = E_G - \frac{R}{n^2} \qquad \text{where} \qquad R = \frac{\mu e^4}{2\hbar^2 \varkappa^2} \tag{3.23}$$

For s-states in the continuum we have:

$$|\tilde{F}(0)|^2 = \frac{\pi\alpha e^{\pi\alpha}}{N\Omega \sinh \pi\alpha} \tag{3.24}$$

where $\alpha = \frac{k_0}{k}$, $k_0 = \frac{1}{a_0}$. Hence in the allowed case for discrete levels:

$$\langle n0 | \underline{\epsilon}.\underline{p} | 0 \rangle = \sqrt{N\Omega}\, \frac{1}{\sqrt{\pi a_0^3 n^3}}\, \underline{\epsilon}.\underline{p}_{cv} \tag{3.25}$$

and for the continuum:

$$\langle n0 | \underline{\epsilon}.\underline{p} | 0 \rangle = \sqrt{\frac{\pi\alpha e^{\pi\alpha}}{\sinh \pi\alpha}}\, \underline{\epsilon}.\underline{p}_{cv} \tag{3.26}$$

The discrete levels therefore have f-values:

$$f_n = \frac{2N\Omega}{\hbar\pi m a_0^3 n^3 \omega} |p_{cv}|^2 \tag{3.27}$$

Close to the absorption edge a large number of discrete lines overlap and they may be treated as a continuum having a density of states $\left[\frac{dE}{dn}\right]^{-1}$. The discrete energy levels are given by $E = -\frac{R}{n^2}$, where R is the effective Rydberg unit of energy defined in (3.23), so that the density of states is:

$$S_n(E) = \left[\frac{dE}{dn}\right]^{-1} = \frac{n^3}{2R} \tag{3.28}$$

The absorption coefficient in this region is therefore:

$$K = \frac{4\pi\mu e^2 k_0}{m^2 h^2 c\,\omega\,\eta} \left| p_{-cv} \right|^2 \qquad (3.29)$$

independent of energy. In the true continuum the coefficient is:

$$K = \frac{e^2}{m^2 c\,\omega\,\eta} \left(\frac{2\mu}{h^2}\right)^{\frac{3}{2}} \left| p_{-cv} \right|^2 \frac{\pi\alpha e^{\pi\alpha}}{\sinh \pi\alpha} \left(h\omega - E_G\right)^{\frac{1}{2}} \qquad (3.30)$$

We observe that for small α , or high energies, well away from the absorption edge this tends to the coefficient (3.18) so that the Coulomb interaction does not affect the shape in this region. For large α (3.30) tends to:

$$K = \frac{4\pi\mu e^2 k_0}{m^2 h^2 c\,\omega\,\eta} \left| p_{-cv} \right|^2$$

so that (3.29) and (3.30) join up smoothly at the absorption edge.

For the forbidden case it is the hydrogen-like p-states which contribute to the absorption. For the discrete states:

$$\left| \underline{\nabla}\, \tilde{F}_n(\underline{r}) \right|^2_{r=0} = \frac{h^2(n^2-1)}{3\pi a_0^5 n^5} \qquad (3.31)$$

so that the lines have f-values:

$$f_n = \frac{2(n^2-1)h}{3\pi m\omega a_0^5 n^5} \left| \underline{M}_{cv} \right|^2 N\Omega \qquad (3.32)$$

and lines again occur at the energies (3.23) but with the n = 1 line now missing. Close to the absorption edge the lines again overlap to

form a pseudo-continuum and the absorption coefficient in this region is:

$$K = \frac{4\pi\mu e^3 k_0^3}{3m^2 c\omega\eta}\left[1 + \frac{\hbar\omega - E_G}{R}\right] \tag{3.33}$$

For the continuum p-states:

$$\left|\underline{\pi}\,\tilde{F}(\underline{r})\right|^2_{r=0} = \frac{\pi(1+\alpha^2)\alpha e^{\pi\alpha}\hbar^2 k^2}{3\,N\Omega\sinh\pi\alpha} \tag{3.34}$$

so that the absorption coefficient in the true continuum is:

$$K = \frac{e^2\hbar^2}{3m^2 c\omega\eta}\left(\frac{2\mu}{\hbar^2}\right)^{\frac{5}{2}}\left|\underline{M}_{cv}\right|^2 \frac{\pi(1+\alpha^2)\alpha e^{\pi\alpha}}{\sinh\pi\alpha}\left(\hbar\omega - E_G\right)^{\frac{3}{2}} \tag{3.35}$$

We observe that the Coulomb interaction again produces no change in the shape of the absorption well away from the edge [cf. (3.20)] and that (3.33) and (3.35) join up smoothly at the edge.

(iii) Coulomb interaction neglected. (Elliott, McLean and Macfarlane[10])

With the Coulomb term removed, the Hamiltonian of equation (3.12) can be written in the form:

$$\mathcal{H} = \frac{1}{2\mu}\left[-i\hbar\nabla + \frac{e}{2c}\,\underline{H}\times\underline{r}\right]^2 + \frac{ie\hbar}{m_h c}\,\underline{H}.\underline{r}\times\nabla \tag{3.36}$$

The first part of this Hamiltonian is just that of a free particle in a magnetic field and this problem is treated in appendix 2. The eigenvalues are there shown to be:

$$E = \hbar\omega_c\left[N + \tfrac{1}{2}\right] + \frac{\hbar^2 k^2}{2\mu} \qquad N = 0, 1, 2, \ldots \tag{3.37}$$

where ω_c is the cyclotron frequency, and the eigenfunctions are:

$$M > 0 \qquad \psi_{NM} = (-i)^N N'_{NM}\, e^{iM\phi}\, \sigma^{\frac{1}{2}M}\, e^{-\frac{1}{2}\sigma}\, L_N^M(\sigma)\, e^{ikz} \tag{3.38}$$

$$M < 0 \qquad \psi_{NM} = (-i)^N N''_{NM}\, e^{iM\phi}\, \sigma^{-\frac{1}{2}M}\, e^{-\frac{1}{2}\sigma}\, L_{N-M}^{-M}(\sigma)\, e^{ikz} \tag{3.39}$$

where:

$$N'^2_{NM} = \frac{1}{2\pi\lambda^2 L_z}\,\frac{\lfloor N-M}{(\lfloor N)^3}, \quad N''^2_{NM} = \frac{1}{2\pi\lambda^2 L_z}\,\frac{\lfloor N}{(\lfloor N-M)^3}, \quad \sigma = \frac{\rho^2}{2\lambda^2}, \quad \lambda^2 = \frac{\hbar c}{eH}$$

and (ρ, ϕ, z) define a cylindrical polar co-ordinate system with the z-axis in the direction of the magnetic field. $\hbar k$ is the component of the momentum of the particle along the z-axis, and M takes all integral values consistent with $M \leq N$. Each energy level of the system therefore has an infinite degeneracy corresponding to the possible values of the angular momentum quantum number M.

The effect of the second term in the Hamiltonian (3.36) is to lift this M degeneracy. The term may be written:

$$-\frac{eH}{m_h c}\left(\underline{r} \times \underline{p}\right)_z$$

But $\left(\underline{r} \times \underline{p}\right)_z$ is just the angular momentum about the z-axis and its eigenvalues are therefore $\hbar M$. The eigenvalues of the total Hamiltonian (3.36) are hence:

$$E = \hbar\omega_c\left[N + \tfrac{1}{2}\right] - \frac{e\hbar H}{m_h c} M + \frac{\hbar^2 k^2}{2\mu} \tag{3.40}$$

The eigenfunctions are still given by (3.38) and (3.39) so that the solutions of (3.12) for this case are $\tilde{F}_{NM}(\underline{r}) = \psi_{NM}$.

We are now in a position to calculate the absorption coefficients. For the allowed case we require $\tilde{F}_{NM}(0)$. This is non-zero only for states having M = 0 in which case:

$$\tilde{F}_{N0}(0) = (-i)^N \sqrt{\frac{eH}{2\pi\hbar c L_z}} \tag{3.41}$$

To obtain the absorption coefficient the contributions of type (3.13) from each value of N must be added together. This gives:

$$K = \frac{e^3 H \sqrt{2\mu}}{2m^2c^2\omega\hbar^2\eta} |P_{cv}|^2 \sum_N \left[\hbar\omega - E_G - (N+\tfrac{1}{2})\hbar\omega_c\right]^{-\frac{1}{2}} \tag{3.42}$$

where we have used the density of states (3.14) and the energy conservation relation:

$$\hbar\omega = E_G + \hbar\omega_c\left[N+\tfrac{1}{2}\right] + \frac{\hbar^2k^2}{2\mu}$$

For the forbidden case we require values of $\left[\bar{\pi}\,\tilde{F}_{NM}(\underline{r})\right]_{r=0}$. The absorption coefficient now depends on the polarisation of the incident radiation. It is seen from equation (3.10) that for the case of spherical bands $\underline{M}_{cv}$ is parallel to the polarization $\underline{\epsilon}$. Now:

$$\underline{M}_{cv}.\underline{\pi} = M^z_{cv}\pi_z + \tfrac{1}{2}\left(M^+_{cv}\pi_- + M^-_{cv}\pi_+\right) \tag{3.43}$$

where:

$$M^{\pm}_{cv} = M^x_{cv} \pm i M^y_{cv} \quad , \quad \pi_{\pm} = \pi_x \pm i\pi_y \tag{3.44}$$

For light polarized parallel to the magnetic field only the first term in (3.43) contributes, and we have:

$$\left[\bar{\pi}_z\,\tilde{F}_{NM}(\underline{r})\right]_{r=0} = \hbar k\,(-i)^N \sqrt{\frac{eH}{2\pi\hbar c L_z}}\,\delta_{M0} \tag{3.45}$$

Hence the absorption coefficient is:

$$K = \frac{e^3 H (2\mu)^{\frac{1}{2}}}{2 m^2 c^2 \omega \hbar^2 \eta} \left| M_{cv}^2 \right|^2 \sum_N \left[\hbar\omega - E_G - \left(N + \tfrac{1}{2}\right) \hbar\omega_c \right]^{\frac{1}{2}} \tag{3.46}$$

For light polarized perpendicular to the magnetic field the second term in (3.43) contributes. Using (A2.41) and (A2.42):

$$\left.\begin{aligned} \pi_- \tilde{F}_{NM} &= \frac{\hbar}{\lambda} \sqrt{2N}\ \tilde{F}_{N-1,M-1} \\ \pi_+ \tilde{F}_{NM} &= \frac{\hbar}{\lambda} \sqrt{2(N+1)}\ \tilde{F}_{N+1,M+1} \end{aligned}\right\} \tag{3.47}$$

Hence:

$$\left[\pi_- \tilde{F}_{NM}(\underline{r}) \right]_{r=0} = (-i)^{N-1} \frac{eH}{c} \frac{1}{\sqrt{\pi L_z}} \sqrt{N}\ \delta_{M,1} \tag{3.48}$$

and:

$$\left[\pi_+ \tilde{F}_{NM}(\underline{r}) \right]_{r=0} = (-i)^{N+1} \frac{eH}{c} \frac{1}{\sqrt{\pi L_z}} \sqrt{N+1}\ \delta_{M,-1} \tag{3.49}$$

where we have used the result: $L_N^0(0) = \underline{|N}$. Hence the coefficient is:

$$K = \frac{e^4 H^2 \sqrt{2\mu}}{4 m^2 c^3 \hbar \omega \eta} \left[\left| M_{cv}^x \right|^2 + \left| M_{cv}^y \right|^2 \right] \sum_{N=0}^{\infty} (N+1) \left\{ \left[\hbar\omega - E_G - \hbar\omega_c \left(N + \tfrac{1}{2}\right) - \frac{e\hbar H}{m_h c} \right]^{-\frac{1}{2}} \right. \tag{3.50}$$
$$\left. + \left[\hbar\omega - E_G - \hbar\omega_c \left(N + \tfrac{1}{2}\right) - \frac{e\hbar H}{m_e c} \right]^{-\frac{1}{2}} \right\}$$

It is seen that in a magnetic field the absorption edge is shifted from the frequency given by $\hbar\omega = E_G$. At the edge the absorption coefficient is either zero or infinite in this theory.

Chapter 4. ABSORPTION IN A HIGH MAGNETIC FIELD.

1. Introduction. It is shewn in (A2.27) that the smallest energy which a free particle in a magnetic field can have is $\frac{1}{2}\hbar\omega_c$; we call this the zero point energy and we use it as a measure of the strength of the magnetic field. The binding energy of the exciton in zero magnetic field is just the effective Rydberg unit of energy R defined in (3.23). It is convenient to define a quantity β as follows:

$$\beta = \frac{\frac{1}{2}\hbar\omega_c}{R} = \frac{\varkappa^2\hbar^3 H}{\mu^2 e^3 c} \qquad (4.1)$$

Equation (3.12) is:

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{ie\hbar}{2c}\,\frac{m_e - m_h}{m_e m_h}\,\underline{H}.\underline{r}\times\nabla + \frac{e^2}{8\mu c^2}\left(\underline{H}\times\underline{r}\right)^2 - \frac{e^2}{\varkappa r}\right\}\tilde{F}_n(\underline{r}) = E_n\tilde{F}_n(\underline{r}) \qquad (4.2)$$

We propose to consider here the solutions of this equation for the case $\beta \gg 1$. For such values of β , corresponding to high magnetic fields, the Coulomb energy is small in comparison with the magnetic energy, and the Coulomb interaction can be treated by perturbation theory. The solution of (4.2) with the Coulomb term removed has been derived in chapter 3, the eigenvalues being given by (3.40) and the eigenfunctions by (3.38) and (3.39). The energy level scheme for the first few N and M values is shewn in figure 1. Each line in the diagram represents the lower edge of a continuum of levels which

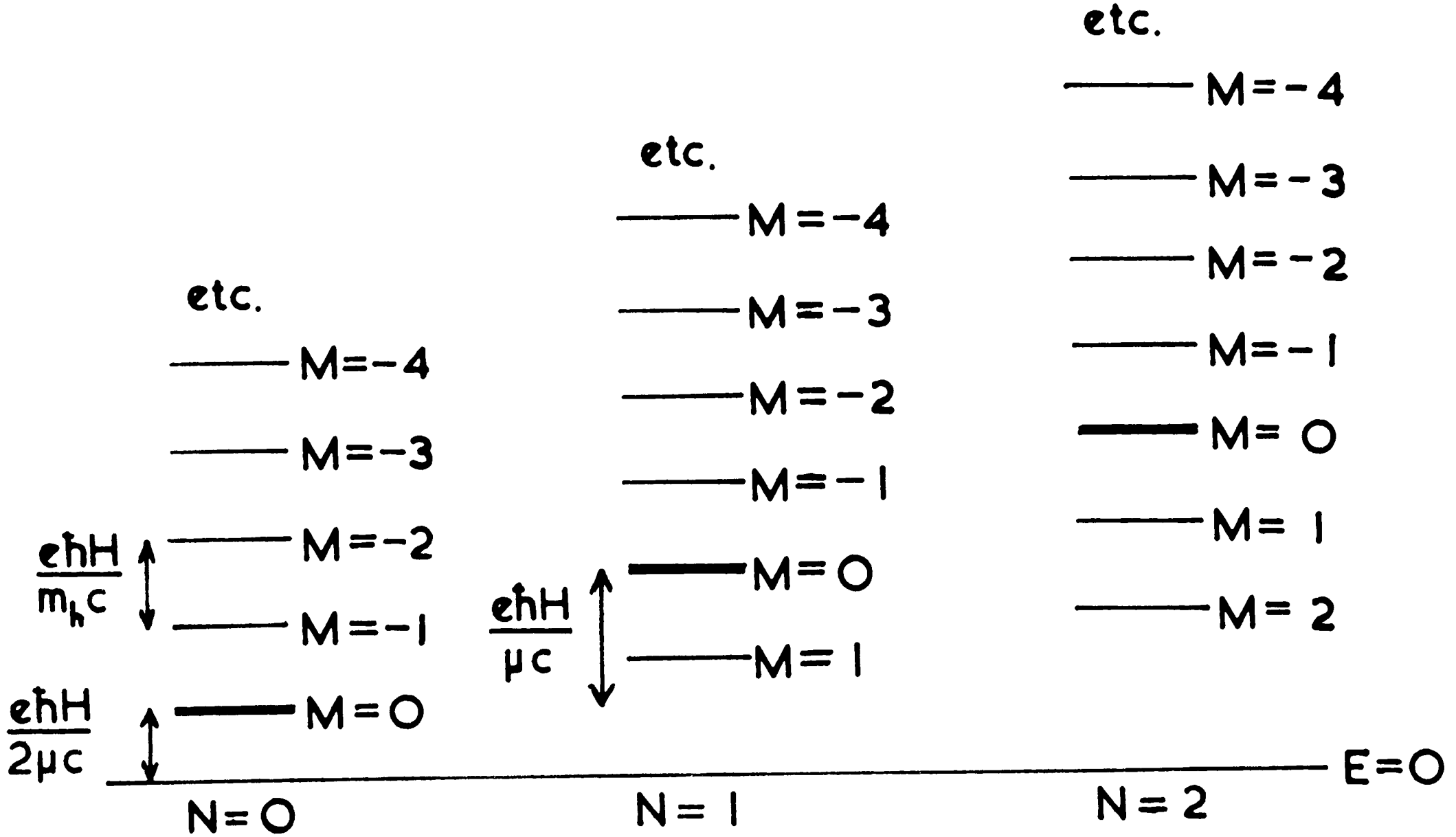

etc.
M=-4
M=-3
M=-2
M=-1
M=0
eħH/m_hc
eħH/2μc
N=0
etc.
M=-4
M=-3
M=-2
M=-1
M=0
M=1
eħH/μc
N=1
etc.
M=-4
M=-3
M=-2
M=-1
M=0
M=1
M=2
E=0
N=2

FIGURE 1

arises because the motion of the particle in the direction of the magnetic field is free, giving rise to the term $\frac{\hbar^2 k^2}{2\mu}$ in the energy expression (3.40). The thicker lines in the diagram are the levels of a completely free particle of mass μ in a magnetic field. The ladders of levels for the different values of N have been separated horizontally in the figure for the sake of clarity.

The above level diagram has ignored the existence of the Coulomb attraction term in (4.2). The main effect of this attraction in high magnetic fields is to remove the freedom of motion along the direction of the field and thus cause bound states to appear below the continuum edges. The form of perturbation theory which we use to take into account the Coulomb interaction is due to Schiff and Snyder[17].

2. Effective Potentials. Since $\beta \gg 1$ the electron is controlled mainly by the magnetic field and it makes many oscillations in this field during the time it takes to make one oscillation due to the influence of the Coulomb field. Put another way, during a time $1/\omega_c$ the Coulomb interaction produces a negligible effect on the motion of the electron. This enables a type of Born-Oppenheimer separation of the wave-equation to be made; we solve (4.2) with the Coulomb interaction, and also the term involving z, the co-ordinate in the direction of the magnetic field, removed. This leads to eigenvalues:

$$E_{\rho\phi}^{NM} = \hbar\omega_c\left(N+\tfrac{1}{2}\right) - \frac{e\hbar H}{m_0 c} M \qquad N = 0,1,2,\ldots \qquad (4.3)$$

$$M \leq N$$

and eigenfunctions:

$$M>0 \qquad \psi_{NM}(\rho\phi) = (-i)^N N^{+}_{NM}\, e^{iM\phi}\, \sigma^{\frac{1}{2}M}\, e^{-\frac{1}{2}\sigma}\, L^{M}_{N}(\sigma) \tag{4.4}$$

$$M<0 \qquad \psi_{NM}(\rho\phi) = (-i)^N N^{-}_{NM}\, e^{iM\phi}\, \sigma^{-\frac{1}{2}M}\, e^{-\frac{1}{2}\sigma}\, L^{-M}_{N-M}(\sigma) \tag{4.5}$$

where:

$$N^{+2}_{NM} = \frac{1}{2\pi\lambda^2}\,\frac{\lfloor N-M}{(\lfloor N)^3}\,, \quad N^{-2}_{NM} = \frac{1}{2\pi\lambda^2}\,\frac{\lfloor N}{(\lfloor N-M)^3}\,, \quad \sigma = \frac{\rho^2}{2\lambda^2}\,, \quad \lambda^2 = \frac{\hbar c}{eH}$$

We now use the Coulomb potential to restrict the motion in the z-direction, the effective potential $V_{NM}(z)$ for the z-motion being the average of the Coulomb field over the positions of the electron in the plane perpendicular to the z-axis for each value of z. i.e.

$$\begin{aligned} V_{NM}(z) &= -\iint \psi^{*}_{NM}(\rho\phi)\,\frac{e^2}{\varkappa\sqrt{\rho^2+z^2}}\,\psi_{NM}(\rho\phi)\,\rho\,d\rho\,d\phi \\ &= -\frac{\lambda^2}{\varkappa}\iint \psi^{*}_{NM}(\sigma\phi)\,\frac{e^2}{\sqrt{2\lambda^2\sigma+z^2}}\,\psi_{NM}(\sigma\phi)\,d\sigma\,d\phi \end{aligned} \tag{4.6}$$

The wave-equation for the z-motion is therefore:

$$\left\{-\frac{\hbar^2}{2\mu}\,\frac{d^2}{dz^2} + V_{NM}(z)\right\}\psi^{i}_{NM}(z) = E^{NMi}_{z}\,\psi^{i}_{NM}(z) \tag{4.7}$$

where i enumerates the different eigenfunctions for the z-motion. The total wave-function is:

$$\tilde{F}^{i}_{NM}(\underline{r}) = \psi_{NM}(\rho\phi)\,\psi^{i}_{NM}(z) \tag{4.8}$$

with energy:

$$E^{NMi} = E_{\rho\phi}^{NM} + E_z^{NMi} \tag{4.9}$$

We postpone a discussion of the validity of the above separation of the wave-equation until after we have determined the eigenfunctions $\psi^i_{NM}(z)$. However we may note here that the separation becomes exact when $H \to \infty$. For the only non-zero off-diagonal matrix elements of $-\frac{e^2}{\varkappa r}$ between the states (4.8) are those linking states of the same M, due to the integration over ϕ. But reference to equation (4.3) or to figure 1 shows that in an infinite field such states have an infinite energy separation, while the matrix elements of $1/r$ remain finite. The functions (4.8) are therefore exact eigenfunctions in this case. We can easily determine the form of the effective potential (4.6) in the infinite field limit, for $\lambda^2 \to 0$ as $H \to \infty$ and since the wavefunctions are normalised we have:

$$V_{NM}(z) = -\frac{e^2}{\varkappa|z|} \qquad \text{for all N and M (infinite field)} \tag{4.10}$$

The wave-equation for the z-motion therefore becomes that of the one-dimensional hydrogen atom. We consider this wave-equation in appendix 4 since it provides useful information about the limit to which the absorption tends in very high magnetic fields.

For finite magnetic fields the form of the effective potentials for very large values of z is also easily determined by the same considerations as we used above for large fields:

$$V_{NM}(z) \to -\frac{e^2}{\varkappa|z|} \qquad \text{as } Z \to \infty \text{ for all N and M} \tag{4.11}$$

However when both z and H are finite the form of $V_{NM}(z)$ is somewhat complicated and depends on the values of N and M. We give here the explicit forms of two of the effective potentials:

$$V_{00}(z) = -\frac{e^2}{\varkappa}\frac{\sqrt{2}}{\lambda} e^{z^2/2\lambda^2} Erfc\left(\frac{|z|}{\sqrt{2}\lambda}\right) \tag{4.12}$$

$$V_{11}(z) = V_{0-1}(z) = -\frac{e^2}{\varkappa}\left\{\frac{|z|}{2\lambda^2} + \frac{1}{\sqrt{2}\lambda} e^{z^2/2\lambda^2}\left[1 - \frac{z^2}{\lambda^2}\right] Erfc\left(\frac{|z|}{\sqrt{2}\lambda}\right)\right\} \tag{4.13}$$

where:

$$Erfc(x) = \int_x^\infty e^{-t^2} dt = \frac{\sqrt{\pi}}{2} - \int_0^x e^{-t^2} dt \tag{4.14}$$

Note that:

$$V_{00}(0) = -\frac{e^2}{\varkappa}\sqrt{\frac{\pi}{2}}\frac{1}{\lambda} \qquad \left[\frac{d}{dz} V_{00}(z)\right]_{z=0} = \frac{e^2}{\varkappa\lambda^2} \tag{4.15}$$

$$V_{11}(0) = -\frac{1}{2}\frac{e^2}{\varkappa}\sqrt{\frac{\pi}{2}}\frac{1}{\lambda} \qquad \left[\frac{d}{dz} V_{11}(z)\right]_{z=0} = 0 \tag{4.16}$$

The two effective potentials are shewn in figure 2, V(z) being measured in units of $e^2/\varkappa\lambda$. The slope of the potential function at z = 0 is non-vanishing only for states having M = 0.

The potentials given in (4.12) and (4.13) allow an investigation of the three lowest groups of levels of the system and

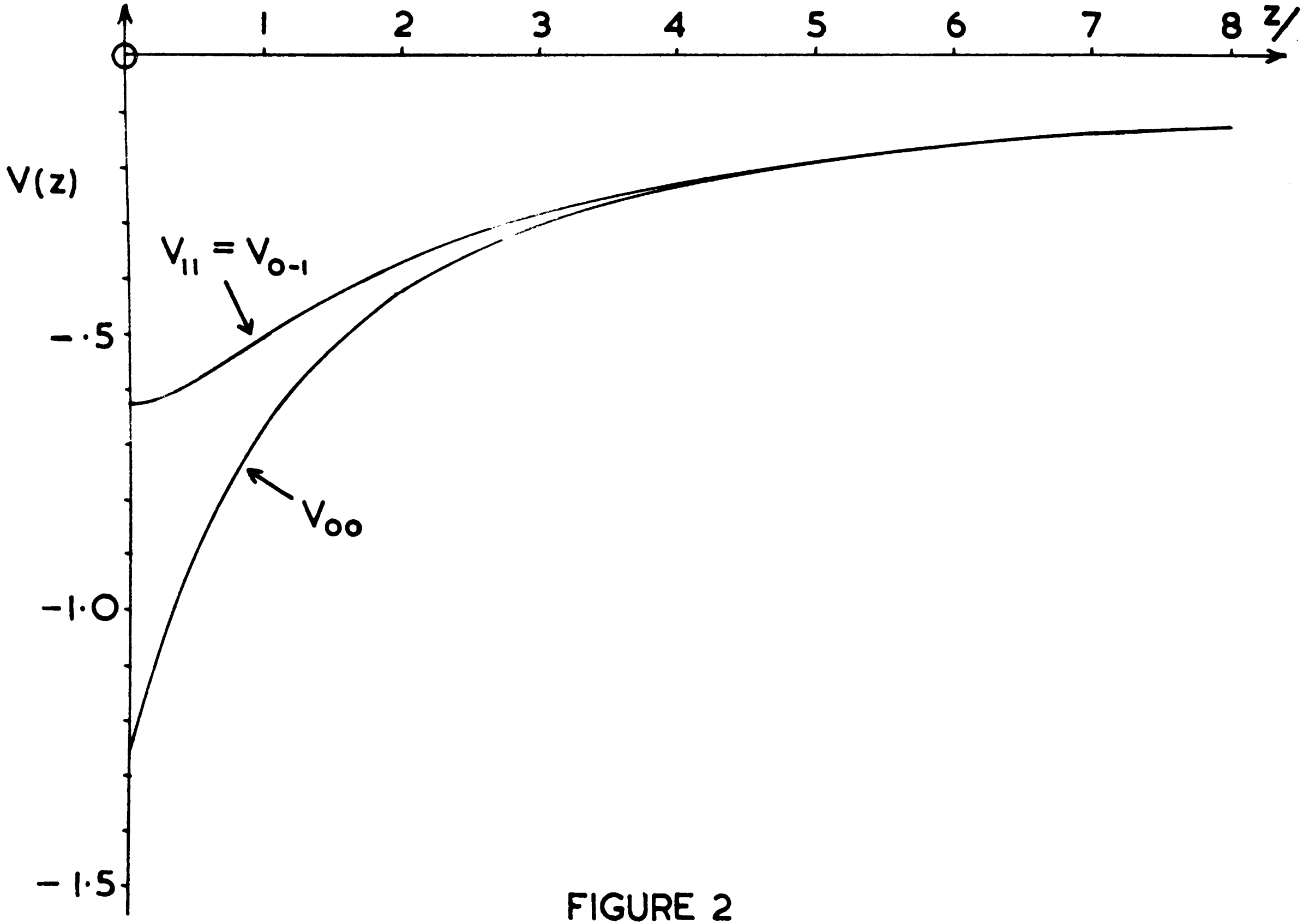


FIGURE 2

these groups are the most important ones. We have shown in chapter 3 that only states having M = -1, 0 or +1 can be excited by electric dipole absorption. Now apart from the three lowest groups of levels, all discrete states of the system having M = -1, 0 or +1 have energies equal to the energies of continuum states belonging to a lower group of levels with the same M value, (see figure 1). As a first correction to the perturbation method outlined above states of the same M value but with different N quantum numbers interact through the Coulomb term in the Hamiltonian since this term is diagonal only for states with the same N and M quantum numbers. These higher discrete states therefore have certain probabilities of transition into the continua of lower groups of levels at the same energy value. This effect is similar to the Auger effect in atomic spectra where a discrete state having energy greater than the ionization energy of the atom can be excited. In cases of this type the high energy discrete states give rise to observable absorption lines only if the line widths due to the probabilities of transition to continuum states are sufficiently small. The order of magnitude of such line widths for the present problem is discussed in section 7 of this chapter. In any case, even when this line width is small the discrete states belonging to the lowest three groups of levels are the ones most likely to be observed experimentally.

As the value of N increases and the value of M decreases the mathematical form of the effective potential becomes more complicated, though its general shape remains the same.

3. Approximate Effective Potentials. It is of course not possible to solve the z-motion wave-equation (4.7) analytically with complicated potential functions like (4.12) and (4.13). However these potentials may be closely approximated by expressions of the form:

$$V(z) = -\frac{e^2}{\kappa(B\lambda + |z|)} + \frac{AB\lambda e^2}{\kappa(B\lambda + |z|)^2} \qquad (4.17)$$

where A and B are constants independent of both field and position, chosen to give closest fit with the required exact potential. For example if we choose $A = \frac{1}{2}$, then the slope of the potential at $z = 0$ is zero as required for $V_{NM}(z)$ when the quantum number M is non-zero. We defer until chapter 5 a consideration of the magnitude of the error introduced by this further approximation.

Introducing (4.17) into the wave-equation (4.7):

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dz^2} - \frac{e^2}{\kappa(a+|z|)}\psi - \frac{Ae^2}{\kappa(a+|z|)^2}\psi = E_z\psi \qquad (4.18)$$

where we have omitted subscripts and also set $B\lambda = a$ for brevity.

Equation (4.18) can be solved analytically and it has solutions corresponding to both bound and free states. We consider these two types of solution separately.

4. Bound States. Introduce a quantity α by putting:

$$E_z = -\frac{\hbar^2 k_0^2}{2\mu\alpha^2} \qquad \text{where } k_0 = \frac{1}{a_0},\ a_0 = \frac{\hbar^2\kappa}{\mu e^2} \qquad (4.19)$$

Also changing the variable to:

$$x = \frac{2k_0}{\alpha}\left(a + |z|\right) \tag{4.20}$$

the wave-equation (4.18) becomes:

$$\frac{d^2\psi}{dx^2} - \frac{1}{4}\psi + \frac{\alpha}{x}\psi - \frac{2Aak_0}{x^2}\psi = 0 \tag{4.21}$$

Define:

$$m = \sqrt{\frac{1}{4} + 2Aak_0} = \sqrt{\frac{1}{4} + \frac{2AB}{\beta^{\frac{1}{2}}}} \tag{4.22}$$

since:

$$\lambda k_0 = \frac{1}{\beta^{\frac{1}{2}}} \tag{4.23}$$

using (4.1) and (4.19). Introducing m into (4.21):

$$\frac{d^2\psi}{dx^2} - \frac{1}{4}\psi + \frac{\alpha}{x}\psi - \frac{m^2 - \frac{1}{4}}{x^2}\psi = 0 \tag{4.24}$$

This has the form of Whittaker's equation (see appendix 3). We are looking for bound states so we require a solution of (4.24) which tends to zero as x tends to infinity. Such a solution, for positive or negative z, is:

$$\psi = W_{\alpha,m}(x) = W_{\alpha,m}\left[\frac{2k_0}{\alpha}\left(a + |z|\right)\right] \tag{4.25}$$

for by (A3.8):

$$W_{\alpha,m}(x) \to x^{\alpha} e^{-\frac{1}{2}x} \qquad \text{as} \quad x \to \infty \tag{4.26}$$

The other independent solution of (4.24) diverges like $x^{-\alpha} e^{\frac{1}{2}x}$ for large x and is therefore not suitable for a bound state wave-function. Equation (4.24) has no singularities, except for an irregular singular

point at infinite x, since the point $x = 0$ is excluded by the definition (4.20). Further, the potential of the problem is invariant under the reflection $Z \longrightarrow -Z$. It follows that the wave-functions must be continuous with continuous slope, and must have either even or odd parity. These conditions lead to a discrete eigenvalue spectrum since they can only be satisfied for certain values of α. For a state of odd parity, α must be such that:

$$W_{\alpha,m}\left[\frac{2k_0 a}{\alpha}\right] = 0 \tag{4.27}$$

while for a state of even parity we must have:

$$\frac{d}{dz} W_{\alpha,m}\left[\frac{2k_0}{\alpha}(a+|z|)\right]_{z=0} = 0 \tag{4.28}$$

In these two equations both a and m depend on the strength of the magnetic field so that the values of α for which they can be satisfied vary with field. We show in figure 3 the qualitative way in which the solutions of (4.27) and (4.28) for α depend on the value of a for small α. For a given value of a the strength of the magnetic field is known since:

$$a = B\lambda = B\sqrt{\frac{\hbar c}{eH}} \tag{4.29}$$

and hence m can be calculated using (4.22). The lines in figure 3 labelled O correspond to solutions of equation (4.27) and those labelled E to solutions of equation (4.28). For any given value of the magnetic field H, and hence of a, there is an infinite number of bound state solutions of equation (4.21), neglecting the finite extent

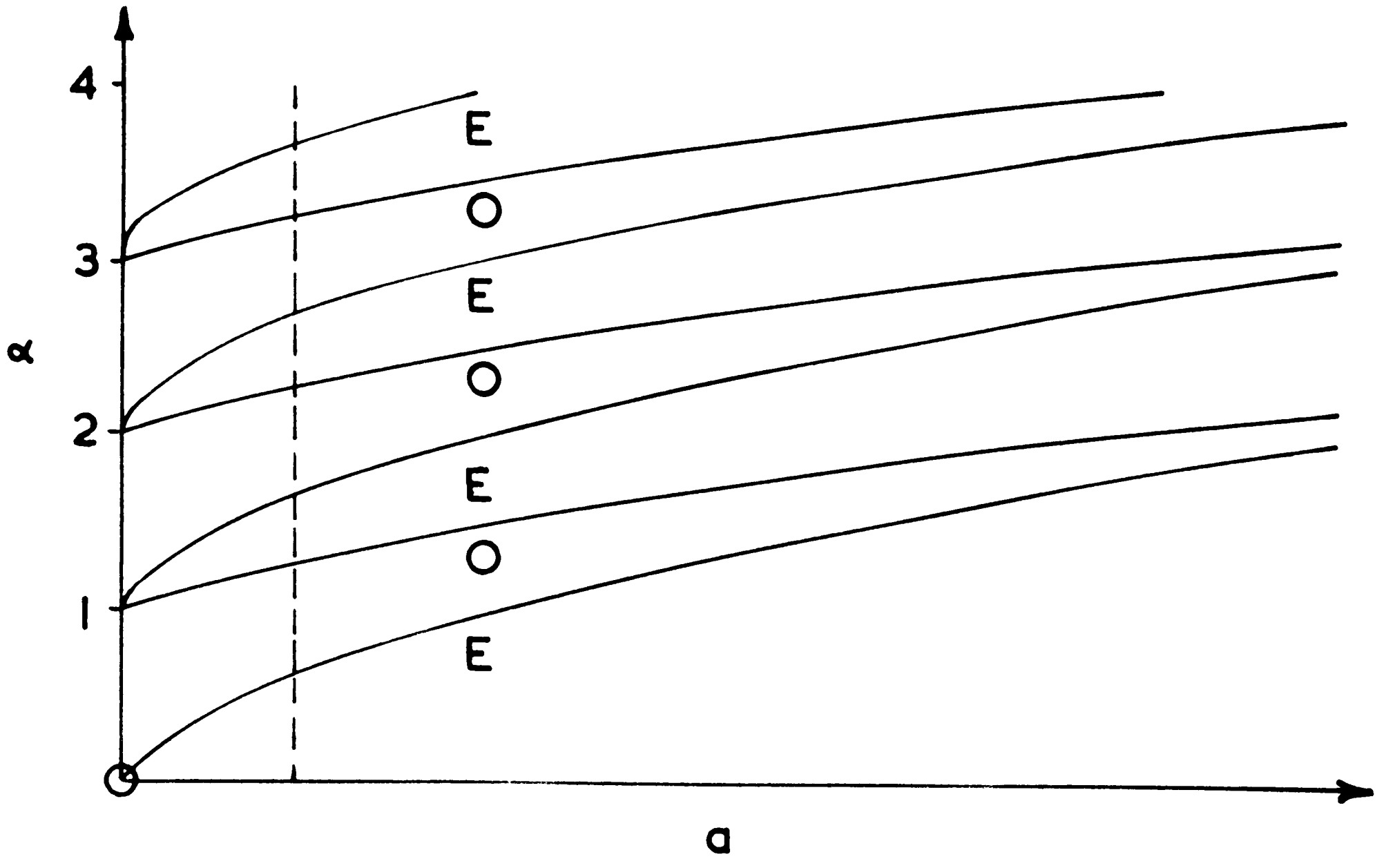


FIGURE 3

of the crystal containing the exciton. In an infinite magnetic field, i.e. $\alpha = 0$, there are degenerate pairs of states having positive integral values of α and therefore eigenvalues equal to the Balmer energies. In addition there is a single even state having an infinite binding energy. These results for infinite field are derived in appendix 4.

As the field decreases from infinity the values of α increase. For a given value of α the number of solutions of (4.27) and (4.28) is finite and for $\nu < \alpha < \nu + 1$ where $\nu = 0, 1, 2, \ldots$ there are ν solutions of (4.27) and $\nu + 1$ solutions of (4.28). However not all these solutions are physically meaningful, for the present theory is valid only for $\beta >> 1$, and there is therefore a physical upper bound to the value of α . The approximate position of this upper bound is marked in figure 3 by a vertical dashed line. We see that for a given α there are at most two field strengths for which the eigenvalue equations can be satisfied.

It is convenient to specify the bound states by means of a quantum number K , which is equal to the number of nodes in the wave-function for the s-motion. Consider the two states which have $\nu < \alpha < \nu + 1$ where as before $\nu = 0, 1, 2, \ldots$

$$\left.\begin{array}{ll} \text{For even states:} & K = 2\nu \\ \text{For odd states:} & K = 2\nu - 1 \end{array}\right\} \qquad (4.30)$$

At $\alpha = \nu$ two nodes in the even states come together but we retain the above definition of K .

We use the quantum number K for the index i of equations (4.7), (4.8) and (4.9), writing the normalised z-wave-functions as $\psi^K_{NM}(z)$ and their energies as E_z^{NMK}. The three quantum numbers N, M and K are sufficient to specify all the bound states of the system uniquely. Unfortunately the normalisation integral for the wave-function (4.25) cannot be evaluated in closed form, except for the infinite magnetic field limit.

We have seen that for the magnetic field strengths which we are considering here, there are just two bound states, one even and the other odd, lying between adjacent Balmer energies. It follows that close to the continuum edge $E_z = 0$ it is possible to define a density of bound states which is the same for both even and odd states and is given by (3.28):

$$S_\alpha(E) = \frac{\alpha^3}{2R} \tag{4.31}$$

By the use of (4.19) and (4.29) it is possible to convert figure 3 relating α and a to the schematic diagram figure 4 relating the energy levels to the magnetic field strength measured by β. Accurate graphs of this type are obtained in chapter 5 by numerical calculation.

5. Free States. We now look for solutions of the wave-equation (4.18) corresponding to free states. Put:

$$E_z = \frac{\hbar^2 k^2}{2\mu} = \frac{\hbar^2 k_0^2}{2\mu\alpha^2} \tag{4.32}$$

where $\hbar k$ is the momentum of the system along the direction of the

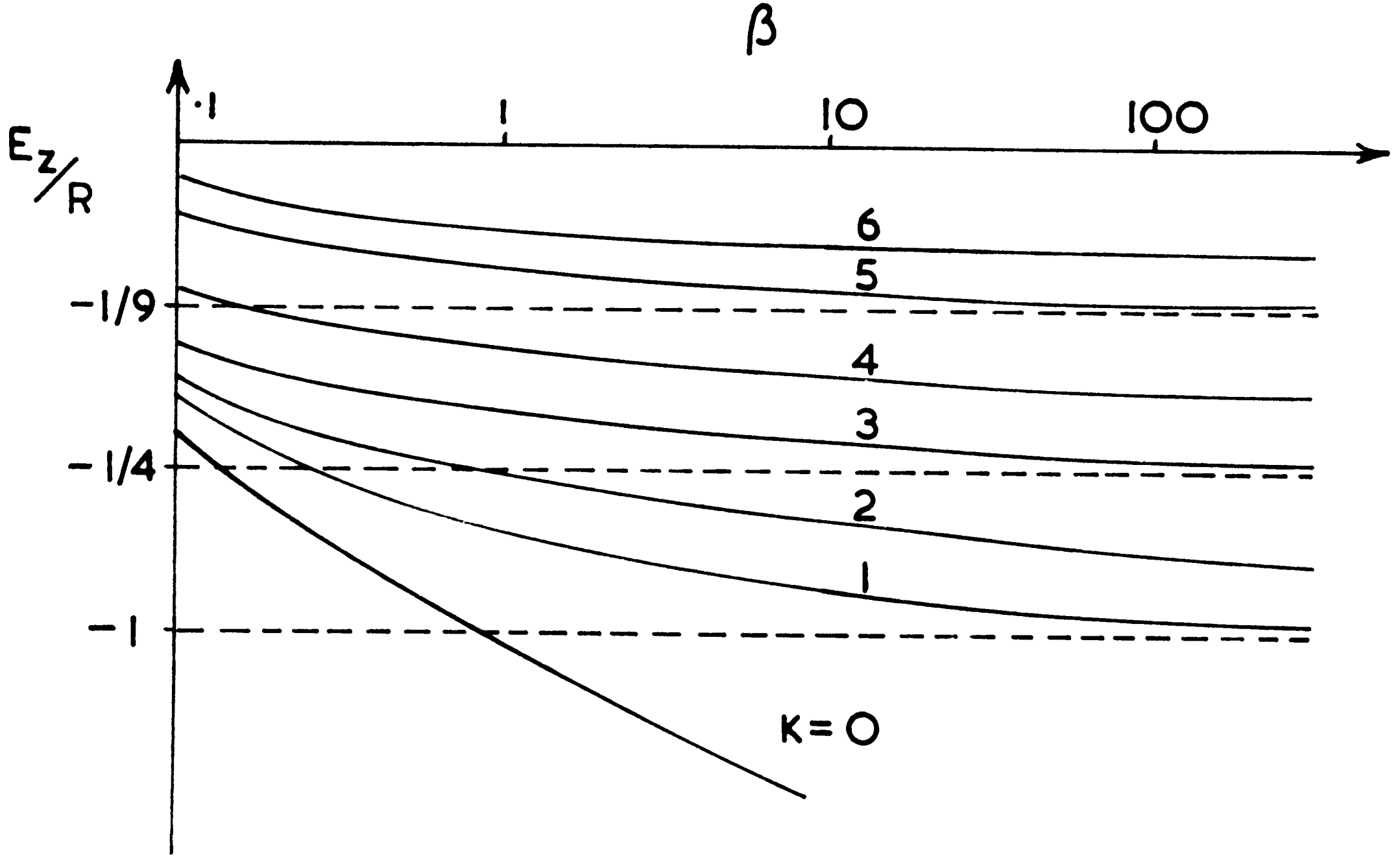


FIGURE 4

magnetic field. Introducing a variable:

$$x = \frac{2ik_0}{\alpha}(a+|z|) \tag{4.33}$$

the wave-equation (4.18) becomes:

$$\frac{d^2\psi}{dx^2} - \frac{1}{4}\psi - \frac{i\alpha}{x}\psi - \frac{2Aak_0}{x^2}\psi = 0 \tag{4.34}$$

Defining a quantity m as in (4.22) this is:

$$\frac{d^2\psi}{dx^2} - \frac{1}{4}\psi - \frac{i\alpha}{x}\psi - \frac{m^2-\frac{1}{4}}{x^2}\psi = 0 \tag{4.35}$$

This is again a form of Whittaker's equation, but this time there are two acceptable independent solutions, since we are not imposing any boundary condition at infinite x. We take the functions defined in appendix 3 as $W_{-i\alpha,m}(x)$ and $V_{-i\alpha,m}(x)$ for the two independent solutions. These have the following asymptotic forms:

$$W_{-i\alpha,m}(x) \rightarrow x^{-i\alpha}e^{-\frac{1}{2}x} = e^{-i\alpha\log x - \frac{1}{2}x} \tag{4.36}$$

$$V_{-i\alpha,m}(x) \rightarrow x^{i\alpha}e^{\frac{1}{2}x}e^{\pi\alpha} = e^{i\alpha\log x + \frac{1}{2}x + \pi\alpha} \tag{4.37}$$

For the remainder of this section we shall drop the subscripts on V and W. From these two solutions of (4.35) we can form an even wave-function:

$$\psi^e(z) = N^e\left\{V\left[\frac{2ik_0}{\alpha}(a+|z|)\right]W'\left[\frac{2ik_0a}{\alpha}\right] - W\left[\frac{2ik_0}{\alpha}(a+|z|)\right]V'\left[\frac{2ik_0a}{\alpha}\right]\right\} \tag{4.38}$$

and an odd wave-function:

$$\psi^o(z) = N^o\tau_2\left\{V\left[\frac{2ik_0}{\alpha}(a+|z|)\right]W\left[\frac{2ik_0a}{\alpha}\right] - W\left[\frac{2ik_0}{\alpha}(a+|z|)\right]V\left[\frac{2ik_0a}{\alpha}\right]\right\} \tag{4.39}$$

where $\tau_z = 1$ for $z > 0$ and $\tau_z = -1$ for $z < 0$,

and:

$$W'\left[\frac{2ik_0a}{\alpha}\right] = \frac{d}{dz}\left\{W\left[\frac{2ik_0}{\alpha}(a+|z|)\right]\right\}_{z=0} \qquad \text{similarly} \quad V'\left[\frac{2ik_0a}{\alpha}\right]$$

N^e and N^o are normalisation constants to be determined.

The asymptotic forms of these two wave-functions may be obtained by use of (4.36) and (4.37). For the even function:

$$\psi^e(z) \to N^e e^{\frac{\pi\alpha}{2}} \left\{W'\left[\frac{2ik_0a}{\alpha}\right] e^{i\frac{k_0}{\alpha}(a+|z|)+i\alpha\log\frac{2k_0}{\alpha}(a+|z|)}\right. \tag{4.40}$$

$$\left. - V'\left[\frac{2ik_0a}{\alpha}\right] e^{-i\frac{k_0}{\alpha}(a+|z|)-i\alpha\log\frac{2k_0}{\alpha}(a+|z|)}\right\}$$

We wish to normalize the wave-functions to a length L_z. Now their asymptotic forms are oscillatory functions with a constant amplitude, and provided that L_z is sufficiently large the contribution to the normalisation integral from the region where (4.40) does not hold is entirely negligible. We therefore evaluate the integral using the asymptotic form of $\psi^e(z)$ which gives:

$$\int_{L_z} \psi^{e*}(z)\,\psi^e(z)\,dz = L_z N^{e2} e^{\pi\alpha}\left\{W'^*\left[\frac{2ik_0a}{\alpha}\right]W'\left[\frac{2ik_0a}{\alpha}\right] + V'^*\left[\frac{2ik_0a}{\alpha}\right]V'\left[\frac{2ik_0a}{\alpha}\right]\right\}$$

$$= 1 \tag{4.41}$$

The normalisation integral for the odd wave-function may be similarly evaluated, and we finally obtain for the two normalized wave-functions:

$$\psi^{e}(z) = \frac{e^{-\frac{\pi\alpha}{2}}}{\sqrt{L_z}} \frac{\left\{V\left[\frac{2ik_0}{\alpha}(a+|z|)\right]W'\left[\frac{2ik_0a}{\alpha}\right] - W\left[\frac{2ik_0}{\alpha}(a+|z|)\right]V'\left[\frac{2ik_0a}{\alpha}\right]\right\}}{\sqrt{\left|W'\left[\frac{2ik_0a}{\alpha}\right]\right|^2 + \left|V'\left[\frac{2ik_0a}{\alpha}\right]\right|^2}} \tag{4.42}$$

$$\psi^{o}(z) = \gamma_z \frac{e^{-\frac{\pi\alpha}{2}}}{\sqrt{L_z}} \frac{\left\{V\left[\frac{2ik_0}{\alpha}(a+|z|)\right]W\left[\frac{2ik_0a}{\alpha}\right] - W\left[\frac{2ik_0}{\alpha}(a+|z|)\right]V\left[\frac{2ik_0a}{\alpha}\right]\right\}}{\sqrt{\left|W\left[\frac{2ik_0a}{\alpha}\right]\right|^2 + \left|V\left[\frac{2ik_0a}{\alpha}\right]\right|^2}} \tag{4.43}$$

For $\alpha \ll 1$, or $k \gg k_0$, well away from the continuum edge the wave-functions are unaffected by the Coulomb potential, for it is seen by use of (4.36) and (4.37) that:

$$\left.\begin{aligned} \psi^{e}(z) &\to -\frac{i}{\sqrt{\tfrac{1}{2}L_z}} \cos\frac{k_0 z}{\alpha} \\ \psi^{o}(z) &\to \frac{i}{\sqrt{\tfrac{1}{2}L_z}} \sin\frac{k_0 z}{\alpha} \end{aligned}\right\} \quad \alpha \to 0 \tag{4.44}$$

and these are just free particle wave-functions.

6. Absorption Coefficients. Using the wave-functions derived in this chapter it is possible to write down formal expressions for line intensities and absorption coefficients with the aid of (3.11) and (3.13). We shall carry out numerical calculations for the three lowest groups of levels, i.e. N = M = 0, N = M = 1 and N = 0, M = -1, since these are the most important ones as discussed in section 2, so we here concern ourselves with these particular levels. There are three

cases to consider: allowed absorption, forbidden absorption with the radiation polarized along the direction of the magnetic field and forbidden absorption with radiation polarized perpendicular to the field.

(i) Allowed Absorption. In this case the most important contribution to the absorption arises from the even states of the N = M = 0 group. For this group of levels the total wave-functions are:

$$\tilde{F}^{i}_{oo}(\underline{r}) = \frac{1}{\sqrt{2\pi\lambda^2}}\, e^{-\frac{1}{4}\sigma}\, \psi^{i}_{oo}(z) \tag{4.45}$$

with energies:

$$E^{ooi} = \tfrac{1}{2}\hbar\omega_c + E_z^{ooi} \tag{4.46}$$

where E_z^{ooi} is given by (4.19) for bound states and (4.32) for free states. Now $\psi^{i}_{oo}(0)$ is non-zero only for even states, so for discrete levels, using (3.11):

$$\langle K0|\underline{\epsilon}\cdot\underline{p}|0\rangle = \tilde{F}^{K}_{oo}(0)\sqrt{N\Omega}\;\underline{\epsilon}\cdot\underline{p}_{cv} = \sqrt{\frac{N\Omega}{2\pi\lambda^2}}\,\psi^{K}_{oo}(0)\,\underline{\epsilon}\cdot\underline{p}_{cv} \qquad K = 0, 2, 4 \ldots \tag{4.47}$$

and for the continuum:

$$\langle \kappa 0|\underline{\epsilon}\cdot\underline{p}|0\rangle = \tilde{F}^{k}_{oo}(0)\sqrt{N\Omega}\;\underline{\epsilon}\cdot\underline{p}_{cv} = \sqrt{\frac{N\Omega}{2\pi\lambda^2}}\,\psi^{e}_{oo}(0)\,\underline{\epsilon}\cdot\underline{p}_{cv} \tag{4.48}$$

Consider first the discrete levels. A series of lines will be observed at energies:

$$\hbar\omega = E_G + \tfrac{1}{2}\hbar\omega_c + E_z^{ooK} \qquad K = 0, 2, 4, \cdots \tag{4.49}$$

and with intensities proportional to the square of (4.47). By (4.25):

$$\psi^{K}_{oo}(z) = N W_{\alpha,m}(x) = \frac{N}{\pi}\cos\pi(\alpha+m)\,\Gamma\left(\tfrac{1}{2}+\alpha+m\right)\Gamma(-2m)\,M_{\alpha,m}(x) + \frac{N}{\pi}\cos\pi(\alpha-m)\,\Gamma\left(\tfrac{1}{2}+\alpha-m\right)\Gamma(2m)\,M_{\alpha,-m}(x) \tag{4.50}$$

where N is a normalisation constant, and we have used the definition (A3.6) of W with some manipulation of the gamma functions. If $\psi^{\kappa}_{00}(z)$ is to be an even function then W must satisfy the condition (4.28) that its derivative with respect to z at z = 0 must be zero. Denoting this differentiation by a prime and using (4.50) the condition for an even function is:

$$\cos\pi(\alpha+m)\,\Gamma\left(\tfrac{1}{2}+\alpha+m\right)\Gamma(-2m)\,M'_{\alpha,m}\left(\frac{2k_0a}{\alpha}\right) + \cos\pi(\alpha-m)\,\Gamma\left(\tfrac{1}{2}+\alpha-m\right)\Gamma(2m)\,M'_{\alpha,-m}\left(\frac{2k_0a}{\alpha}\right) = 0 \tag{4.51}$$

If we write this equation symbolically as:

$$A\cos\pi(\alpha+m) + B\cos\pi(\alpha-m) = 0$$

then elementary trigonometry gives the results:

$$\cos\pi(\alpha+m) = -\frac{2B\sin\pi m\cos\pi m}{\sqrt{A^2+B^2+2AB\cos 2\pi m}} \qquad \cos\pi(\alpha-m) = \frac{2A\sin\pi m\cos\pi m}{\sqrt{A^2+B^2+2AB\cos 2\pi m}}$$

(4.51) may therefore be used to eliminate the cosine terms from (4.50):

$$NW_{\alpha,m}(x) = \frac{N}{2m\,M_1(\alpha,m)}\,\Gamma\left(\tfrac{1}{2}+\alpha+m\right)\Gamma\left(\tfrac{1}{2}+\alpha-m\right)\left\{M_{\alpha,m}\left[\frac{2k_0}{\alpha}(a+|z|)\right]M'_{\alpha,-m}\left[\frac{2k_0a}{\alpha}\right] - M_{\alpha,-m}\left[\frac{2k_0}{\alpha}(a+|z|)\right]M'_{\alpha,m}\left[\frac{2k_0a}{\alpha}\right]\right\} \tag{4.52}$$

where:

$$M_1^2(\alpha,m) = A^2+B^2+2AB\cos 2\pi m \qquad \begin{cases} A = \Gamma\left(\tfrac{1}{2}+\alpha+m\right)\Gamma(-2m)\,M'_{\alpha,m}\left[\frac{2k_0a}{\alpha}\right] \\ B = \Gamma\left(\tfrac{1}{2}+\alpha-m\right)\Gamma(2m)\,M'_{\alpha,-m}\left[\frac{2k_0a}{\alpha}\right] \end{cases} \tag{4.53}$$

and we have used the relation:

$$\Gamma(2m)\,\Gamma(-2m) = -\frac{\pi}{2m \sin 2\pi m} \tag{4.54}$$

Using (A3.10) $\psi^{K}_{00}(0)$ takes on a very simple form:

$$\psi^{K}_{00}(0) = N W_{\alpha,m}\left(\frac{2k_0 a}{\alpha}\right) = -\frac{2k_0 N}{\alpha M_1(\alpha,m)}\,\Gamma\left(\tfrac{1}{2}+\alpha+m\right)\Gamma\left(\tfrac{1}{2}+\alpha-m\right) \tag{4.55}$$

This is now in a form very suitable for numerical calculations, provided that the normalization constant N can be evaluated. We have stated above that the normalization integral for $W_{\alpha,m}(x)$ has not been carried out for general values of α and m. However for special values of α and m the integral can be done and the result is given in (A3.30). The important properties of $W_{\alpha,m}(x)$, such as its asymptotic form and the positions of its zeros, vary in a smooth way with α and m and these properties do not show any singular behaviour at the values of α and m for which the normalization integral can be carried out. Since the value of the integral for the special α and m is also a smoothly varying function of α and m, it should be a good approximation to assume that (A3.30) holds for the intermediate values of α and m, as well as for the special values. This assumption may in fact be exactly correct, though it has not been found possible to prove it mathematically.

To normalise $\psi^{K}_{00}(z)$ we really require the integral (A3.30) with values $-\frac{2k_0 a}{\alpha} < x < \frac{2k_0 a}{\alpha}$ excluded from the range of integration. However numerical calculation shows that the contribution to the normalisation integral from this range of x values is negligible

except for the $K = 0$ state, and we therefore make the approximation:

$$N = \sqrt{\frac{k_0}{2\alpha^2}} \left[\Gamma\left(\tfrac{1}{2} + \alpha + m\right) \Gamma\left(\tfrac{1}{2} + \alpha - m\right) \right]^{-\frac{1}{2}} \tag{4.56}$$

Hence:

$$\tilde{F}^{K}_{00}(0) = \frac{1}{\sqrt{2\pi\lambda^2}} \psi^{K}_{00}(0) = -\frac{1}{\alpha^2 M_1(\alpha, m)} \sqrt{\frac{\beta}{\pi a_0^5}} \sqrt{\Gamma\left(\tfrac{1}{2}+\alpha+m\right)\Gamma\left(\tfrac{1}{2}+\alpha-m\right)} \tag{4.57}$$

Substitution of this expression into (4.47) gives the required electric dipole matrix elements and hence line intensities can be calculated if the variation in α with field [given by solution of (4.51)] is known.

Close to the absorption edge a large number of discrete lines overlap to form a pseudo-continuum having a density of states $S_\alpha(E)$ given by (4.31) i.e. $\alpha^3/2R$. The absorption coefficient in this region is therefore proportional to:

$$S_\alpha(E) \left| \langle K0 | \epsilon . p | 0 \rangle \right|^2 = N\Omega \frac{\mu\beta}{\pi \hbar^2 a_0^3} \frac{\Gamma\left(\tfrac{1}{2}+\alpha+m\right)\Gamma\left(\tfrac{1}{2}+\alpha-m\right)}{\alpha M_1^2(\alpha, m)} \left| p_{cv} \right|^2 \tag{4.58}$$

using (3.13), (4.23) and (4.47).

For the wave-functions of the true continuum, using (4.42) and (A3.11):

$$\psi^{e}_{00}(0) = -\frac{2ike^{\frac{\pi\alpha}{2}}}{\sqrt{L_z}} \left[\left| W'\left(\frac{2ik_0 a}{\alpha}\right) \right|^2 + \left| V'\left(\frac{2ik_0 a}{\alpha}\right) \right|^2 \right]^{-\frac{1}{2}} \tag{4.59}$$

Using the density of states (3.14) this gives:

$$S_1(E)\left|\langle \alpha 0|\underline{\epsilon}.\underline{p}|0\rangle\right|^2 = N\Omega\,\frac{\mu\beta}{\pi^2\hbar^2 a_0^3}\,\frac{e^{\pi\alpha}}{\alpha}\,\frac{|p_{cv}|^2}{\left|w'\left(\frac{2ik_0a}{\alpha}\right)\right|^2+\left|v'\left(\frac{2ik_0a}{\alpha}\right)\right|^2} \qquad (4.60)$$

The expressions (4.58) and (4.60) for the absorption coefficients below and above the absorption edge cannot be simplified any further by analytic means. In the next chapter we determine the absorption coefficient close to the edge numerically by expanding the two expressions in power series of $1/\alpha^2$. In this way it is found that the absorption coefficient is a continuous function of energy at the edge and also has continuous slope there.

(ii) Forbidden Absorption $\underline{\epsilon} \parallel \underline{H}$. The absorption depends on $\left[\pi_z \psi^i_{00}(z)\right]_{z=0}$ i.e. on $\left[-i\hbar\frac{d}{dz}\psi^i_{00}(z)\right]_{z=0}$, and the most important contribution comes from the odd states of the group N = M = 0. The theory follows through in much the same way as for case (i). The discrete levels again give rise to a series of lines at the energies (4.49), but it is now the states of odd K which contribute. The dipole matrix elements for the discrete states are:

$$\langle K0|\underline{\epsilon}.\underline{p}|0\rangle = -\sqrt{\frac{N\Omega}{2\pi\lambda^2}}\;i\hbar M^z_{cv}\left[\frac{d}{dz}\psi^K_{00}(z)\right]_{z=0} \qquad K = 1,3,\ldots \qquad (4.61)$$

and for the continuum states:

$$\langle \alpha 0|\underline{\epsilon}.\underline{p}|0\rangle = -\sqrt{\frac{N\Omega}{2\pi\lambda^2}}\;i\hbar M^z_{cv}\left[\frac{d}{dz}\psi^0_{00}(z)\right]_{z=0} \qquad (4.62)$$

Equations similar to those for case (i) are easily derived and we quote

them without proof. For the discrete levels:

$$\left[\pi_z \tilde{F}^{\kappa}_{oo}(\underline{r})\right]_{\underline{r}=0} = -\frac{i\hbar}{\sqrt{2\pi\lambda^2}}\left[\frac{d}{dz}\psi^{\kappa}_{oo}(z)\right]_{z=0} = -\frac{i\hbar}{a^2 M_2(\alpha,m)}\sqrt{\frac{\beta}{\pi a_0^5}}\sqrt{\Gamma(\tfrac{1}{2}+\alpha+m)\Gamma(\tfrac{1}{2}+\alpha-m)} \quad (4.63)$$

where: $\kappa = 1, 3, \ldots$

$$M_2^2(\alpha,m) = C^2 + \mathcal{D}^2 + 2C\mathcal{D}\cos 2\pi m \qquad \begin{cases} C = \Gamma(\tfrac{1}{2}+\alpha+m)\Gamma(-2m)M_{\alpha,m}\left(\dfrac{2k_0a}{\alpha}\right) \\ \mathcal{D} = \Gamma(\tfrac{1}{2}+\alpha-m)\Gamma(2m)M_{\alpha,-m}\left(\dfrac{2k_0a}{\alpha}\right) \end{cases} \quad (4.64)$$

Close to the absorption edge, where the discrete lines overlap to form a continuum, the absorption coefficient is proportional to:

$$S_\alpha(E)\left|\langle \kappa 0|\underline{\epsilon}.\underline{p}|0\rangle\right|^2 = N\Omega\,\frac{\hbar\beta}{\pi a_0^3}\,\frac{\Gamma(\tfrac{1}{2}+\alpha+m)\Gamma(\tfrac{1}{2}+\alpha-m)}{\alpha M_2^2(\alpha,m)}\left|M_{cv}^z\right|^2 \quad (4.65)$$

and in the true continuum using (4.43):

$$S_1(E)\left|\langle \alpha 0|\underline{\epsilon}.\underline{p}|0\rangle\right|^2 = N\Omega\,\frac{\hbar\beta}{\pi^2 a_0^3}\,\frac{e^{\pi\alpha}}{\alpha}\,\frac{\left|M_{cv}^z\right|^2}{\left|W\left(\frac{2ik_0a}{\alpha}\right)\right|^2 + \left|V\left(\frac{2ik_0a}{\alpha}\right)\right|^2} \quad (4.66)$$

The expressions for the absorption coefficient above and below the edge again join up smoothly as will be shown in the next chapter.

It is of interest to compare the orders of magnitude of the absorption coefficients in the allowed and forbidden cases. p_{cv} is of order $1/L$, where L is the lattice constant, while M_{cv} is of order unity [see (3.10)]. Also:

$$\frac{d}{dz}\psi^{i}_{oo}(z) \sim \frac{1}{a_0}\psi^{i}_{oo}(z)$$

The absorption in this forbidden case is therefore weaker on the whole than that in the allowed case by a factor of order [lattice constant/effective Bohr radius]^2.

(iii) Forbidden Absorption $\underline{\epsilon} \perp \underline{H}$. For left circularly polarised radiation the even states of the N = 0, M = -1 group contribute to the absorption, while for right circularly polarised radiation it is the even states of the N = M = 1 group which contribute. The form of the absorption is the same for both polarisations, except that in the latter case the energy at which the absorption takes place is lower by an amount $\frac{e\hbar H}{c}\left[\frac{1}{m_h} - \frac{1}{m_e}\right]$. We need therefore only consider one of the polarisations and we choose right circular polarisation. Now:

$$\pi_- \tilde{F}^i_{\perp\perp}(\underline{r}) = \pi_- \psi_{\perp\perp}(\rho\phi)\,\psi^i_{\perp\perp}(z)$$

$$= \frac{\hbar}{\lambda}\sqrt{2}\,\psi_{00}(\rho\phi)\,\psi^i_{\perp\perp}(z) \qquad (4.67)$$

using (4.8) and (A2.42). Hence:

$$\left[\pi_- \tilde{F}^i_{\perp\perp}(\underline{r})\right]_{r=0} = \frac{\hbar}{\lambda^2}\frac{1}{\sqrt{\pi}}\,\psi^i_{\perp\perp}(0) \qquad (4.68)$$

$\psi^i_{\perp\perp}(0)$ may be calculated by the same methods as were used in case (i) for calculating $\psi^i_{00}(0)$. For the bound states:

$$\left[\pi_- \tilde{F}^K_{\perp\perp}(\underline{r})\right]_{r=0} = -\frac{\beta\hbar}{\alpha^2 M_1(\alpha,m)}\sqrt{\frac{2}{\pi a_0^7}}\sqrt{\Gamma\left(\tfrac{1}{2}+\alpha+m\right)\Gamma\left(\tfrac{1}{2}+\alpha-m\right)} \qquad K=0,2,\ldots \qquad (4.69)$$

where $M_1(\alpha,m)$ is defined in (4.53). Of course the relationship of m with β, as given by (4.22), is different to what it was for case (i) since the effective potential (4.17) is different for the N = M = 1 states. The energies at which the lines are observed are:

$$\hbar\omega = E_G + \tfrac{3}{2}\hbar\omega_c - \frac{e\hbar H}{m_h c} + E_Z^{\perp\perp K} \qquad K = 0, 2, 4, \ldots \qquad (4.70)$$

and the intensities are proportional to the square of (4.69).

Close to the absorption edge, where the discrete lines overlap to form a continuum, the absorption coefficient is proportional to:

$$S_\alpha(E)\left|\langle K0|\underline{\epsilon}.\underline{p}|0\rangle\right|^2 = N\Omega\frac{\mu\beta^2}{2\pi a_0^5}\frac{\Gamma(\frac{1}{2}+\alpha+m)\Gamma(\frac{1}{2}+\alpha-m)}{\alpha M_1^2(\alpha,m)}\left|M_{cv}^{+}\right|^2 \qquad (4.71)$$

where we have used (3.11) and (3.13). In the true continuum:

$$S_1(E)\left|\langle\alpha 0|\underline{\epsilon}.\underline{p}|0\rangle\right|^2 = N\Omega\frac{\mu\beta^2}{2\pi^2 a_0^5}\frac{e^{\pi\alpha}}{\alpha}\frac{\left|M_{cv}^{+}\right|^2}{\left|\omega'\left(\frac{2ik_0a}{\alpha}\right)\right|^2+\left|V'\left(\frac{2ik_0a}{\alpha}\right)\right|^2} \qquad (4.72)$$

To calculate the order of magnitude of the absorption coefficient in this case we observe that:

$$\pi_-\psi_{11}(\rho,\phi)\psi_{11}^{i}(z) \sim \frac{h}{\lambda}\psi_{00}(\rho,\phi)\psi_{11}^{i}(z)$$

The absorption in this forbidden case is therefore on the whole weaker than that in the allowed case by a factor of order $\left[\text{lattice constant/radius of magnetic orbit}\right]^2$.

This completes the formal treatment of the absorption coefficients. Various graphs of the coefficients computed from the above expressions by numerical methods are presented in chapter 5.

7. High Energy Discrete States. The occurrence of bound states having energies lying in the continua of lower groups of levels has been pointed out in section 2. The line widths of such discrete levels due to the probability of transition into a continuum state can be

easily estimated. The numerical results of chapter 5 lead to the expectation that only the ground state, i.e. the $K = 0$ state, of each N,M group will be observed in an experiment since this state gives rise to an absorption line which is much more intense than the lines due to the excited states within a group. We therefore consider as an example the ground state of the $N = 1$, $M = 0$ group which is level with the continuum of the $N = M = 0$ group (see figure 1); other cases may be dealt with in a similar manner.

For $\beta >> 1$ the continuum state we are interested in has a wave-vector $k >> k_0$ and we therefore take a simple cosine function for its z-dependence [see (4.44)]:

$$\tilde{F}^{e}_{oo}(\underline{r}) = \frac{1}{\sqrt{2\pi\lambda^2}} e^{-\frac{1}{2}\sigma} \frac{1}{\sqrt{\frac{1}{2}L_z}} \cos kz \qquad (4.73)$$

For the bound state it is a good approximation to assume a simple exponential dependence on s:

$$\tilde{F}^{o}_{10}(\underline{r}) = \frac{1}{\sqrt{2\pi\lambda^2}} e^{-\frac{1}{2}\sigma} (1-\sigma) \frac{1}{\sqrt{\alpha a_0}} e^{-\frac{|z|}{\alpha a_0}} \qquad (4.74)$$

The probability of transition from the discrete to the continuum state is then:

$$P = \frac{2\pi}{\hbar} S_1(E) |M|^2 \qquad (4.75)$$

where M is the matrix element of the Coulomb attraction:

$$M = -\int \tilde{F}^{e\,*}_{oo}(\underline{r}) \frac{e^2}{\varkappa r} \tilde{F}^{o}_{10}(\underline{r})\, d\underline{r} \qquad (4.76)$$

In estimating the value of this matrix element we proceed as in sections

2 and 3 of this chapter. First carry out the ρ, ϕ part of the integral (4.76), obtaining a complicated function of z similar to the effective potentials of section 2. Approximate this function by a simpler expression as in section 3, and finally carry out the z part of the integral (4.76). For the particular case we are considering here the ρ, ϕ part of the integral yields a function of z which is the difference of the effective potentials $V_{00}(z)$ and $V_{11}(z)$ [see (4.12), (4.13) and figure 2] . This function can be roughly approximated by:

$$-\frac{e^2}{\varkappa}\frac{\lambda^2}{(b+|z|)^3} \qquad \text{where} \quad b^3 = \sqrt{\frac{2}{\pi}}\, 2\lambda^3 \tag{4.77}$$

so that:

$$M \sim -\frac{e^2\lambda^2 2}{\varkappa\sqrt{\frac{1}{2}L_z a_0 \alpha}} \int_0^\infty \cos kz\; e^{-\frac{z}{2a_0}} \frac{1}{(b+z)^3}\, dz \tag{4.78}$$

Put:

$$I = \int_0^\infty \cos kz\; e^{-\frac{z}{2a_0}} \frac{a_0^2}{(b+z)^3}\, dz \tag{4.79}$$

It remains to estimate the order of magnitude of this integral I. Now $k \sim 1/\lambda$ and $b \sim \lambda$ by (4.77) so that:

$$I \sim \int_0^\infty \cos\sqrt{\beta}\frac{z}{a_0}\; e^{-\frac{z}{2a_0}} \frac{1}{\left(\frac{1}{\sqrt{\beta}}+\frac{z}{a_0}\right)^3}\, d\left(\frac{z}{a_0}\right) \qquad \text{using (4.23)}$$

Hence:

$$I \sim \int_0^\infty \cos y \; e^{-\frac{y}{\sqrt{\beta}\alpha}} \frac{\beta}{(1+y)^3} \, dy \qquad \text{where} \quad y = \sqrt{\beta}\,\frac{z}{a_0}$$

$$\sim \int_0^\infty \frac{\beta}{(1+y)^3} \, dy \sim \frac{\beta}{2} \tag{4.80}$$

since the cosine and exponential factors have not fallen much below their unit values at y = 0 in the region where the inverse cube factor is significant. Hence substituting into (4.78):

$$M = -\frac{e^2\lambda^2\beta}{\pi a_0^2 \sqrt{\frac{1}{2}L_{2\alpha}\alpha a_0}} = -2R\sqrt{\frac{2a_0}{L_{2\alpha}}} \tag{4.81}$$

where we have used (3.23) and (4.23). It is noteworthy that M depends on the magnetic field strength only through the very weak field dependence of α . Substituting into (4.75) from (3.14) and (4.81) and using the definition (4.1) of β :

$$p = \frac{2\sqrt{2}R}{\alpha\hbar\beta^{\frac{1}{2}}} \tag{4.82}$$

The line width is therefore:

$$\Delta E \sim \frac{2\sqrt{2}R}{\alpha\beta^{\frac{1}{2}}} \sim 2\sqrt{-\frac{2RE_2^{100}}{\beta}} \tag{4.83}$$

The method of estimating the integral I is such as to give a rather larger value than the exact one, particularly for the smaller values of β , so that the line width is somewhat smaller than (4.83). The variation of α with field for the ground state of the N = 1,

M = 0 group of levels has not been calculated but it will be about the same as for the ground states of the two groups of levels for which numerical information is given in chapter 5. Referring to figures 6 and 7 we see that the absorption line due to the 100 state will be quite considerably broadened for the lower values of β plotted in the graphs, though it should be narrow enough for observation at fields corresponding to values of β at the higher end of the β scale. Similar considerations may be expected to apply to absorption lines due to the other discrete states which are degenerate with continuum states having the same M quantum number.

Chapter 5. NUMERICAL RESULTS AND DISCUSSION.

1. Bound Exciton States. Numerical calculations have been carried out for the three lowest groups of levels, i.e. the $N = M = 0$, $N = M = 1$ and $N = 0$, $M = -1$ groups. Corresponding levels in the last two groups have the same energies relative to their continuum edges and they also give rise to lines of the same intensity, due to the fact that the effective potentials for the s-motion of these two groups of states are the same [see (4.13)]. We therefore restrict our attention to the $N = M = 0$ and $N = M = 1$ levels.

The first step in carrying out numerical calculations is to fit approximate potentials $V(s)$ of the type (4.17) to the exact potentials $V_{00}(s)$ and $V_{11}(s)$. We have two arbitrary parameters A and B at our disposal, and we choose these in such a way that the exact and approximate potential curves have the same slope at the origin and enclose equal areas with the axis of s. $V_{00}(s)$ and the approximation to it are displayed in figure 5, where the potential is in units of $e^2/\varkappa\lambda$.

Having determined A and B the two quantities $\alpha = \beta\lambda$ and m defined in (4.22) can be calculated for any given value of the magnetic field and we are now in a position to set about solving the eigenvalue equations (4.27) and (4.28) for α and hence finding the

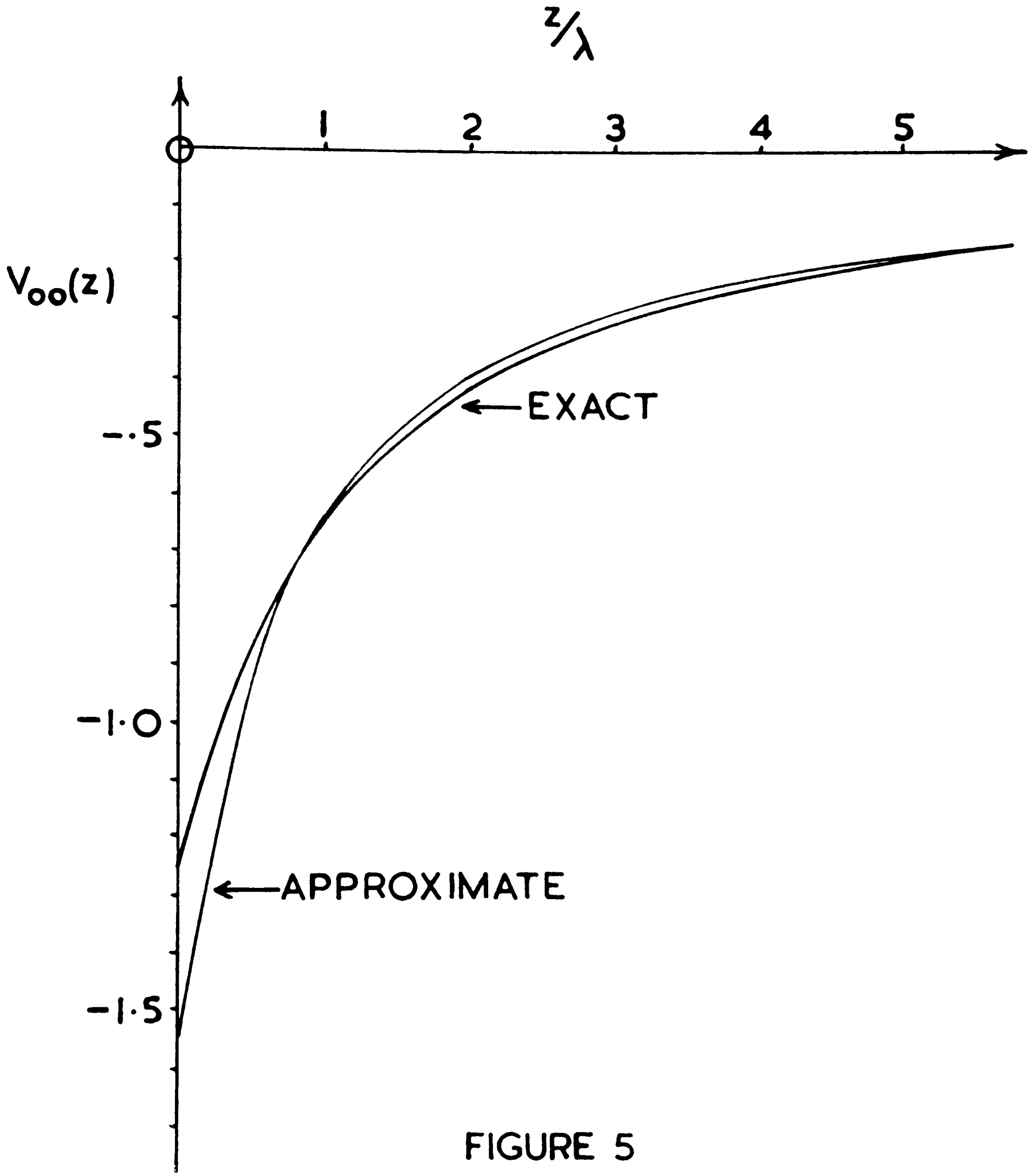


FIGURE 5

binding energy using (4.19). If the Whittaker functions were tabulated fairly completely it would be an easy matter to find the solutions of the eigenvalue equations. However there are only a few tables of Whittaker functions of the type required for treating attractive Coulomb fields[18] and these are of use largely for $K = 0$ states. For the remaining states it is necessary to use the series expansion of $W_{\alpha,m}(x)$ which can be obtained by combination of (A3.2), (A3.3), (A3.4) and (A3.6). Fortunately the value of x at which $W_{\alpha,m}(x)$ must be evaluated, i.e. $\frac{2k_0 a}{\alpha}$, is small being less than about .25 for $\beta > 2$, so that the series expansion converges rapidly.

The variations of bound state energies with magnetic field calculated in this way are shown in figures 6 and 7. The groups of three numbers attached to the lines denote the quantum numbers NMK for the corresponding energy levels. In figure 6 the levels 000 and 002 are the lowest two levels which can be observed if the absorption is allowed while 001 is the lowest observable level if the absorption is forbidden and the polarisation of the radiation is parallel to the magnetic field. For forbidden absorption and polarization perpendicular to the field direction the two lines 110 and 112 (or 0-10 and 0-12) whose energies are given in figure 7 are those of lowest energy. The level 111 cannot be investigated experimentally so its energy has not been calculated. In both figures the level of lowest energy has infinite binding energy in an infinite magnetic field while the levels of higher energy illustrated tend to the first Balmer energy in the infinite field limit and have the line

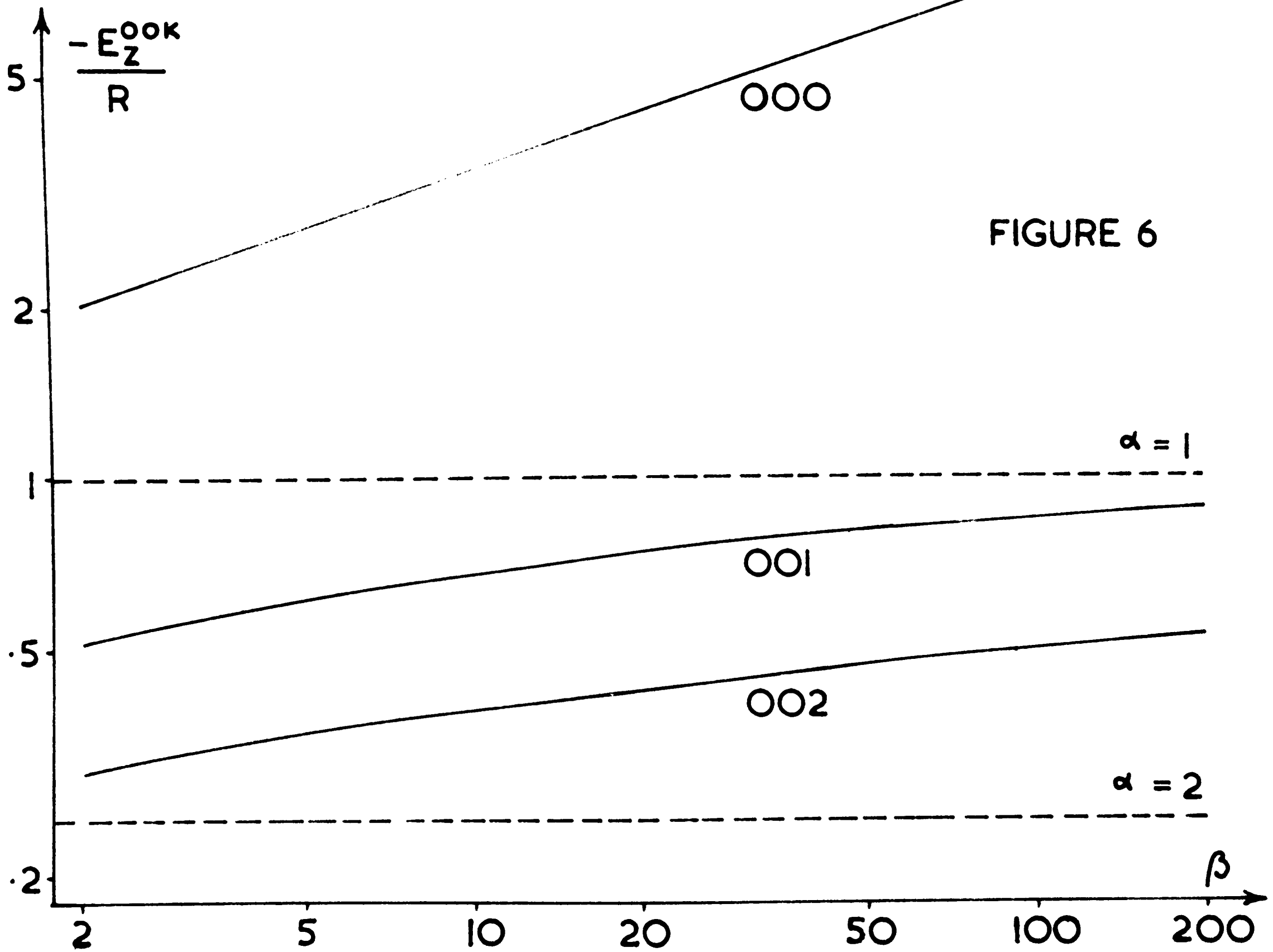


FIGURE 6

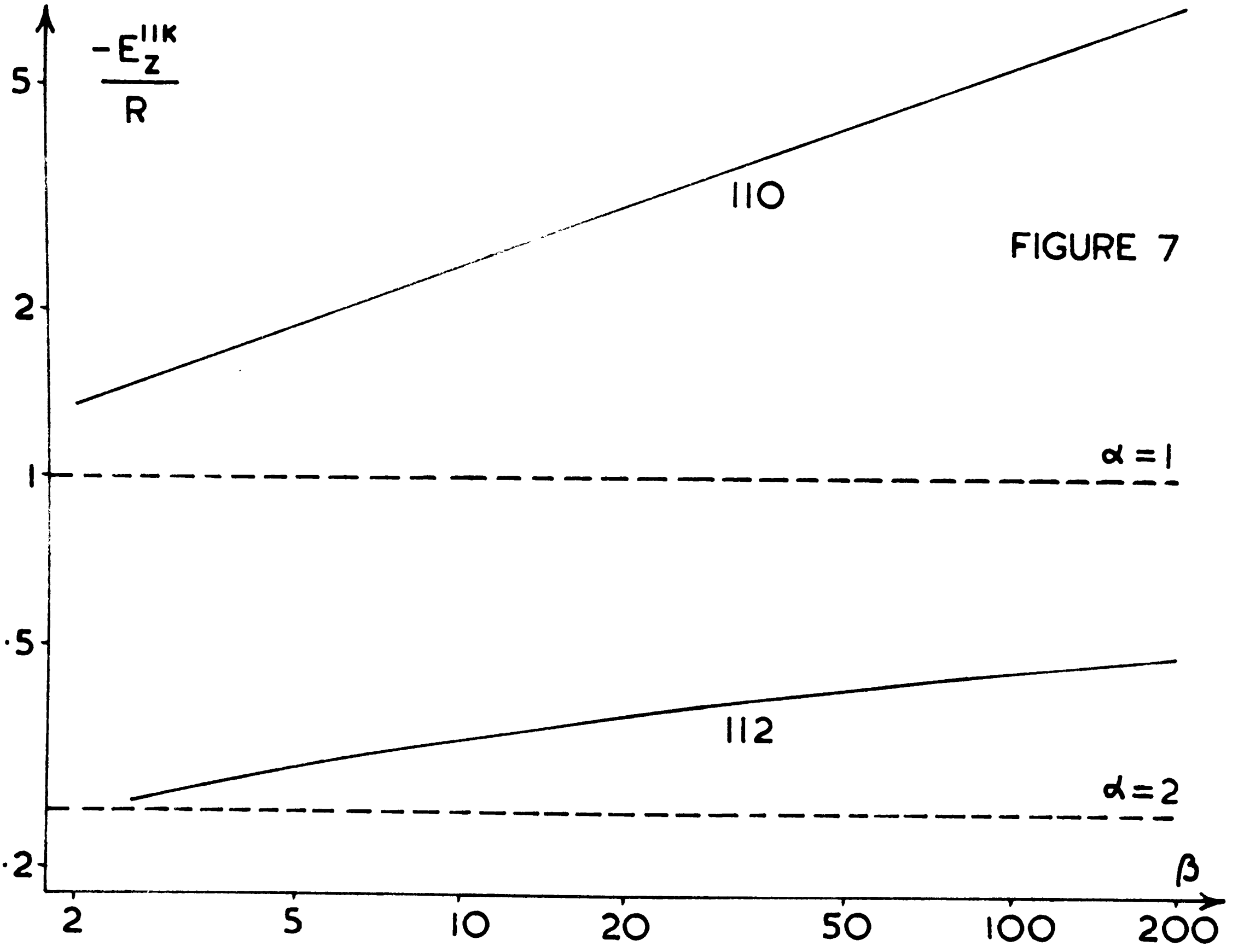


FIGURE 7

marked $\alpha = 1$ as an asymptote (see appendix 4).

For each of the levels of figure 6 the z part of the wave-function is plotted in figure 8 for some value of the magnetic field fixed by the fact that tables of the Whittaker function are available only for these values.

The variation of the f-values of the absorption lines due to these three levels with magnetic field is shewn in figure 9. The expressions (4.57) and (4.63) have been evaluated by again making use of the tables[18] and the series expansion for $W_{d,m}(x)$. For the states 000 and 002 the quantity $a_0^3 \left|\tilde{F}^K_{00}(0)\right|^2$ is plotted on the vertical axis while for the state 001 this axis represents the dimensionless quantity $a_0^5 \left|\frac{d}{dz}\tilde{F}^K_{00}(r)\right|^2_{r=0}$. The intensities of absorption in the allowed and forbidden cases cannot be directly compared in this graph since the quantities plotted here are multiplied by different factors in forming the f-values in the two cases [see (3.11) and (3.21)]. As discussed at the end of section 6(ii) of chapter 4 the absorption in the forbidden case is on the whole weaker than that in the allowed case by a factor of order $\left[\text{ lattice constant/effective Bohr radius }\right]^2$.

For the forbidden case with the radiation polarized perpendicular to the field direction the variation in f-value of the 110 and 112 lines is similar to that of the 000 and 002 lines respectively but multiplied by an extra factor of order $\left(\frac{L}{\lambda}\right)^2$ [see end of section 6(iii) chapter 4]. Since $\frac{1}{\lambda^2} = \frac{\beta}{a_0^2}$ the f-value rises more rapidly with increasing magnetic field in this case than in the other two cases.

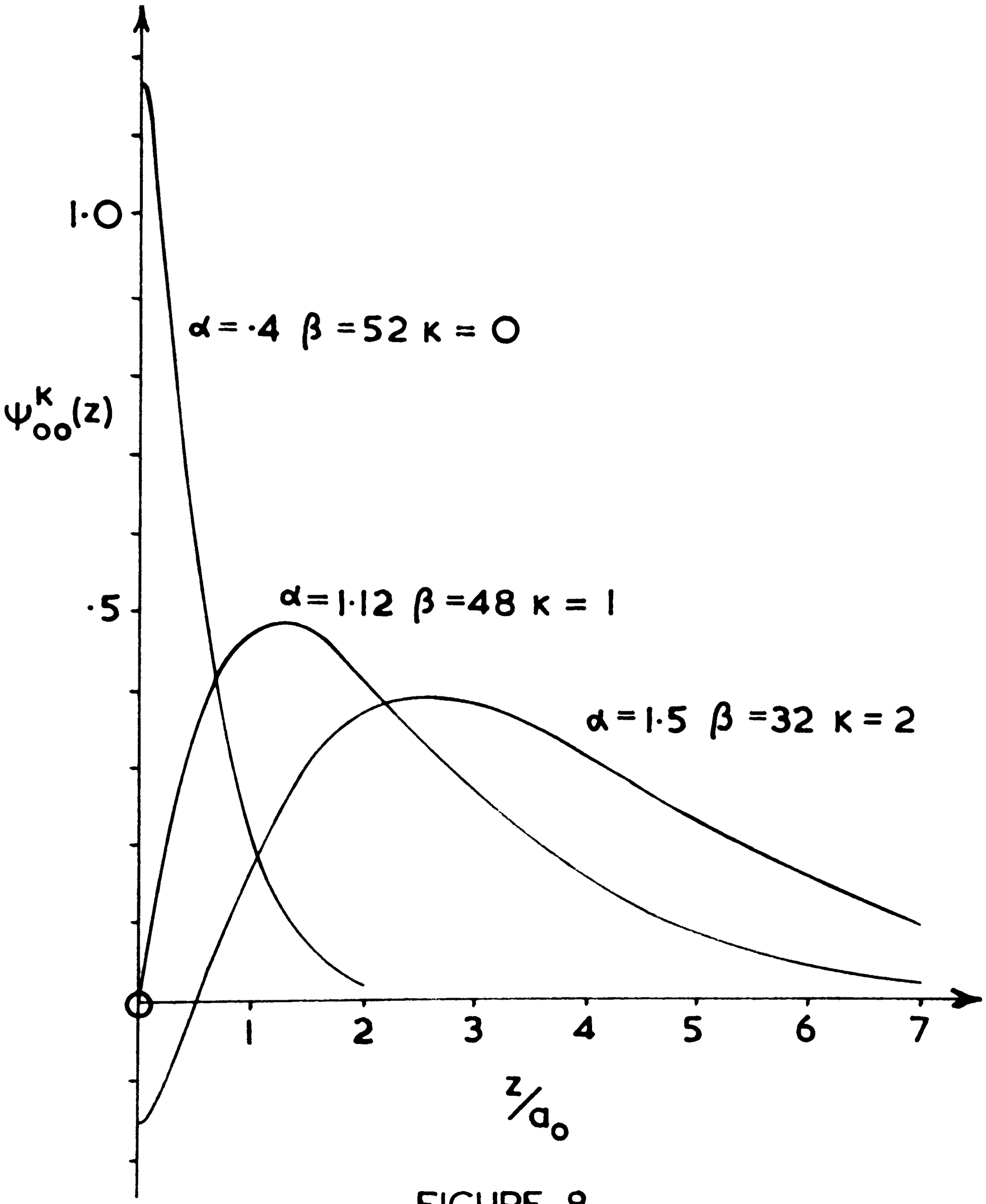


FIGURE 8

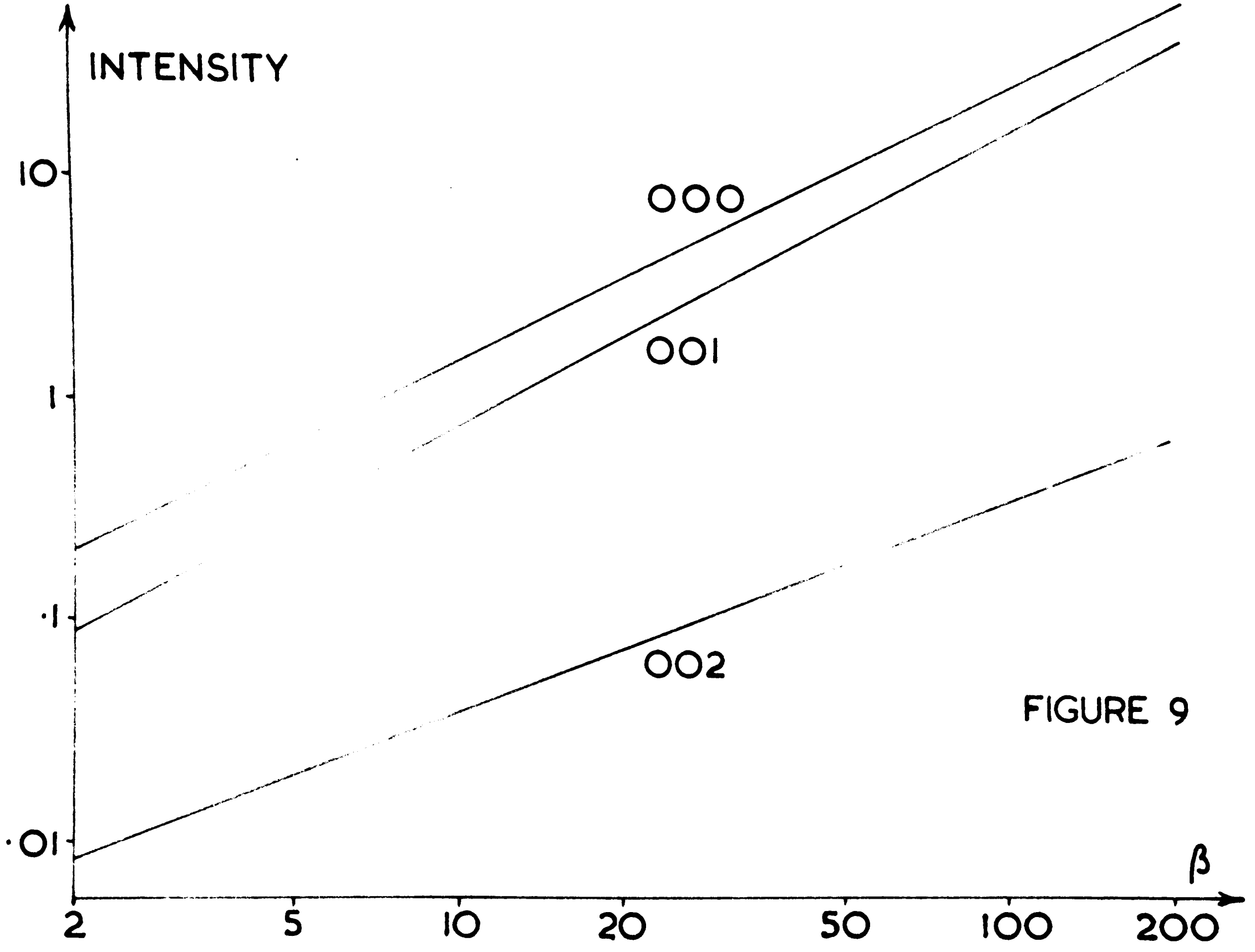


FIGURE 9

2. Free Exciton States. General expressions for absorption coefficients due to optical excitation of continuum exciton states have been given in section 6 of chapter 4. There are also expressions in this section for the absorption coefficients in the region below the absorption edge where the discrete energy levels are sufficiently close together to give rise to a continuous absorption. Both types of absorption coefficient involve the evaluation of a confluent hypergeometric function at some value of its argument depending on the distance from the absorption edge. The required functions are again not tabulated. However, useful information about the absorption can be obtained by expanding the absorption coefficient in a power series of the energy separation from the absorption edge. Taking the first two terms in such a series gives the value of the absorption coefficient at the edge and its slope there.

We consider first the region below the edge and for definiteness we will take the absorption to be forbidden, with the polarization of the radiation parallel to the magnetic field. The absorption coefficient is therefore given by (4.65) with the definition (4.64). The energy separation from the absorption edge is proportional to $1/\alpha^2$ by (4.19), and we therefore require to expand the various functions appearing in (4.65) in power series of $1/\alpha^2$.

Now:

$$M_{\alpha,m}\left(\frac{2k_0a}{\alpha}\right) = \left(\frac{2k_0a}{\alpha}\right)^{\frac{1}{2}+m}\Gamma(2m+1)(2k_0a)^{-m}\left\{ J_{2m}(\sqrt{8k_0a}) + \left(\frac{k_0a}{\alpha}\right)^2\left[\frac{1}{3}(2k_0a)^{-\frac{1}{2}}J_{2m+1}(\sqrt{8k_0a}) + \frac{2m-1}{6}(2k_0a)^{-1}J_{2m+2}(\sqrt{8k_0a})\right] + O\left(\frac{1}{\alpha^4}\right)\right\} \tag{5.1}$$

where:

$$J_\nu(y) = \sum_{n=0}^{\infty}(-1)^n\left(\frac{1}{2}y\right)^{2n+\nu}\frac{1}{\Gamma(n+\nu+1)\,\underline{|n}} \tag{5.2}$$

is a Bessel function. The first two terms in this expansion of $M_{\alpha,m}$ can be easily obtained by writing down the series defined by (A3.2) and (A3.4) for the case $X = \frac{2k_0a}{\alpha}$ and collecting together the terms involving the required powers of α. A similar expression for $M_{\alpha,-m}$ is given by reversing the sign of m in (5.1). The series expansions of the gamma functions in (4.65) are also required:

$$\Gamma\left(\tfrac{1}{2}+\alpha+m\right) = e^{-\alpha}\,\alpha^{\alpha+m}\,e^{-\frac{1}{2\alpha}\left(\frac{1}{2}-m\right)\left(\frac{1}{2}+m\right)}\,e^{\frac{1}{12\alpha}}\sqrt{2\pi}\left[1-\frac{1}{\alpha^2}\frac{m}{24}\left(4m^2-1\right)+O\left(\frac{1}{\alpha^4}\right)\right] \tag{5.3}$$

obtained from Stirling's expansion (see Erdélyi et al.[19]), and similarly for $\Gamma\left(\frac{1}{2}+\alpha-m\right)$.

Using the above expansions (4.65) may be evaluated as a power series in $1/\alpha^2$, and the corresponding expressions (4.58) and (4.71) for the other two cases can be treated in the same way. In all three cases it is found that the series are of the form:

$$S_\alpha(E)\left|\langle k0|\underline{\epsilon}.\underline{p}|0\rangle\right|^2 = A + \frac{B}{\alpha^2} + O\left(\frac{1}{\alpha^4}\right) \tag{5.4}$$

where A and B depend on the magnetic field but not on the energy, being different functions in the three cases. We shall not write down the functional forms of A and B since they are very complicated.

The absorption coefficients for the region above the edge can be similarly calculated. $W_{-i\lambda,m}$ and $V_{-i\lambda,m}$ are given in terms of $M_{-i\lambda,m}$ and $M_{-i\lambda,-m}$ by (A3.6) and (A3.7) so that a series expansion of type (5.1) can be used again. The expressions (4.60), (4.66) and (4.72) can be expanded in power series of $1/\lambda^2$ and in all three cases the result is of the form:

$$S_1(E)\left|\langle \lambda 0 | \xi \cdot p | 0 \rangle\right|^2 = A - \frac{B}{\lambda^2} + O\left(\frac{1}{\lambda^4}\right) \qquad (5.5)$$

where A and B are the same functions as occurred for the same case in the expression (5.4) for the region below the edge.

(5.4) and (5.5) show that the absorption coefficient has a finite value at the absorption edge and is continuous there, having also a continuous derivative with respect to energy. These properties seem to be characteristic of a theory which takes account of the Coulomb attraction of the pair of particles forming the exciton. In chapter 3 section 2(iii) the absorption coefficients in a magnetic field but ignoring the Coulomb interaction were shown to be either zero or infinite at the absorption edge. Similarly the absorption coefficients in zero magnetic field [chapter 3 section 2(i)] ignoring the Coulomb interaction are zero at the edge, but taking the Coulomb interaction into account [chapter 3 section 2(ii)] gives absorption coefficients which are finite and continuous at the edge

and have continuous slope.

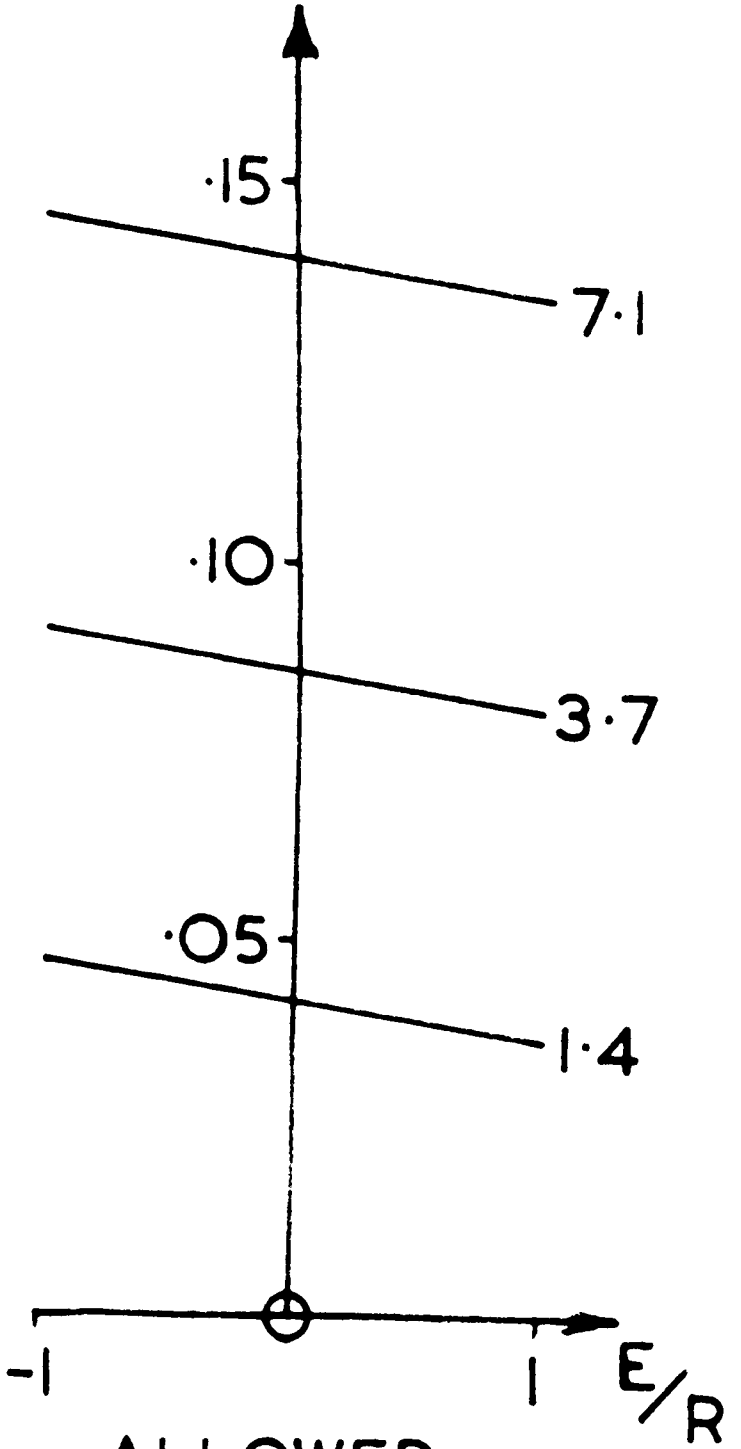
Figure 10 illustrates the value and slope of the absorption coefficients at the edge for the three cases, for several values of the magnetic field. The magnetic field strengths are indicated by the values of β which are shown at the right hand ends of the curves. The ordinate is drawn at the absorption edge and the energy of absorption increases towards the right. The absorption is shown in the graph as if the linear dependence on E extends out to the points $E = \pm R$. This is done so as to show up clearly the slope of the coefficient at the edge; of course higher terms than the second in the expansion of the absorption coefficient in powers of $1/a^2$ become important before the point $E = R$, and discrete lines appear before a distance R below the edge.

The vertical axes in the figure represent the following quantities:

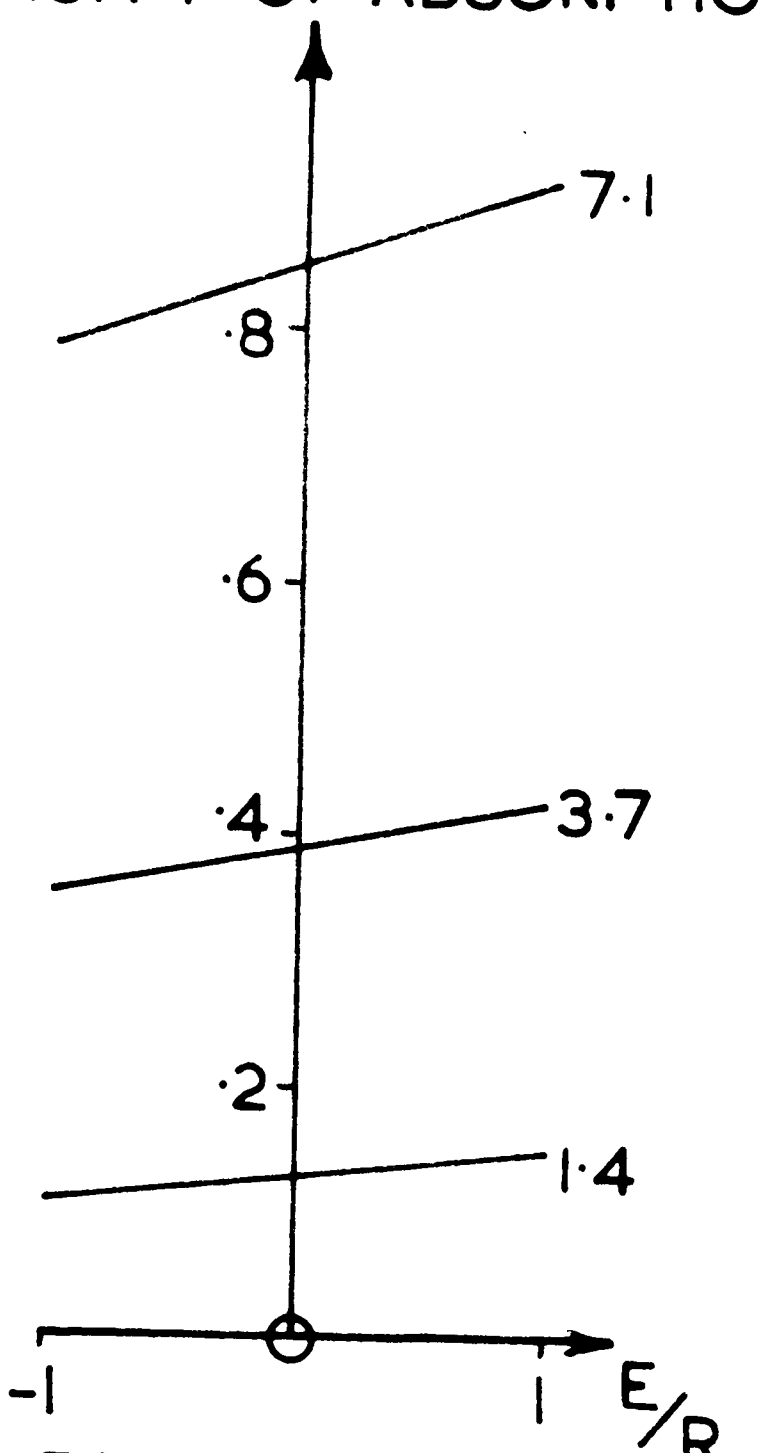
(i) Allowed	(ii) Forbidden $\epsilon \parallel H$	(iii) Forbidden $\epsilon \perp H$
$\frac{k^2 a_0}{\mu} S_1(E) \left\| \tilde{F}^e_{00}(0) \right\|^2$	$\frac{a_0^3}{\mu} S_1(E) \left\| \pi_z \tilde{F}^o_{00}(\underline{r}) \right\|^2_{r=0}$	$\frac{a_0^3}{\mu} S_1(E) \left\| \pi_- \tilde{F}^e_{11}(\underline{r}) \right\|^2_{r=0}$ $= \frac{a_0^3}{\mu} S_1(E) \left\| \pi_+ \tilde{F}^e_{0-1}(\underline{r}) \right\|^2_{r=0}$

In comparing the absorption in the three cases it must be remembered that to form absorption coefficients from the quantities plotted in figure 10 it is necessary to multiply them by expressions having the relative orders of magnitude 1, $\left(\frac{L}{a_0}\right)^2$ and $\left(\frac{L}{a_0}\right)^2$

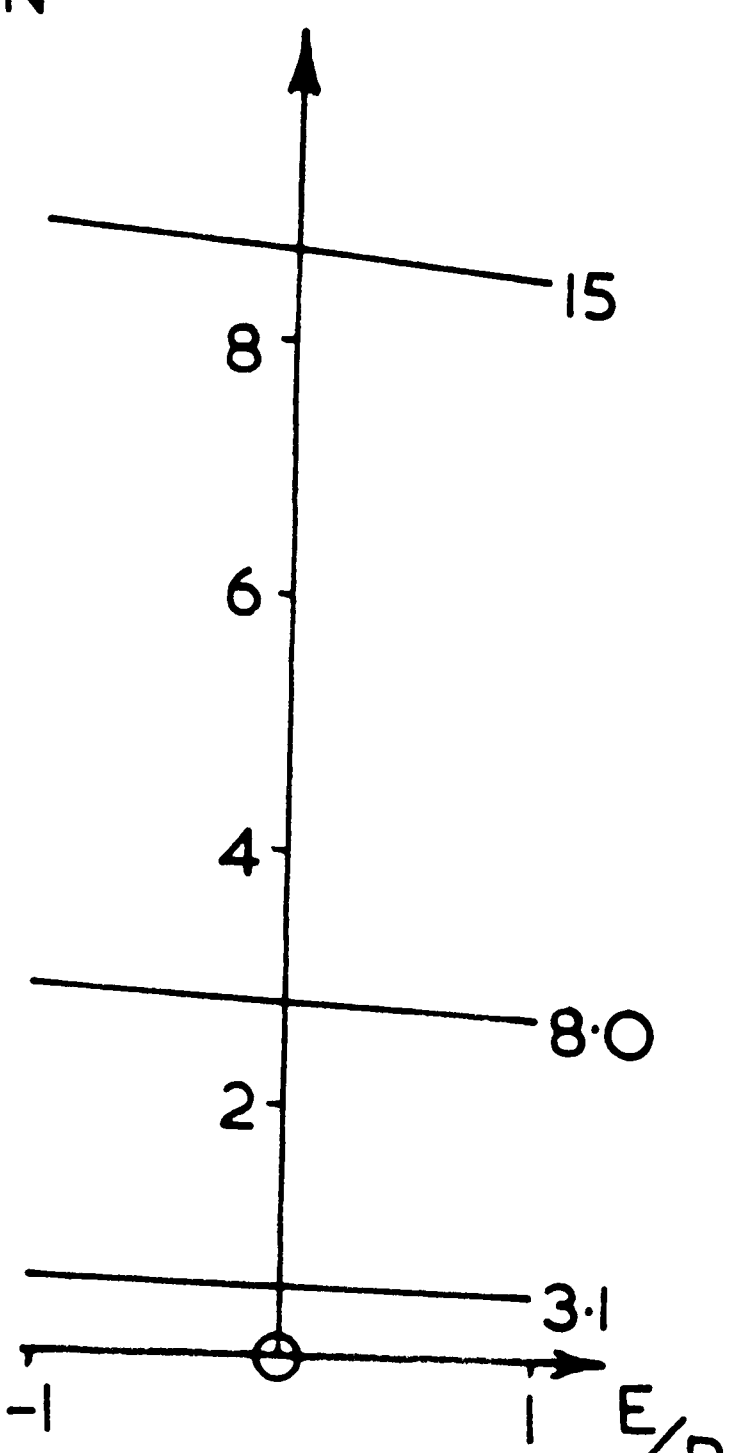
INTENSITY OF ABSORPTION



ALLOWED



FORBIDDEN $\epsilon \parallel \underline{H}$



FORBIDDEN $\epsilon \perp \underline{H}$

FIGURE 10

respectively, so that the absorption in the forbidden cases is much weaker than in the allowed case.

The above numerical results are discussed in section 4.

3. Accuracy of the Method. In the perturbation theory method presented in chapter 4 for treating excitons in a high magnetic field two main approximations were made and we are now in a position to consider their validity.

The first approximation arose from the separation of the envelope function of the exciton into a part depending only on the co-ordinate in the direction of the magnetic field and a part depending only on the co-ordinates in a plane perpendicular to the field, as in equation (4.8). The error involved in this separation depends upon the size of the non-diagonal matrix elements of $-e^2/\varkappa r$ linking the approximate eigenfunctions thus obtained. The orders of magnitude of these matrix elements may be estimated in much the same way as was used to estimate line widths in section 7 of chapter 4. We consider as an example the perturbation of the ground state of the N = M = 0 group of levels by higher states having M = 0. The most important perturbing state would be expected to be the ground state of the N = 1, M = 0 group of levels. We approximate these two ground state wave-functions by:

$$\tilde{F}^{0}_{00}(\underline{r}) = \frac{1}{\sqrt{2\pi\lambda^2}}\, e^{-\frac{1}{2}\sigma}\, \frac{1}{\sqrt{a_0 a_0}}\, e^{-\frac{|z|}{a_0 a_0}} \qquad (5.6)$$

$$\tilde{F}^{0}_{10}(\underline{r}) = \frac{1}{\sqrt{2\pi\lambda^2}}\, e^{-\frac{1}{2}\sigma}(1-\sigma)\,\frac{1}{\sqrt{\alpha_1 a_0}}\, e^{-\frac{|z|}{\alpha_1 a_0}} \tag{5.7}$$

and we require the matrix element:

$$M = -\int \tilde{F}^{0*}_{10}(\underline{r})\,\frac{e^2}{\varkappa r}\,\tilde{F}^{0}_{00}(\underline{r})\,d\tau \tag{5.8}$$

Using the same argument as led to (4.78) this approximately reduces to:

$$M = -\frac{2e^2\lambda^2}{\varkappa a_0\sqrt{\alpha_0\alpha_1}}\int_0^\infty e^{-\frac{z}{a_0}\left(\frac{1}{\alpha_0}+\frac{1}{\alpha_1}\right)}\,\frac{1}{(b+z)^3}\,dz \tag{5.9}$$

where:

$$b^3 = \sqrt{\frac{8}{\pi}}\,\lambda^3$$

The integral can be approximated in the same way as the integral I of (4.79) and (4.80) leading to:

$$M \sim -\frac{2R}{\sqrt{\alpha_0\alpha_1}} \tag{5.10}$$

The shift in the energy of the 000state due to perturbation by the 100 state is therefore:

$$\Delta E \sim -\frac{4R^2}{\alpha_0\alpha_1 \hbar\omega_c} = -\frac{2R}{\alpha_0\alpha_1\beta} = -\frac{2\bar{E}}{\beta} \tag{5.11}$$

where $\bar{E}$ is the geometric mean of the binding energies of the two states involved. The value of the integral in (5.9) has again been slightly overestimated so that the shift in energy will be slightly less than (5.11).

The perturbation of the 000 state by the other even states

of the N = 1, M = 0 group is considerably less than this since the wave-functions of these other states are much less concentrated at small values of z where the inverse cube factor in (5.9) is important. The perturbations due to N00 states for N greater than unity will be weaker because the energy separation between the 000 state and the perturbing state is greater (being $\sim N\hbar\omega_c$), and also because the overlap between the ρ, ϕ parts of the approximate wave-functions becomes smaller as N increases.

The energy shift in the 000 state is therefore of the order of twice its unperturbed binding energy divided by β . As might have been expected our calculation of energy values is poor for small values of β , at least for the ground state. It improves as β increases becoming good for the higher values of β .

We have shewn that the matrix elements of $-\frac{e^2}{\kappa r}$ between states of the N = M = 0 and N = 1, M = 0 groups are approximately the same as those of: $$-\frac{e^2}{\kappa}\frac{\lambda^2}{(\lambda+|z|)^3}$$ between the z components of the wave-functions. This interaction potential extends over a distance of order λ along the z-axis and as we have seen its perturbing effect is quite large for the ground state when β is not very much larger than unity. However, for the higher excited states within a group the maximum amplitude in the z component of the wave-function occurs at a z co-ordinate of order αa_0 so that the effect of the perturbing potential, which is localized about the origin, decreases with increasing α . Indeed,

however small the magnetic field may be, causing a large value of λ, there are always some bound states close to the continuum edge whose value of α is sufficiently large for their energy to be accurately given by the approximation of chapter 4. This approximation was in fact first introduced by Schiff and Snyder[17] to treat states close to the continuum edge in a magnetic field such that $\beta \ll 1$. However the approximation to the wave-functions is a poor one for such low magnetic fields even for states of high α, and this is also true of the continuum wave-functions. Our method of calculating absorption coefficients therefore does not hold in the region $\beta < 1$. Similar remarks apply to the interaction between other N,M groups of levels.

Returning to the case $\beta \gg 1$ we remark finally that our method of approximation is better for groups of levels having $M \neq 0$, since in this case the 'centrifugal barrier' keeps the ρ, ϕ part of the wave-function away from the origin where the $-e^2/\chi r$ perturbation is most important.

The second main approximation in the perturbation theory method of chapter 4 is the replacement of the exact effective potentials, like (4.12) and (4.13), by approximate effective potentials of the type (4.17). Here it is possible to make an accurate assessment of the error involved for Keyes[11] has solved the Schrödinger equation for the s-motion for the energy of the ground state 000 using the exact effective potential $V_{00}(s)$ of equation (4.12). An electronic computor was used in these calculations, the result of which is shown in figure 11 by the continuous line. The isolated points

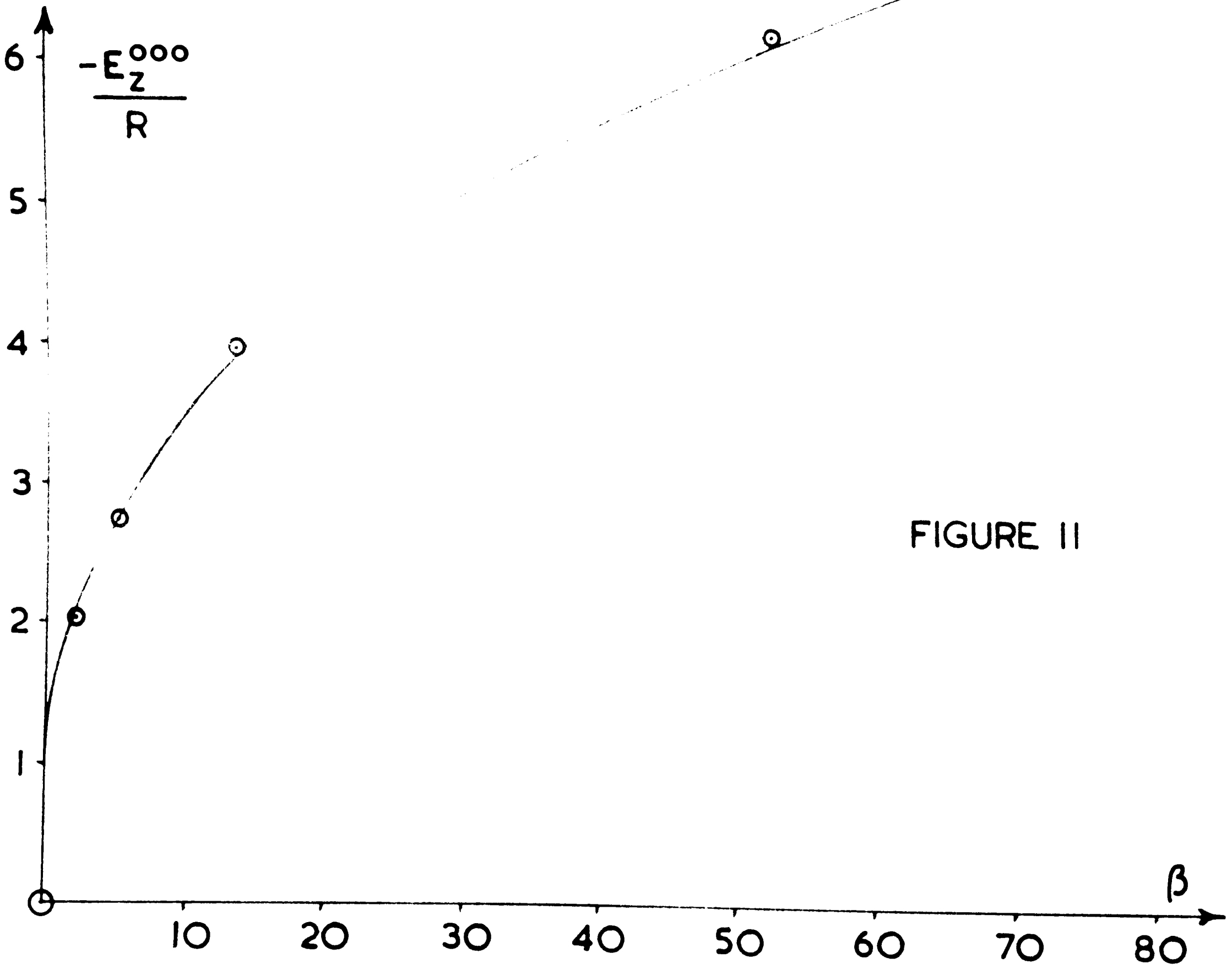


FIGURE 11

represent the results of the present calculation. The disagreement between the two calculations is seen to be of the order of two per cent.

For the excited states no direct estimate of the error involved in using an approximate effective potential can be made. However we can be quite certain that the error will be less than for the ground state since the excited state wave-functions are much less concentrated in the region close to the origin where the approximation to the exact potential is poorest (see figures 5 and 8).

4. Discussion of Results. Numerical data on the absorption spectrum of a semiconductor due to its lowest lying exciton levels have been presented in sections 1 and 2 of this chapter. The information given there may be supplemented by the fact mentioned at the end of section 5 chapter 4 that in the energy range well above the absorption edge, where $k >> k_0$, the s part of the wave-function is unaffected by the Coulomb interaction. It follows that in this region the results of section 2(iii) chapter 3 hold. In particular, for the cases illustrated in figure 10 the variation of absorption coefficient K with energy in the region well above the absorption edge is as follows:

(i)	Allowed	$K \propto H E^{-\frac{1}{2}}$
(ii)	Forbidden $\underline{\epsilon} \parallel \underline{H}$	$K \propto H E^{\frac{1}{2}}$
(iii)	Forbidden $\underline{\epsilon} \perp \underline{H}$	$K \propto H^2 E^{-\frac{1}{2}}$

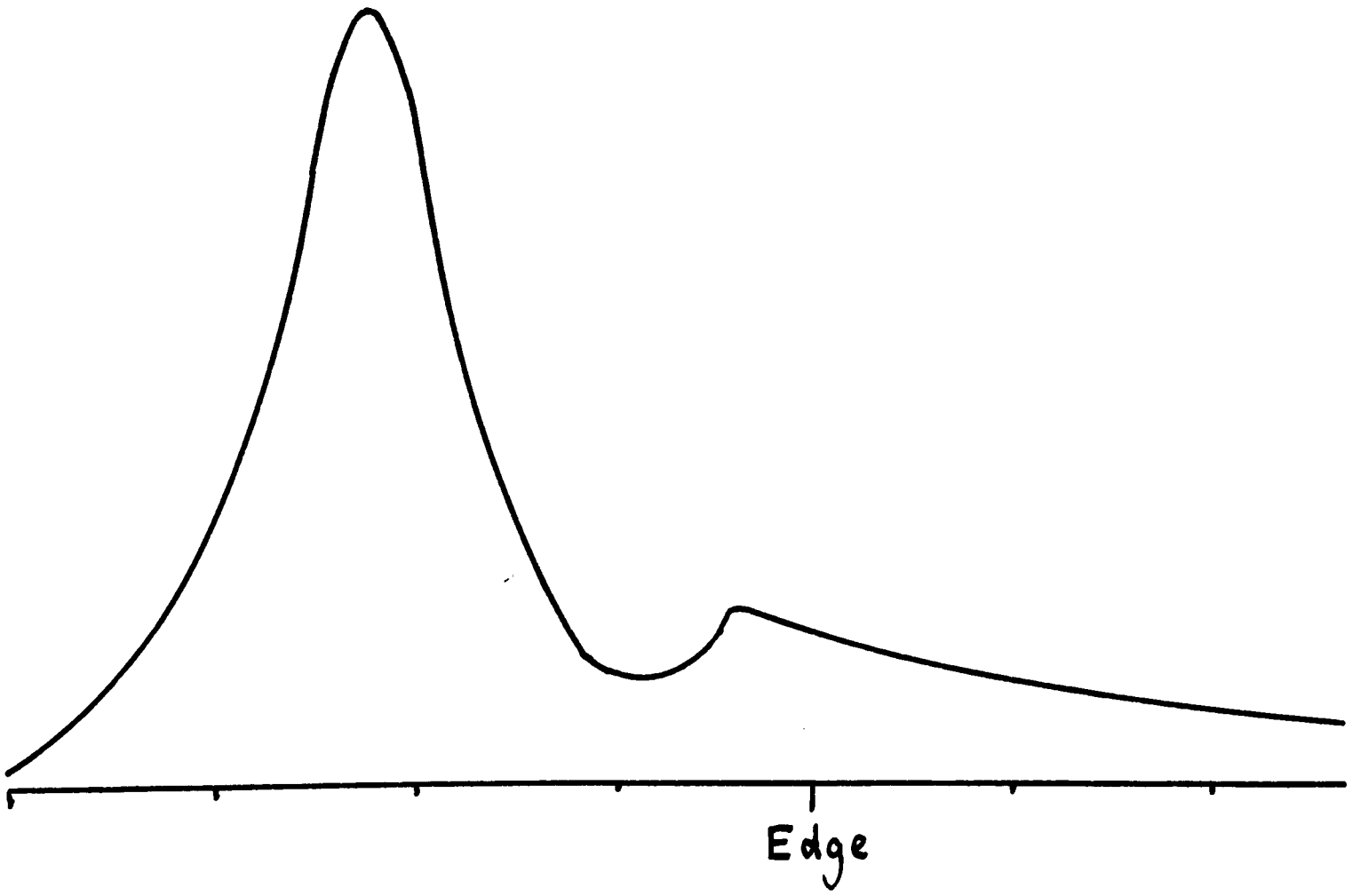
Combining the known forms of the absorption spectrum close to and well

above the edge it is possible to gain a fairly complete impression of the form of the absorption in the entire region above the edge.

The absorption edge itself is not distinguished by any striking change in the absorption coefficient which is continuous with continuous slope at the edge in all three cases. Experimentally the edge could not be located and the only way in which its position could be determined would be by measuring the positions of the absorption lines below the edge due to the bound exciton states and using theoretical values for their binding energies. Of these absorption lines below the edge, that having the smallest frequency is the most intense, and its intensity relative to the other lines increases with magnetic field, at least in the allowed case (see figure 9). At high values of β , in the allowed case, the first absorption line is about a hundred times more intense than the second absorption line. Under experimental conditions then, the absorption spectrum due to the lowest observable N,M group of levels might show a single relatively intense line joined on its high frequency side to a 'shoulder' arising from unresolved excited discrete states and the continuous states above the absorption edge.

The area enclosed by an absorption line due to a bound exciton state in a graph of absorption coefficient against photon energy is given by an expression similar to (3.13) but with the density of states S(E) omitted. It is therefore possible to compare the intensities of absorption in the discrete and continuous regions. If the ordinate in figure 9 is multiplied by a factor 2 then

figures 9 and 10 are in the same system of units and the intensities may be compared if line widths are assumed for the discrete lines. The following sketch shows roughly the form of the absorption coefficient for β about 2 in the allowed case assuming a line width of about R for the peak due to the 000 state. The horizontal axis is divided into energy units R.



We have so far considered only the contribution to the absorption spectrum arising from the lowest observable group of levels in each case. Let us consider the allowed case for definiteness, though our remarks will apply mutatis mutandis to the other two cases. All the groups of levels having M = 0 make a contribution to the absorption coefficient. We have not calculated the form of the

spectrum for $N \gg 1$ but we may take it to be qualitatively similar to that for N = 0, although the lines in the absorption spectrum may be substantially broadened as discussed in section 7 chapter 4. The complete absorption spectrum therefore consists of a part due to the N = 0 levels followed at higher energies by somewhat similar absorption patterns spaced at energy intervals of $\hbar\omega_c$ (see figure 1). In the contribution of one of these higher groups of levels to the absorption spectrum perhaps all that would be observed experimentally would be a single broadened line due to the ground state of the group, and the complete spectrum arising from these higher groups would show a series of lines, one from each ground state. These lines will be fairly evenly spaced since the separation $\hbar\omega_c$ between adjacent groups is much larger than the binding energy $\sim R$ of the states within a group for $\beta \gg 1$.

Neglect of the Coulomb interaction was shown in section 2(iii) chapter 3 to lead to a theory which predicts peaks at energies $(N+\frac{1}{2})\hbar\omega_c$ above the zero field position of the absorption edge. It was stated in chapter 1 that on the basis of this type of theory the position of the zero field absorption edge could be determined by extrapolation of the position of a peak corresponding to a given N quantum number at various magnetic fields. The theory presented here shows that if the magnetic field measurements are carried out in a region where $\beta \gg 1$ then the observed peaks will probably lie slightly below the energies $(N+\frac{1}{2})\hbar\omega_c$ by an amount of the order of the binding energy of the ground exciton state for the

group II. Since this binding energy increases less rapidly than linearly with increasing field (see figure 6), an extrapolation to zero field gives a lower energy than the correct one for the absorption edge. The value obtained for the forbidden energy gap in this way is therefore slightly smaller than the correct one.

5. Experimental Work. Exciton absorption in a magnetic field has so far been observed in only two semiconductors, and for neither of these is the theory presented in this thesis really applicable. In the case of cuprous oxide the energy bands appear to have the simple shape assumed in our theoretical discussion but unfortunately magnetic fields high enough to attain the condition $\beta \gg 1$ are out of the question for this substance. In the case of germanium, on the other hand, the condition $\beta > 1$ has been achieved experimentally, but the structure of the valence band is so complicated that the present theory can have only qualitative application. For a detailed comparison of theory with experiment we must therefore await measurements on a substance which combines the virtues of cuprous oxide and germanium without having their accompanying vices. However we shall briefly comment on the measurements on these two semiconductors.

(1) Cuprous Oxide. The magnetic field corresponding to $\beta = 1$ is 6,500,000 gauss, so that the condition $\beta \ll 1$ holds in all experimental work. We have not made any calculation of the intensity or shape of the absorption spectrum for such values of the magnetic

field, but we will show how effective masses may be obtained from observations on the bound exciton states. The eigenvalue equation for the exciton binding energies is (3.12):

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2+\frac{ie\hbar}{2c}\frac{m_e-m_h}{m_e m_h}\underline{H}\cdot\underline{r}\times\nabla+\frac{e^2}{8\mu c^2}(\underline{H}\times\underline{r})^2-\frac{e^2}{\varkappa r}\right\}\tilde{F}_n(\underline{r})=E_n\tilde{F}_n(\underline{r}) \qquad (5.12)$$

The magnetic field terms can be treated by perturbation theory as in the case of the hydrogen atom and give rise to Zeeman and quadratic Zeeman effects (see Schiff[20]).

The most complete experimental measurements are those reported by Gross[1]. No linear Zeeman effect is observed in Cu_2O so we may conclude that $m_e = m_h$. For the quadratic effect we require the matrix elements of the term in H^2 between the appropriate hydrogen-like exciton wave-functions. In cuprous oxide the absorption is thought to be forbidden[9] and so it is the p-states which are responsible for the observed absorption lines [see section 2(ii) chapter 3]. For the case of p-states having $m = 0$, the diagonal matrix elements of $r^2\sin^2\theta$ are:

$$n^2(n^2-1)a_0^2$$

n being the principal quantum number, so that the quadratic Zeeman shift, being the matrix element of $\frac{e^2H^2}{8\mu c^2}r^2\sin^2\theta$, is:

$$\Delta E = \frac{H^2\hbar^4\varkappa^2}{8\mu^3c^2e^2}n^2(n^2-1) \qquad (5.13)$$

In zero field the exciton levels show hydrogenic spacings to a good approximation so that the effective Rydberg energy R of (3.23) can

also be measured experimentally. With a knowledge of ΔE and R both μ and $\varkappa$ can be calculated, and using the results of Gross:

$$\varkappa \sim 8 \quad \text{and} \quad \mu \sim \cdot 42 m_0 \quad \text{so that} \quad m_e = m_h \sim \cdot 84 m_0$$

This calculated value of the dielectric constant is in good agreement with the value obtained by direct measurement.

Above the absorption edge, in the region of continuum exciton states, a series of peaks at fairly constant spacing is observed, the energy separations between adjacent peaks being about $\frac{eH}{\mu c}$ with the value of μ given above. This observation indicates that for $\beta \ll 1$ the continuum states of the exciton give rise to absorption maxima, in contrast to the case $\beta \gg 1$.

(ii) Germanium. Measurements of the absorption spectrum of germanium have been carried out in magnetic field strengths up to about 40,000 gauss by Zwerdling et al.[4] The magnetic field corresponding to $\beta = 1$ is 8,900 gauss so that this highest field corresponds to a value of β of about 4. Altogether measurements have been made at three field strengths having $\beta > 2$.

The observed absorption spectrum is very complicated owing to the fourfold degeneracy of the valence band in germanium. In addition, the experimental arrangements used in the above measurements have been criticised[21] on the grounds that the specimen of germanium used was in a state of non-uniform strain due to its mounting. It has been demonstrated that in a zero magnetic field the experimental method of Zwerdling et al. leads to a shift in the

position of the absorption spectrum to higher energies and also to the appearance of a spurious absorption band close to the absorption edge. The agreement of the experimental spectrum with the theoretical spectrum as predicted in section 2(ii) chapter 3 is destroyed by the use of strained crystals[21].

For these reasons little agreement would also be expected between theory and experiment for the magnetic field case. However, some of the predictions of the theory are found to receive qualitative verification. The lowest line of the spectrum has roughly the form shewn in the sketch on page 87, although the intensity of the line relative to the shoulder seems to be smaller in the experimental results. In this connection however, we may note that the extra absorption band introduced by strain appears at about the position of the shoulder so that its greater intensity in the experimental measurements may well be spurious. As far as can be judged on the basis of measurements at only three magnetic field strengths, the intensity of the lowest line of the spectrum increases with field in roughly the manner indicated in figure 9 for the 000 line. The higher energy lines of the spectrum increase in breadth with distance from the absorption edge.

Appendix 1. Absorption Coefficient in a Solid.

Consider a solid of volume $V = L^3$, dielectric constant $\varkappa$ and permeability μ. Maxwell's equations for the radiation field in the solid are:

$$\nabla \times \underline{E} = -\frac{1}{c}\frac{\partial \underline{B}}{\partial t} \qquad \nabla . \underline{D} = 0 \tag{A1.1}$$

$$\nabla \times \underline{H} = \frac{1}{c}\frac{\partial \underline{D}}{\partial t} \qquad \nabla . \underline{B} = 0 \tag{A1.2}$$

where:

$$\underline{D} = \varkappa \underline{E} \qquad \underline{B} = \mu \underline{H} \tag{A1.3}$$

Taking zero scalar potential and a vector potential $\underline{A}$, we have:

$$\underline{B} = \nabla \times \underline{A} \tag{A1.4}$$

$$\underline{E} = -\frac{1}{c}\frac{\partial \underline{A}}{\partial t} \tag{A1.5}$$

We choose the Coulomb gauge:

$$\nabla . \underline{A} = 0 \tag{A1.6}$$

and then using all the above equations $\underline{A}$ satisfies:

$$\nabla^2 \underline{A} - \frac{\varkappa\mu}{c^2}\frac{\partial^2 \underline{A}}{\partial t^2} = 0 \tag{A1.7}$$

The field energy is given by the usual expression:

$$\mathcal{E} = \frac{1}{8\pi}\int_V \left(\underline{D} . \underline{E} + \underline{B} . \underline{H}\right) d\tau \tag{A1.8}$$

We expand the vector potential in plane waves:

$$\underline{A} = \sum_{\lambda} \left[a_\lambda \underline{A}_\lambda + a_\lambda^* \underline{A}_\lambda^* \right] \tag{A1.9}$$

where the a_λ are independent of position and:

$$\underline{A}_\lambda = \sqrt{\frac{4\pi c^2}{\varkappa V}}\, \underline{\epsilon}_\lambda\, e^{i\underline{k}_\lambda \cdot \underline{r}} \tag{A1.10}$$

The plane waves must be transverse, i.e. $\underline{\epsilon}_\lambda \perp \underline{k}_\lambda$, in order that the vector potential should satisfy (A1.6). The normalisation of (A1.10) will be justified later. The $\underline{A}_\lambda$ clearly satisfy:

$$\nabla^2 \underline{A}_\lambda + k_\lambda^2 \underline{A}_\lambda = 0 \tag{A1.11}$$

It then follows from (A1.7) that:

$$\frac{d^2 a_\lambda}{dt^2} + \omega_\lambda^2 a_\lambda = 0 \tag{A1.12}$$

with a similar equation for a_λ^*, where ω_λ is given by:

$$|k_\lambda| = \frac{2\pi}{\lambda} = \frac{\omega_\lambda \sqrt{\varkappa\mu}}{c} \tag{A1.13}$$

since the velocity of light in the solid is $c/\sqrt{\varkappa\mu}$. Instead of a_λ and a_λ^* we may work with two canonically conjugate variables:

$$Q_\lambda = a_\lambda + a_\lambda^* \qquad P_\lambda = -i\omega_\lambda (a_\lambda - a_\lambda^*) \tag{A1.14}$$

$$\text{i.e.} \quad a_\lambda = \tfrac{1}{2}\left[Q_\lambda + \frac{i}{\omega_\lambda} P_\lambda \right] \qquad a_\lambda^* = \tfrac{1}{2}\left[Q_\lambda - \frac{i}{\omega_\lambda} P_\lambda \right] \tag{A1.15}$$

The Hamiltonian is:

$$\mathcal{H}_\lambda = \tfrac{1}{2}\left[P_\lambda^2 + \omega_\lambda^2 Q_\lambda^2 \right] = \omega_\lambda^2 \left[a_\lambda a_\lambda^* + a_\lambda^* a_\lambda \right] \tag{A1.16}$$

and it may be easily verified that this leads to the field equation (A1.12) since the Hamiltonian equations are:

$$\frac{\partial \mathcal{H}_\lambda}{\partial Q_\lambda} = -\dot{P}_\lambda = \omega^2 Q_\lambda \qquad \text{(A1.17)}$$

$$\frac{\partial \mathcal{H}_\lambda}{\partial P_\lambda} = \dot{Q}_\lambda = P_\lambda \qquad \text{(A1.18)}$$

The Hamiltonian (A1.16) is quantised by introducing the commutation relations:

$$[P_\lambda, Q_\lambda] = -i\hbar$$

$$[P_\lambda, Q_\mu] = [P_\lambda, P_\mu] = [Q_\lambda, Q_\mu] = 0 \qquad \text{(A1.19)}$$

The problem is that of a harmonic oscillator and the eigenvalues are:

$$\mathcal{E}_\lambda = \hbar\omega_\lambda\left(n_\lambda + \tfrac{1}{2}\right) \qquad n_\lambda = 0, 1, 2, \ldots \qquad \text{(A1.20)}$$

The a_λ can be represented by the usual matrices:

$$\langle n_\lambda | a_\lambda | n_\lambda + 1 \rangle = \sqrt{\frac{\hbar(n_\lambda+1)}{2\omega_\lambda}} = \langle n_\lambda + 1 | a_\lambda^* | n_\lambda \rangle \qquad \text{(A1.21)}$$

all the other matrix elements being zero.

In order to expand $\underline{E}$ in the $\underline{A}_\lambda$ we need to know how to represent $\dot{a}_\lambda$ when the system is quantised. Using equations (A1.15), (A1.17) and (A1.18) we obtain the correspondence:

$$\dot{a}_\lambda \rightarrow -i\omega_\lambda a_\lambda \qquad \dot{a}_\lambda^* \rightarrow i\omega_\lambda a_\lambda^* \qquad \text{(A1.22)}$$

Hence using (A1.4) and (A1.5):

$$\underline{E} = \frac{i}{c}\sum_\lambda \omega_\lambda \left[a_\lambda \underline{A}_\lambda - a_\lambda^* \underline{A}_\lambda^*\right] \qquad \text{(A1.23)}$$

$$\underline{B} = i \sum_{\lambda} \left[a_\lambda \underline{k}_\lambda \times \underline{A}_\lambda - a_\lambda^* \underline{k}_\lambda \times \underline{A}_\lambda^* \right] \tag{A1.24}$$

Substituting these expansions into (A1.8):

$$\mathcal{E} = \frac{1}{8\pi} \sum_{\lambda} \int_V \left[\frac{\kappa \omega_\lambda^2}{c^2} + \frac{k_\lambda^2}{\mu} \right] \left[a_\lambda^* a_\lambda + a_\lambda a_\lambda^* \right] \underline{A}_\lambda \cdot \underline{A}_\lambda^* \, d\tau$$

$$= \sum_{\lambda} \omega_\lambda^2 \left[a_\lambda a_\lambda^* + a_\lambda^* a_\lambda \right] = \sum_{\lambda} \mathcal{H}_\lambda = \sum_{\lambda} \mathcal{E}_\lambda \tag{A1.25}$$

using (A1.16) and (A1.20). We have therefore shewn that the normalisation of (A1.10) is correct since it leads to the correct value for the field energy.

The interaction between the radiation field and the electronic system is represented by:

$$\mathcal{H}_I = \frac{e}{mc} \, \underline{p} \cdot \underline{A} \tag{A1.26}$$

For the case of photon absorption we require matrix elements of the type:

$$\langle a, n_\lambda - 1 | \mathcal{H}_I | b, n_\lambda \rangle = \frac{e}{mc} \sqrt{\frac{4\pi c^2}{\kappa V}} \sqrt{\frac{\hbar n_\lambda}{2\omega_\lambda}} \int_V \psi_a^* \, \underline{p} \cdot \underline{\epsilon}_\lambda \, e^{i \underline{k}_\lambda \cdot \underline{r}} \, \psi_b \, d\tau$$

$$= \frac{e}{m} \sqrt{\frac{2\pi \hbar n_\lambda}{\kappa V \omega_\lambda}} \langle a | \underline{p} \cdot \underline{\epsilon}_\lambda | b \rangle \tag{A1.27}$$

where we have made the dipole approximation, taking only the first term in the expansion of $e^{i \underline{k}_\lambda \cdot \underline{r}}$. a and b represent the final and initial electronic states and n_λ is the initial number of photons of wavelength λ. We have used (A1.10) and (A1.21).

The transition probability per unit time is:

$$W = \frac{2\pi}{\hbar} \rho_E \left| \langle | \mathcal{H}_I | \rangle \right|^2 \qquad (A1.28)$$

where $\rho_E \, dE$ is the number of photon states with energy between E and E + dE. Now if we assume periodic boundary conditions for $\underline{A}$ and take axes parallel to the edges of our cubic box V, then the allowed values of the components of $\underline{k}_\lambda$ are:

$$k_{\lambda x} = \frac{2\pi}{L} n_{\lambda x}, \quad k_{\lambda y} = \frac{2\pi}{L} n_{\lambda y}, \quad k_{\lambda z} = \frac{2\pi}{L} n_{\lambda z}$$

where the n's are intogers. Hence:

$$\omega_\lambda^2 = \left(\frac{2\pi c}{L\sqrt{\varkappa\mu}} \right)^2 \left(n_{\lambda x}^2 + n_{\lambda y}^2 + n_{\lambda z}^2 \right)$$

If the number of radiation oscillators having frequency between ω_λ and $\omega_\lambda + d\omega_\lambda$ and propagation vector within a solid angle $d\Omega$ is $\rho_{\omega_\lambda} \, d\omega_\lambda \, d\Omega$, then:

$$\rho_{\omega_\lambda} \, d\omega_\lambda \, d\Omega = 4\pi n_\lambda^2 \, dn_\lambda \, \frac{d\Omega}{4\pi} = \omega_\lambda^2 \, d\omega_\lambda \, d\Omega \, V \left(\frac{\sqrt{\varkappa\mu}}{2\pi c} \right)^3 \qquad (A1.29)$$

where $n_\lambda^2 = n_{\lambda x}^2 + n_{\lambda y}^2 + n_{\lambda z}^2$. Since $E_\lambda = \hbar \omega_\lambda$, we have:

$$\rho_E \, dE \, d\Omega = \frac{\omega_\lambda^2}{\hbar} \, dE \, d\Omega \left(\frac{\sqrt{\varkappa\mu}}{2\pi c} \right)^3 V \qquad (A1.30)$$

The transition probability per unit time for radiation propagating in a given direction is therefore:

$$W \, d\Omega = \frac{e^2}{m^2} \frac{\omega_\lambda}{2\pi c^3 \hbar} \frac{(\varkappa\mu)^{\frac{3}{2}}}{\varkappa} \left| \langle a | \underline{p} \cdot \underline{\epsilon}_\lambda | b \rangle \right|^2 n_\lambda \, d\Omega \qquad (A1.31)$$

The energy absorbed per unit time is:

$$\hbar\omega_\lambda W d\Omega = \frac{e^2}{m^2}\frac{\omega_\lambda^2}{2\pi c^3}\frac{(n\mu)^{\frac{3}{2}}}{n}|\langle a|p\cdot\varepsilon_\lambda|b\rangle|^2 n_\lambda d\Omega \qquad (A1.32)$$

Now the amount of energy in the photon beam crossing unit area in unit time is:

$$I(\omega_\lambda)d\omega_\lambda = n_\lambda \hbar\omega_\lambda \frac{c}{\sqrt{n\mu}}\frac{1}{V}\rho_{\omega_\lambda} d\omega_\lambda\, d\Omega$$

$$= n_\lambda \hbar\omega_\lambda^3 \frac{n\mu}{8\pi^3 c^2} d\omega_\lambda\, d\Omega \qquad (A1.33)$$

Suppose that the number of final states a which can be reached from the same initial state b, such that the energy difference between the two states lies between E and E + dE is S(E)dE. We call S(E) the density of final states. Then using (A1.32) and (A1.33), the energy absorbed per unit time per unit energy range is:

$$\frac{4\pi^2 e^2}{\hbar\omega_\lambda m^2 c}\frac{\sqrt{n\mu}}{n}\overline{|\langle a|p\cdot\varepsilon_\lambda|b\rangle|^2}\, I(\omega_\lambda) S(E)$$

where the bar over the square of the matrix element indicates that it is to be averaged over the final states. We define the absorption coefficient K to be the energy absorbed per unit volume per unit time per unit energy range when the radiation crossing unit area in unit time has unit energy for a unit energy range. Hence:

$$K = \frac{4\pi^2 e^2}{\omega_\lambda m^2 c V}\frac{\sqrt{n\mu}}{n}\overline{|\langle a|p\cdot\varepsilon_\lambda|b\rangle|^2}\, S(E) \qquad (A1.34)$$

Note that this expression has dimensionality $1/L$ in accord with its definition. In semiconductors we can normally put $\mu = 1$ so that the refractive index is $\eta = \sqrt{n}$.

Appendix 2. The Free Particle in a Uniform Magnetic Field.

We consider a particle of mass μ and charge $-e$. The Hamiltonian of the system is:

$$\mathcal{H} = \frac{\Pi^2}{2\mu} \tag{A2.1}$$

where $\underline{\Pi}$ is the effective momentum:

$$\underline{\Pi} = \underline{p} + \frac{e}{c}\underline{A} \tag{A2.2}$$

and the symbol $\underline{p}$ represents the momentum operator. The eigenfunctions of this Hamiltonian can be found in two ways, either by solving the differential equation or by operator methods. The former method gives the eigenfunctions most directly and we shall consider this first. However the operator method, apart from being more elegant, also gives many additional results, and we shall therefore go on to present an alternative solution by this method.

The equation we wish to solve is:

$$\frac{1}{2\mu}\left[-i\hbar\nabla + \frac{e}{c}\underline{A}\right]^2\psi = E\psi \tag{A2.3}$$

We take the direction of the field to lie along the z-axis of a cylindrical polar co-ordinate system ρ, ϕ, z and we choose the following gauge for the vector potential:

$$A_\rho = 0 \qquad A_\phi = \tfrac{1}{2}\rho H \qquad A_z = 0 \tag{A2.4}$$

where H is the magnitude of the field. The wave equation then becomes:

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2}+\frac{\partial^2\psi}{\partial z^2}\right]-\frac{ie\hbar H}{2\mu c}\frac{\partial\psi}{\partial\phi}+\frac{e^2H^2}{8\mu c^2}\rho^2\psi=E\psi \qquad (A2.5)$$

Make the substitutions:

$$\psi(\rho,\phi,z)=e^{ikz}\,e^{iM\phi}\,\frac{1}{\rho}F(\rho) \qquad (A2.6)$$

$$E=E_{\rho\phi}+\frac{\hbar^2k^2}{2\mu} \qquad (A2.7)$$

where M must be integral for a single-valued wave-function. Then (A2.5) becomes:

$$-\frac{\hbar^2}{2\mu}\left[\frac{d^2F}{d\rho^2}-\frac{1}{\rho}\frac{dF}{d\rho}+\frac{F}{\rho^2}\right]+\frac{\hbar^2}{2\mu}\frac{M^2}{\rho^2}F+\frac{e\hbar H}{2\mu c}MF+\frac{e^2H^2}{8\mu c^2}\rho^2F=E_{\rho\phi}F \qquad (A2.8)$$

Introduce a new variable:

$$\sigma=\frac{eH}{2\hbar c}\rho^2 \qquad (A2.9)$$

Then:

$$\frac{e\hbar H}{2\mu c}\left[\frac{d^2F}{d\sigma^2}-\frac{1}{4}F-\frac{MF}{2\sigma}+\frac{1-M^2}{4\sigma^2}F\right]=-\frac{E_{\rho\phi}}{2\sigma}F \qquad (A2.10)$$

This is now in the form of Whittaker's equation (see appendix 3). If we put:

$$E_{\rho\phi}=\frac{e\hbar H}{2\mu c}(2N+1) \qquad (A2.11)$$

then the solutions of (A2.10) may be written:

$$M_{\frac{1}{2}(2N+1-M),\frac{1}{2}M}(\sigma)=e^{-\frac{1}{2}\sigma}\,\sigma^{\frac{1}{2}(M+1)}\,{}_1F_1(M-N,M+1;\sigma) \qquad (A2.12)$$

$$M_{\frac{1}{2}(2N+1-M),-\frac{1}{2}M}(\sigma)=e^{-\frac{1}{2}\sigma}\,\sigma^{\frac{1}{2}(-M+1)}\,{}_1F_1(-N,-M+1;\sigma) \qquad (A2.13)$$

If the wave-function is to represent a bound state, its value must tend to zero as σ tends to infinity. It follows from the properties of the confluent hypergeometric function that this can only be if N is zero or a positive integer, being greater than or equal to M, in which case these functions become associated Laguerre polynomials (see appendix 3). Since M is an integer the two solutions of the wave equation given above are not independent but we give them both because the first form can be converted at once into an associated Laguerre polynomial for the case $M>0$ using (A3.27) and (A3.28), while for $M<0$ the second form is most convenient. The second independent solution of the Whittaker equation is not a suitable wave-function since it diverges for large σ.

Collecting together the terms in the solution, normalising the resulting wave-function and putting in a convenient phase factor, we obtain:

$$M \leq N \begin{cases} M>0 & \psi_{NM} = (-i)^N N'_{NM}\, e^{iM\phi}\, \sigma^{\frac{1}{2}M}\, e^{-\frac{1}{2}\sigma}\, L_N^M(\sigma)\, e^{ikz} \qquad (A2.14) \\ M<0 & \psi_{NM} = (-i)^N N''_{NM}\, e^{iM\phi}\, \sigma^{-\frac{1}{2}M}\, e^{-\frac{1}{2}\sigma}\, L_{N-M}^{-M}(\sigma)\, e^{ikz} \qquad (A2.15) \end{cases}$$

where:

$$N'^{2}_{NM} = \frac{1}{2\pi\lambda^2 L_z}\,\frac{\lfloor N-M}{(\lfloor N)^3}, \quad N''^{2}_{NM} = \frac{1}{2\pi\lambda^2 L_z}\,\frac{\lfloor N}{(\lfloor N-M)^3}, \quad \lambda^2 = \frac{\hbar c}{eH} \qquad (A2.16)$$

and L_z is the z-dimension of the volume to which the particle is confined.

The method we have used to obtain these wave-functions is

similar to that of Dingle[22]. We shall now obtain the same results by the operator methods introduced by Johnson and Lippmann[23].

The operator $\underline{\Pi}$ defined in (A2.2) satisfies the commutation relations:

$$\underline{\Pi} \times \underline{\Pi} = -i\frac{e\hbar}{c}\underline{H} \tag{A2.17}$$

The equation of motion is:

$$\dot{\underline{\Pi}} = -\frac{1}{i\hbar}\left[\mathcal{H}, \underline{\Pi}\right] = -\frac{1}{2i\hbar\mu}\left[\Pi^2, \underline{\Pi}\right] = \frac{e}{\mu c}\underline{H} \times \underline{\Pi} \tag{A2.18}$$

where we have used a general relation which holds for any operator:

$$\left[\Pi^2, \underline{\Pi}\right] = \left(\underline{\Pi} \times \underline{\Pi}\right) \times \underline{\Pi} - \underline{\Pi} \times \left(\underline{\Pi} \times \underline{\Pi}\right) \tag{A2.19}$$

We take a Cartesian co-ordinate system with z-axis in the direction of the magnetic field. Writing the equation of motion in components:

$$\dot{\Pi}_x = -\frac{eH}{\mu c}\Pi_y \tag{A2.20}$$

$$\dot{\Pi}_y = \frac{eH}{\mu c}\Pi_x \tag{A2.21}$$

$$\dot{\Pi}_z = 0 \tag{A2.22}$$

Also we have:

$$\mu\dot{\underline{r}} = \underline{\Pi} \tag{A2.23}$$

The equation for the z-motion (A2.22) can be integrated at once to give:

$$\Pi_z = \hbar k \tag{A2.24}$$

The Hamiltonian (A2.1) may be written:

$$\mathcal{H} = \frac{1}{2\mu}\left[\Pi_x^2 + \Pi_y^2\right] + \frac{\Pi_z^2}{2\mu} \tag{A2.25}$$

The x,y part of this Hamiltonian together with the commutation relation

(A2.17) shew that the transverse part of the problem is similar to a harmonic oscillator with conjugate co-ordinates π_x and $\pi_y/\mu\omega_c$ [the oscillator Hamiltonian is $\frac{1}{2\mu}\left(p^2+\mu^2\omega^2q^2\right)$] where ω_c is the cyclotron frequency:

$$\omega_c = \frac{eH}{\mu c} \tag{A2.26}$$

The energy levels of the system are therefore given by:

$$E = \hbar\omega_c\left(N+\tfrac{1}{2}\right) + \frac{\hbar^2k^2}{2\mu} \qquad N = 0, 1, 2, \cdots \tag{A2.27}$$

Combining (A2.20), (A2.21) and (A2.23):

$$\left.\begin{aligned} \frac{d}{dt}\left(\pi_x + \mu\omega_c y\right) &= 0 \\ \frac{d}{dt}\left(\pi_y - \mu\omega_c x\right) &= 0 \end{aligned}\right\} \tag{A2.28}$$

so that:

$$\left.\begin{aligned} \frac{\pi_x}{\mu\omega_c} + y &= y_0 \\ -\frac{\pi_y}{\mu\omega_c} + x &= x_0 \end{aligned}\right\} \tag{A2.29}$$

where x_0 and y_0 are constants. These two integration constants commute with the Hamiltonian and with π_x and π_y, but they do not commute with each other:

$$\left[x_0, y_0\right] = \left[x, \frac{\pi_x}{\mu\omega_c}\right] + \left[y, \frac{\pi_y}{\mu\omega_c}\right] + \left[\frac{\pi_x}{\mu\omega_c}, \frac{\pi_y}{\mu\omega_c}\right] = 2\frac{i\hbar}{\mu\omega_c} - \frac{ie\hbar H}{\mu^2\omega_c^2 c} = i\frac{\hbar c}{eH} \tag{A2.30}$$

(A2.23) and (A2.28) are the same as the classical equations for the system, and we therefore identify x_0 and y_0 with the co-ordinates of the centre of the orbit. The distance r_0 of the centre of the orbit from the origin is given by:

$$r_0^2 = x_0^2 + y_0^2 \tag{A2.31}$$

Equations (A2.30) and (A2.31) again define an eigenvalue problem similar to the harmonic oscillator, with conjugate co-ordinates $\sqrt{2\mu}\,x_0$ and $\hbar y_0/\lambda^2\sqrt{2\mu}$, where λ is a length characteristic of the magnetic field defined in (A2.16). If these co-ordinates are substituted in the harmonic oscillator Hamiltonian, (A2.31) is obtained if the 'frequency' is taken to be $\frac{2\lambda^2}{\hbar}$. The eigenvalues are therefore:

$$r_0^2 = \lambda^2(2L+1) \qquad L = 0,1,2,\ldots \qquad \text{(A2.32)}$$

We observe that although r_0^2 is well defined, the commutator (A2.30) implies that:

$$\Delta x_0\,\Delta y_0 \geq \lambda^2 \qquad \text{(A2.33)}$$

where Δx_0 and Δy_0 are the uncertainties in experimentally possible determinations of x_0 and y_0 . If r' is the radius of the particle's orbit, then using (A2.29):

$$r'^2 = (x-x_0)^2 + (y-y_0)^2 = \frac{1}{\mu^2\omega_c^2}(\pi_x^2+\pi_y^2) = \frac{2\hbar\omega_c}{\mu\omega_c^2}(N+\tfrac{1}{2}) = \lambda^2(2N+1) \qquad \text{(A2.34)}$$

so that r' is exactly known.

The angular momentum about the z-axis is:

$$\hbar M = (\underline{r}\times\underline{p})_z \qquad \text{(A2.35)}$$

It is now convenient to choose a particular gauge for the vector potential. We take:

$$\underline{A} = \tfrac{1}{2}\underline{H}\times\underline{r} \qquad \text{i.e.} \quad A_x = -\tfrac{1}{2}yH,\ A_y = \tfrac{1}{2}xH,\ A_z = 0 \qquad \text{(A2.36)}$$

Then:
$$\hbar M = x\pi_y - y\pi_x - \frac{\mu\omega_c}{2}(x^2+y^2)$$

$$= \frac{\mu\omega_c}{2}(r'^2 - r_0^2) = \hbar(N-L) \qquad \text{(A2.37)}$$

where we have used (A2.29). Now introduce:

$$\bar{\pi}_{\pm} = \bar{\pi}_x \pm i\bar{\pi}_y$$

$$= -i\hbar\left[\frac{\partial}{\partial x} \pm i\frac{\partial}{\partial y} + \frac{1}{2\lambda^2}(x \pm iy)\right] \qquad \text{(A2.38)}$$

$$\bar{\pi}_z = -i\hbar\frac{\partial}{\partial z} \qquad \text{(A2.39)}$$

Suppose that ψ_N is an energy eigenfunction with eigenvalue $\hbar\omega_c\left(N+\frac{1}{2}\right)$. Then $\bar{\pi}_+\psi_N$ and $\bar{\pi}_-\psi_N$ are also eigenfunctions with eigenvalues $\hbar\omega_c\left(N+\frac{1}{2}+1\right)$ and $\hbar\omega_c\left(N+\frac{1}{2}-1\right)$. Let:

$$C\bar{\pi}_+\psi_{N-1} = \psi_N$$

where C is a constant to be determined and suppose that ψ_N and ψ_{N-1} are normalised in the same way so that:

$$CC^*\int\psi^*_{N-1}\,\bar{\pi}_-\bar{\pi}_+\psi_{N-1}\,d\tau = \int\psi^*_N\psi_N\,d\tau$$

But:

$$\bar{\pi}_-\bar{\pi}_+\psi_{N-1} = \left\{\bar{\pi}_x^2 + \bar{\pi}_y^2 + i\left[\bar{\pi}_x, \bar{\pi}_y\right]\right\}\psi_{N-1}$$

$$= \left\{2\mu\hbar\omega_c\left[N+\tfrac{1}{2}-1\right] + \frac{e\hbar H}{c}\right\}\psi_{N-1} = 2N\frac{e\hbar H}{c}\psi_{N-1} \qquad \text{(A2.40)}$$

Hence:

$$C = \frac{1}{\sqrt{2N}}\frac{\lambda}{\hbar}$$

Therefore:

$$\psi_N = \frac{1}{\sqrt{2N}}\frac{\lambda}{\hbar}\bar{\pi}_+\psi_{N-1} \qquad \text{(A2.41)}$$

and similarly:

$$\psi_{N-1} = \frac{1}{\sqrt{2N}}\frac{\lambda}{\hbar}\bar{\pi}_-\psi_N \qquad \text{(A2.42)}$$

The wave-function of the lowest state must satisfy:

$$\pi_- \psi_0 = 0 \tag{A2.43}$$

$$\pi_z \psi_0 = \hbar k \psi_0 \tag{A2.44}$$

Hence:

$$\psi_0 = f(x - iy)\, e^{ikz}\, e^{-\frac{x^2+y^2}{4\lambda^2}} \tag{A2.45}$$

where f is an arbitrary function. This arbitrariness allows us to impose a further condition on the energy eigenfunctions, and so we specify that they shall also be eigenfunctions of r_0^2. Such wave-functions have cylindrical symmetry. Hence for the lowest state:

$$r_0^2 \psi_0 = \lambda^2 (2L+1) \psi_0 \tag{A2.46}$$

Since eigenfunctions of $\mathcal{H}$ and r_0^2 are necessarily eigenfunctions of M by (A2.37) this condition can also be written:

$$\frac{\partial \psi_0}{\partial \phi} = M \psi_0 = -L \psi_0 \tag{A2.47}$$

where ϕ is the angular co-ordinate of a cylindrical polar co-ordinate set ρ, ϕ, z. The normalised solution of (A2.47) is:

$$\psi_{0,L} = \frac{1}{\sqrt{2^{L+1} L_z \pi \lfloor L}}\, \frac{1}{\lambda} \left(\frac{x - iy}{\lambda}\right)^L e^{-\frac{x^2+y^2}{4\lambda^2}}\, e^{ikz} \tag{A2.48}$$

where L_z is again the length of the volume in which the particle is contained. From (A2.41), ψ_{NL} is given by:

$$\psi_{NL} = \frac{1}{\sqrt{2^N \lfloor N}} \left(\frac{\lambda \overline{\pi}_+}{\hbar}\right)^N \psi_{0L} \tag{A2.49}$$

Using the relations:

$$\pi_+ e^{\frac{x^2+y^2}{4\lambda^2}} = e^{\frac{x^2+y^2}{4\lambda^2}} (-i\hbar)\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) \tag{A2.50}$$

this becomes:

$$\psi_{NL} = (-i)^N \frac{1}{\sqrt{2^{N+L+1} L_z \pi \lfloor L \lfloor N}} \frac{1}{\lambda} e^{\frac{x^2+y^2}{4\lambda^2}} e^{ikz} \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^N \left(\frac{x-iy}{\lambda}\right)^L e^{-\frac{x^2+y^2}{2\lambda^2}} \tag{A2.51}$$

$$= (-i)^N \frac{1}{\sqrt{2^{N-L+1} L_z \pi \lfloor L \lfloor N}} \frac{1}{\lambda} \left(\frac{\rho}{\lambda}\right)^{N-L} e^{\frac{\rho^2}{4\lambda^2}} e^{ikz} e^{i(N-L)\phi} \left(\frac{d}{d\frac{\rho^2}{2\lambda^2}}\right)^N e^{-\frac{\rho^2}{2\lambda^2}} \left(\frac{\rho^2}{2\lambda^2}\right)^L$$

since $x + iy$ commutes with $\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)$. This expression may be written in terms of associated Laguerre polynomials which take a different form according as $N \gtrless L$:

$$N > L \qquad \psi_{NL} = (-i)^N N'_{NL} e^{i(N-L)\phi} \sigma^{\frac{1}{2}(N-L)} e^{-\frac{1}{2}\sigma} L_N^{N-L}(\sigma) e^{ikz} \tag{A2.52}$$

$$N < L \qquad \psi_{NL} = (-i)^N N''_{NL} e^{i(N-L)\phi} \sigma^{\frac{1}{2}(L-N)} e^{-\frac{1}{2}\sigma} L_L^{L-N}(\sigma) e^{ikz} \tag{A2.53}$$

where:

$$N'^2_{NL} = \frac{1}{2\pi\lambda^2 L_z} \frac{\lfloor L}{(\lfloor N)^3}, \quad N''^2_{NL} = \frac{1}{2\pi\lambda^2 L_z} \frac{\lfloor N}{(\lfloor L)^3}, \quad \sigma = \frac{\rho^2}{2\lambda^2} \tag{A2.54}$$

Since $M = N - L$ these wave-functions are the same as (A2.14) and (A2.15).

Appendix 3. Properties of the Confluent Hypergeometric Function.

Confluent Hypergeometric functions are solutions of Whittaker's equation:

$$\frac{d^2z}{dx^2} + \left[-\frac{1}{4} + \frac{\alpha}{x} + \frac{\frac{1}{4} - m^2}{x^2} \right] z = 0 \qquad \text{(A3.1)}$$

The nature of the two independent solutions of the equation depends on whether or not m is integral or half-integral. We consider these two cases separately, basing our discussion on the work of Erdélyi et al.[19] and of Whittaker and Watson[24].

Case 1. m not integral or half-integral. The two independent solutions of (A3.1) are:

$$M_{\alpha,m}(x) = e^{-\frac{1}{2}x}\, x^{m+\frac{1}{2}}\, {}_1F_1\left(\tfrac{1}{2} - \alpha + m,\ 2m+1;\ x\right) \qquad \text{(A3.2)}$$

$$M_{\alpha,-m}(x) = e^{-\frac{1}{2}x}\, x^{-m+\frac{1}{2}}\, {}_1F_1\left(\tfrac{1}{2} - \alpha - m,\ -2m+1;\ x\right) \qquad \text{(A3.3)}$$

the notation $M_{\alpha,m}(x)$ being that of Whittaker. In these expressions ${}_1F_1$ is the power series:

$${}_1F_1(a,c;x) = \sum_{r=0}^{\infty} \frac{(a)_r}{(c)_r} \frac{x^r}{\lfloor r} \qquad \text{where } (s)_r = \frac{\Gamma(s+r)}{\Gamma(s)} \qquad \text{(A3.4)}$$

The two solutions (A3.2) and (A3.3) can be easily obtained by series

solution of Whittaker's equation. Erdélyi et al. derive the following asymptotic form:

$$M_{\alpha,m}(x) \to \frac{\Gamma(2m+1)}{\Gamma(\frac{1}{2}+m+\alpha)} e^{i\left(\frac{\pi}{2}-\pi\alpha+\pi m\right)} e^{-\frac{1}{2}x} x^{\alpha} \sum_{n=0}^{M} \frac{\left(\frac{1}{2}-\alpha+m\right)_n \left(\frac{1}{2}-\alpha-m\right)_n}{\lfloor n} (-x)^{-n} + O\left|e^{-\frac{1}{2}x} x^{\alpha-M-1}\right|$$

$$+ \frac{\Gamma(2m+1)}{\Gamma(\frac{1}{2}+m-\alpha)} e^{\frac{1}{2}x} x^{-\alpha} \sum_{n=0}^{N} \frac{\left(\frac{1}{2}+\alpha+m\right)_n \left(\frac{1}{2}+\alpha-m\right)_n}{\lfloor n} x^{-n} + O\left|e^{\frac{1}{2}x} x^{-\alpha-N-1}\right| \qquad (A3.5)$$

$$\text{for } x \to \infty, \quad \Im m\, x > 0, \quad M, N = 0, 1, 2, \ldots$$

The asymptotic form of $M_{\alpha,-m}(x)$ is found by changing the sign of m. Instead of using (A3.2) and (A3.3) as the two independent solutions of the Whittaker equation, it is sometimes more convenient to take linear combinations of $M_{\alpha,m}(x)$ and $M_{\alpha,-m}(x)$ such that the asymptotic form of one combination contains only the positive exponential series of (A3.5) while the asymptotic form of the other contains only the negative exponential series. We accordingly define:

$$W_{\alpha,m}(x) = \frac{\Gamma(-2m)}{\Gamma(\frac{1}{2}-\alpha-m)} M_{\alpha,m}(x) + \frac{\Gamma(2m)}{\Gamma(\frac{1}{2}-\alpha+m)} M_{\alpha,-m}(x) \qquad (A3.6)$$

$$V_{\alpha,m}(x) = -i\left\{\frac{e^{-i\pi m}\Gamma(-2m)}{\Gamma(\frac{1}{2}-m+\alpha)} M_{\alpha,m}(x) + \frac{e^{i\pi m}\Gamma(2m)}{\Gamma(\frac{1}{2}+m+\alpha)} M_{\alpha,-m}(x)\right\} \qquad (A3.7)$$

It can be verified using (A3.5) that these functions have the asymptotic forms:

$$\left.\begin{aligned} W_{\alpha,m}(x) &\to x^{\alpha} e^{-\frac{1}{2}x} \\ V_{\alpha,m}(x) &\to x^{-\alpha} e^{\frac{1}{2}x} e^{i\pi\alpha} \end{aligned}\right\} \quad x \to \infty \qquad \begin{aligned} &(A3.8) \\ &(A3.9) \end{aligned}$$

where we have retained only the dominant term in each case.

The Wronskian of two independent solutions of a differential equation of the type (A3.1) is a constant independent of position, so that the asymptotic forms of the solutions can be used in determining it. In this way it may be established that:

$$M_{\alpha,m}(x)\, M'_{\alpha,-m}(x) - M_{\alpha,-m}(x)\, M'_{\alpha,m}(x) = -2m \qquad (A3.10)$$

$$W_{\alpha,m}(x)\, V'_{\alpha,m}(x) - V_{\alpha,m}(x)\, W'_{\alpha,m}(x) = e^{i\pi\alpha} \qquad (A3.11)$$

where the prime denotes differentiation with respect to x.

Any two of the four solutions $M_{\alpha,m}(x)$, $M_{\alpha,-m}(x)$, $W_{\alpha,m}(x)$ and $V_{\alpha,m}(x)$ are independent.

Case 2. m integral or half-integral. For this case it is most convenient to transform (A3.1) by making the substitutions:

$$z = x^{\frac{1}{2}c} e^{-\frac{1}{2}x} y \quad , \quad a = \tfrac{1}{2} - \alpha + m \quad , \quad c = 2m+1 \qquad (A3.12)$$

whereupon it takes the form:

$$x \frac{d^2y}{dx^2} + (c-x)\frac{dy}{dx} - ay = 0 \qquad (A3.13)$$

This equation can be solved using the method of Frobenius, and since c is an integer one of the solutions is always logarithmic. Consider

first the case where c is a positive integer. Two independent solutions of (A3.13) are:

$$\Psi(a,c,x) = \frac{(-1)^c}{\underline{|c-1}\,\Gamma(1+a-c)}\left\{{}_1F_1(a,c;x)\left[\log x + \psi(a) - \psi(1) - \psi(c)\right] + \sum_{r=1}^{\infty}\frac{(a)_r}{(c)_r}A_r\,\frac{x^r}{\underline{|r}}\right\}$$

$$+\ \frac{\underline{|c-2}}{\Gamma(a)}\sum_{r=0}^{c-2}\frac{(a-c+1)_r}{(2-c)_r}\,\frac{x^{r-c+1}}{\underline{|r}} \qquad \text{(A3.14)}$$

$$\Phi(a,c,x) = \frac{\Gamma(a)}{\Gamma(c)\,\Gamma(0)}\left\{{}_1F_1(a,c;x)\log x + \sum_{s=0}^{-a}\frac{(a)_s}{(c)_s}\,\frac{x^s}{\underline{|s}}\left[\psi(a+s) - \psi(1+s) - \psi(c+s)\right]\right\}$$

$$+\sum_{s=0}^{\infty}\frac{\Gamma(a+s)}{\Gamma(c+s)}\,\frac{x^s}{\underline{|s}} + \frac{\Gamma(1-c+a)}{\Gamma(2-c)}\sum_{s=0}^{c-2}\frac{(a-c+1)_s}{(2-c)_s}\,\frac{x^{s-c+1}}{\underline{|s}} \qquad \text{(A3.15)}$$

In both functions the last summation is to be omitted for c = 1. Also:

$$\psi(r) = \frac{d}{dr}\log\Gamma(r) = \frac{\Gamma'(r)}{\Gamma(r)} \qquad \text{(A3.16)}$$

and:

$$A_r = \sum_{\nu=0}^{r-1}\left[\frac{1}{\nu+a} - \frac{1}{\nu+1} - \frac{1}{\nu+c}\right] \qquad \text{(A3.17)}$$

For c zero or a negative integer it is necessary to make use of the relation:

$$\Psi(a,c,x) = x^{1-c}\,\Psi(a-c+1,\,2-c,\,x) \qquad \text{(A3.18)}$$

before the series expansion (A3.14) can be used, and for these values of c, (A3.15) must be evaluated as a limit.

The asymptotic forms of the two solutions are:

$$\left.\begin{aligned} \Psi(a,c,x) &\to x^{-a} \\ \Phi(a,c,x) &\to x^{a-c}e^{x} \end{aligned}\right\} \quad x \to \infty \qquad \begin{matrix}(A3.19)\\(A3.20)\end{matrix}$$

Although both (A3.14) and (A3.15) appear to contain a logarithmic term, this term always drops out of one or the other depending on the value of the parameter a.

Case 2(i). $a \neq 0, -1, -2, \ldots$. The first and last terms in (A3.15) are zero leaving:

$$\Phi(a,c,x) = \sum_{s=0}^{\infty} \frac{\Gamma(a+s)}{\Gamma(c+s)} \frac{x^s}{\lfloor s} = \frac{\Gamma(a)}{\Gamma(c)} {}_1F_1(a,c;x) \qquad (A3.21)$$

where ${}_1F_1$ is defined in (A3.4). Two independent solutions of the Whittaker equation (A3.1) are therefore:

$$M_{\alpha,m}(x) = e^{-\frac{1}{2}x} x^{m+\frac{1}{2}} {}_1F_1\left(\tfrac{1}{2}-\alpha+m, 2m+1; x\right) \qquad (A3.22)$$

$$W_{\alpha,m}(x) = e^{-\frac{1}{2}x} x^{m+\frac{1}{2}} \Psi\left(\tfrac{1}{2}-\alpha+m, 2m+1; x\right) \qquad (A3.23)$$

It is easily checked that these functions have the same asymptotic forms as the corresponding solutions defined for the case where m is not integral or half-integral.

Case 2(ii). $a = 0, -1, -2, \ldots$. In this case it is the solution Ψ which takes on a simpler form while Φ remains logarithmic. We observe that since:

$$\frac{\psi(a)}{\Gamma(1+a-c)} = (-1)^{a-c}\Gamma(c-a) \qquad \begin{matrix} c = 1, 2, 3, \ldots \\ a = 0, -1, -2, \ldots \end{matrix} \qquad (A3.24)$$

it follows that:

$$\Psi(a,c,x) = (-1)^a (c)_{-a} \, {}_1F_1(a,c;x) \qquad \text{(A3.25)}$$

Two independent solutions of the Whittaker equation (A3.1) are therefore:

$$e^{-\frac{1}{2}x} x^{m+\frac{1}{2}} \Phi\left(\tfrac{1}{2}-\alpha+m, 2m+1, x\right) \qquad \text{(A3.26)}$$

$$W_{\alpha,m}(x) = e^{-\frac{1}{2}x} x^{m+\frac{1}{2}} (-1)^{\frac{1}{2}-\alpha+m} (2m+1)_{-\frac{1}{2}+\alpha+m} \, {}_1F_1\left(\tfrac{1}{2}-\alpha+m, 2m+1; x\right) \qquad \text{(A3.27)}$$

The function (A3.27) is very important in quantum mechanics since it is only for the case 2(ii) that the Whittaker equation has a solution which is everywhere finite with finite slope and tends to zero exponentially at large x, the asymptotic form of $W_{\alpha,m}(x)$ again being given by (A3.8). Also for this case $W_{\alpha,m}(x)$ is simply related to an associated Laguerre polynomial:

$$W_{\alpha,m}(x) = (-1)^{\frac{1}{2}-\alpha-m} \frac{\Gamma\left(\frac{1}{2}+\alpha-m\right)}{\Gamma\left(\frac{1}{2}+\alpha+m\right)} e^{-\frac{1}{2}x} x^{m+\frac{1}{2}} L^{2m}_{-\frac{1}{2}+\alpha+m}(x) \qquad \text{(A3.28)}$$

where:

$$L^n_\ell(x) = \frac{d^n}{dx^n} L_\ell(x) \quad , \quad L_\ell(x) = e^x \frac{d^\ell}{dx^\ell}\left(x^\ell e^{-x}\right) \qquad \text{(A3.29)}$$

The normalisation integral for $W_{\alpha,m}(x)$ can be carried out in this case giving:

$$\int_{-\infty}^{\infty} |W_{\alpha,m}(x)|^2 dx = 4\alpha \, \Gamma\left(\tfrac{1}{2}+\alpha-m\right) \Gamma\left(\tfrac{1}{2}+\alpha+m\right) \qquad \text{(A3.30)}$$

Appendix 4. The One-dimensional Hydrogen Atom Equation.

In an infinite magnetic field the effective potential is given by (4.10) and the wave-equation for the z-motion (4.7) takes the form:

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dz^2} - \frac{e^2}{\varkappa|z|}\psi = E_z\psi \qquad (A4.1)$$

This is just the wave-equation for the one-dimensional hydrogen atom. All the levels of the system are twofold degenerate, except for the ground state which is a state of infinite binding energy localized at the point $z = 0$. We justify these statements by a study of the bound state solutions of (A4.1).

Introduce a quantity α by taking:

$$E_z = -\frac{\mu e^4}{2\hbar^2\varkappa^2\alpha^2} \qquad (A4.2)$$

Define a Bohr length:

$$a_0 = \frac{\hbar^2\varkappa}{\mu e^2} \qquad (A4.3)$$

and change the variable in (A4.1) to:

$$x = \frac{2z}{a_0\alpha} \qquad (A4.4)$$

obtaining:

$$\frac{d^2\psi}{dx^2} - \frac{1}{4}\psi + \frac{\alpha}{|x|}\psi = 0 \qquad (A4.5)$$

The wave-equation has therefore been reduced to Whittaker's form of the confluent hypergeometric equation (A3.1) with m = $\frac{1}{2}$. Consider first the region $x > 0$. We have shewn in appendix 3 that the solution of (A4.5) which tends to zero as x tends to infinity is a function $W_{\alpha,\frac{1}{2}}(x)$ defined by (A3.23) and (A3.14). The following series expansion may be obtained from these two equations:

$$W_{\alpha,\frac{1}{2}}(x) = \frac{e^{-\frac{1}{2}x}}{\Gamma(-\alpha)}\left\{x\,{}_1F_1(1-\alpha,2;x)\left[\log x + \psi(1-\alpha) - \psi(1) - \psi(2)\right] - \frac{1}{\alpha} + \sum_{r=1}^{\infty}\frac{(1-\alpha)_r}{\lfloor r \lfloor r+1}\,A_r\,x^{r+1}\right\} \qquad (A4.6)$$

where:

$$A_r = \sum_{\nu=0}^{r-1}\left[\frac{1}{\nu+1-\alpha} - \frac{1}{\nu+1} - \frac{1}{\nu+2}\right]$$

The function $W_{\alpha,\frac{1}{2}}(x)$ is finite at x = 0 but it has infinite slope there except when α is a positive integer. An acceptable wave-function can therefore only be formed when α is a positive integer $\nu = 1, 2, \cdots$. The bound state energies as given by equation (A4.2) are just the Balmer energies so that the one- and three-dimensional hydrogen atoms have common energy levels. The form of $W_{\alpha,\frac{1}{2}}(x)$ simplifies considerably for these particular values of α. Using (A3.28) we have:

$$W_{\alpha,\frac{1}{2}}(x) = (-1)^{\alpha}\frac{1}{\alpha}\,e^{-\frac{1}{2}x} \times L^1_{\alpha}(x) \qquad \alpha = 1, 2, \cdots \qquad (A4.7)$$

We have therefore shewn that for $x > 0$ the wave-function of the system is:

$$\psi = B e^{-\frac{1}{2}x} \times L^1_\alpha(x) \qquad x = \frac{2z}{\alpha a_0} \qquad \alpha = 1, 2, \cdots \qquad (A4.8)$$

where B is a normalisation constant. Similarly for $x < 0$ it may be shewn that:

$$\psi = C e^{\frac{1}{2}x} \times L^1_\alpha(-x) \qquad (A4.9)$$

C being another normalization constant.

We now require to join together the two solutions (A4.8) and (A4.9) at the point $x = 0$. Since the potential of the problem is invariant under the reflection $z \longrightarrow -z$, we may insist that the wave-functions be either even or odd functions of z. The wave-functions (A4.8) and (A4.9) have finite slopes for small $|x|$, but the wave-equation (A4.5) has a regular singular point at $x = 0$ giving rise to the possibility of a singularity in the second derivative of the wave-function at this point. There is thus some uncertainty as to whether or not (A4.8) and (A4.9) can be joined together to give an even wave-function. To investigate this we consider the problem with the potential slightly different, viz:

$$-\frac{e^2}{\kappa(a+|z|)} \qquad (A4.10)$$

where a is a positive quantity very much smaller than the Bohr length a_0, and which we shall eventually allow to tend to zero so as to reproduce the original potential. For large $|z|$ (A4.10) is little

different from $-\frac{e^2}{\varkappa|z|}$ but the new potential remains finite at z = 0 instead of having a pole.

The wave-equation is still of the form (A4.5) but the variable is now

$$x' = \frac{2}{\alpha a_0}(a + z) \qquad \text{for} \quad z > 0$$
$$x' = -\frac{2}{\alpha a_0}(a - z) \qquad \text{for} \quad z < 0 \tag{A4.11}$$

There is therefore a lower bound of $\frac{2a}{\alpha a_0}$ to the range of values which $|x'|$ can take. The modification we have made to the potential is such that the potential energy of the electron is higher at all points, and we may therefore expect the energy levels of the system to be raised slightly above the Balmer energies. Referring to (A4.2) we see that the values of α for which eigenfunctions can be formed will be slightly higher than the positive integers. This may be conveniently expressed by defining the quantum defect δ_ν of a level as the difference between the value of α to which it corresponds and the integer ν close to α :

$$\delta_\nu = \alpha - \nu \tag{A4.12}$$

For $a << a_0$ we shall have $\delta_\nu << 1$, and $\delta_\nu \to 0$ as $\alpha \to 0$.

The wave-function is still $W_{\alpha,\frac{1}{2}}(|x'|)$ given by (A4.6). α is not now integral so the function has infinite slope at x' = 0, but this does not matter since the point x' = 0 is not included in the physical domain of x'.

The solutions for positive and negative z can be joined

together at $z = 0$ to form both even and odd wave-functions. For an odd state we require:

$$W_{\alpha,\frac{1}{2}}\left(\frac{2a}{\alpha a_0}\right) = 0 \qquad (A4.13)$$

while for an even state:

$$\frac{d}{dx'}\left[W_{\alpha,\frac{1}{2}}(x')\right]_{x'=\frac{2a}{\alpha a_0}} = 0 \qquad (A4.14)$$

These conditions give the eigenvalues of the system for a given value of a. Using (A4.6) we keep only the terms which are dominant when $x = \frac{2a}{\alpha a_0}$ is very small and α is close to a positive integer. The eigenvalue conditions then become:

$$\text{Odd state:} \quad \frac{2a}{\alpha a_0}\psi(1-\alpha) - \frac{1}{\alpha} = 0 \qquad (A4.15)$$

$$\text{Even state:} \quad \log\frac{2a}{\alpha a_0} + \psi(1-\alpha) = 0 \qquad (A4.16)$$

$$\text{Now as} \quad \alpha \longrightarrow \nu, \quad \psi(1-\alpha) \longrightarrow \frac{1}{\alpha-\nu} = \frac{1}{\delta_\nu} \qquad (A4.17)$$

Hence using (A4.15) and (A4.16) the quantum defects are:

$$\text{Odd state:} \quad \delta_\nu = \frac{2a}{a_0} \qquad (A4.18)$$

$$\text{Even state:} \quad \delta_\nu = -\frac{1}{\log\frac{2a}{\alpha a_0}} \qquad (A4.19)$$

Figure 12 shows how the quantum defect δ_1 varies with a/a_0 for both

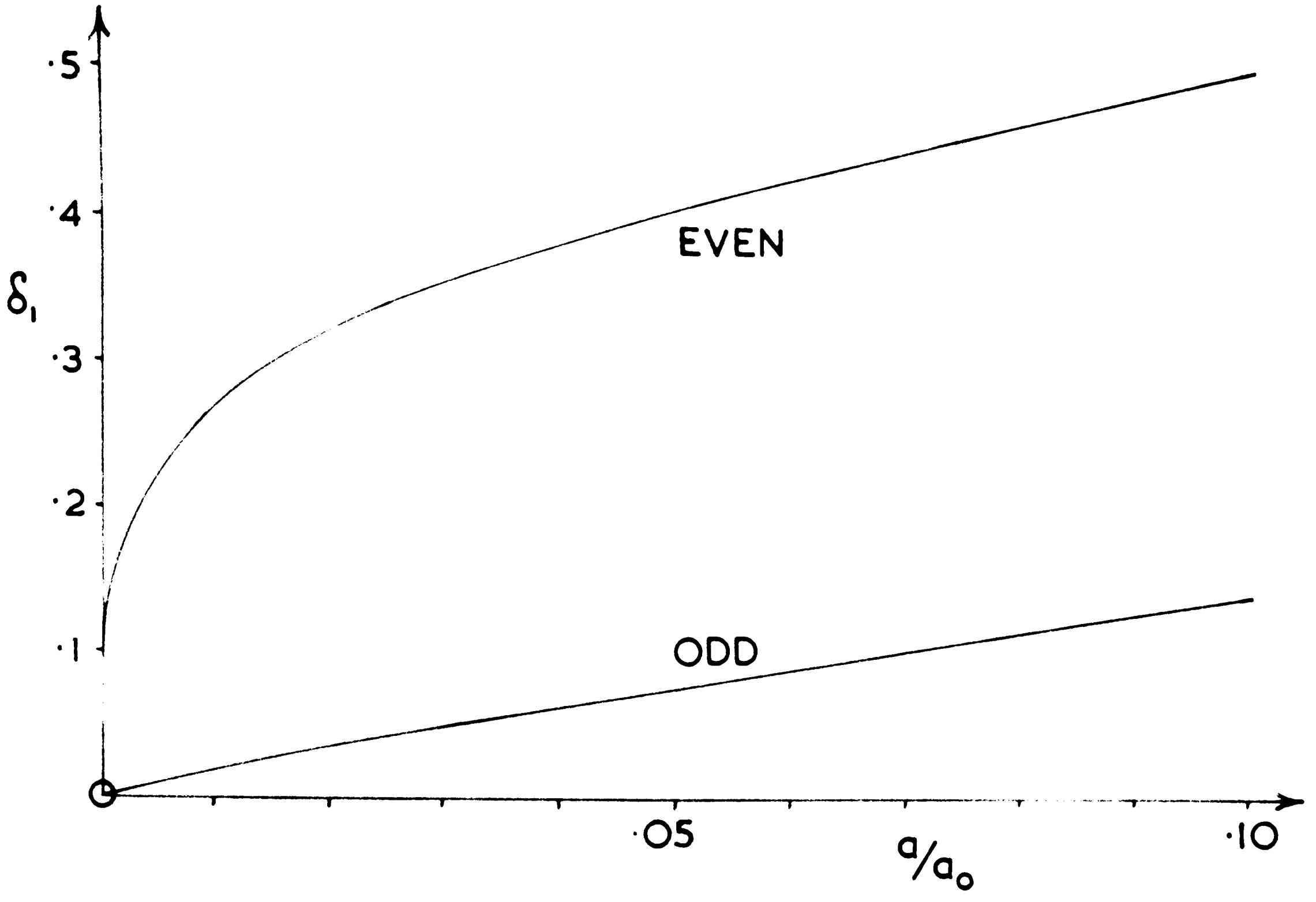


FIGURE 2

the odd and the even state. δ_ν behaves in a similar manner for the other values of ν. The curves were calculated using the complete expression (A4.6) for $W_{\alpha,\frac{1}{2}}(x)$ and not the approximate equations (A4.18) and (A4.19) which hold only at the lower end of the a/a_0 scale where $\delta_1 \ll 1$. Note that the even state quantum defect plunges to zero very steeply close to the origin.

In addition to these series of odd and even states having their quantum numbers α close to the positive integers, there is another state having α close to zero. For such a value of α, $\psi(1-\alpha)$ is no longer an important term in (A4.6), and $1/\alpha$ becomes the dominant term in α. Hence for this case the eigenvalue conditions (A4.13) and (A4.14) become:

$$\text{Odd state:} \quad \frac{2a}{2a_0}\log\frac{2a}{2a_0} - \frac{1}{\alpha} = 0 \qquad \text{(A4.20)}$$

$$\text{Even state:} \quad \log\frac{2a}{2a_0} + \frac{1}{2\alpha} = 0 \qquad \text{(A4.21)}$$

Equation (A4.20) has no solution for $a \ll a_0$, so that there is only one state having $\alpha \ll 1$. This even state is the ground state in the potential (A4.10). Since for $\nu = 0$, α is equal to the quantum defect δ_0, equation (A4.21) can be regarded as an equation for the quantum defect of the ground state.

Since the quantum defect for the even state is always larger than that for the corresponding odd state, the states alternate between even and odd as we move up the energy scale with an even state lowest. Figure 13 shows the odd and even wave-functions

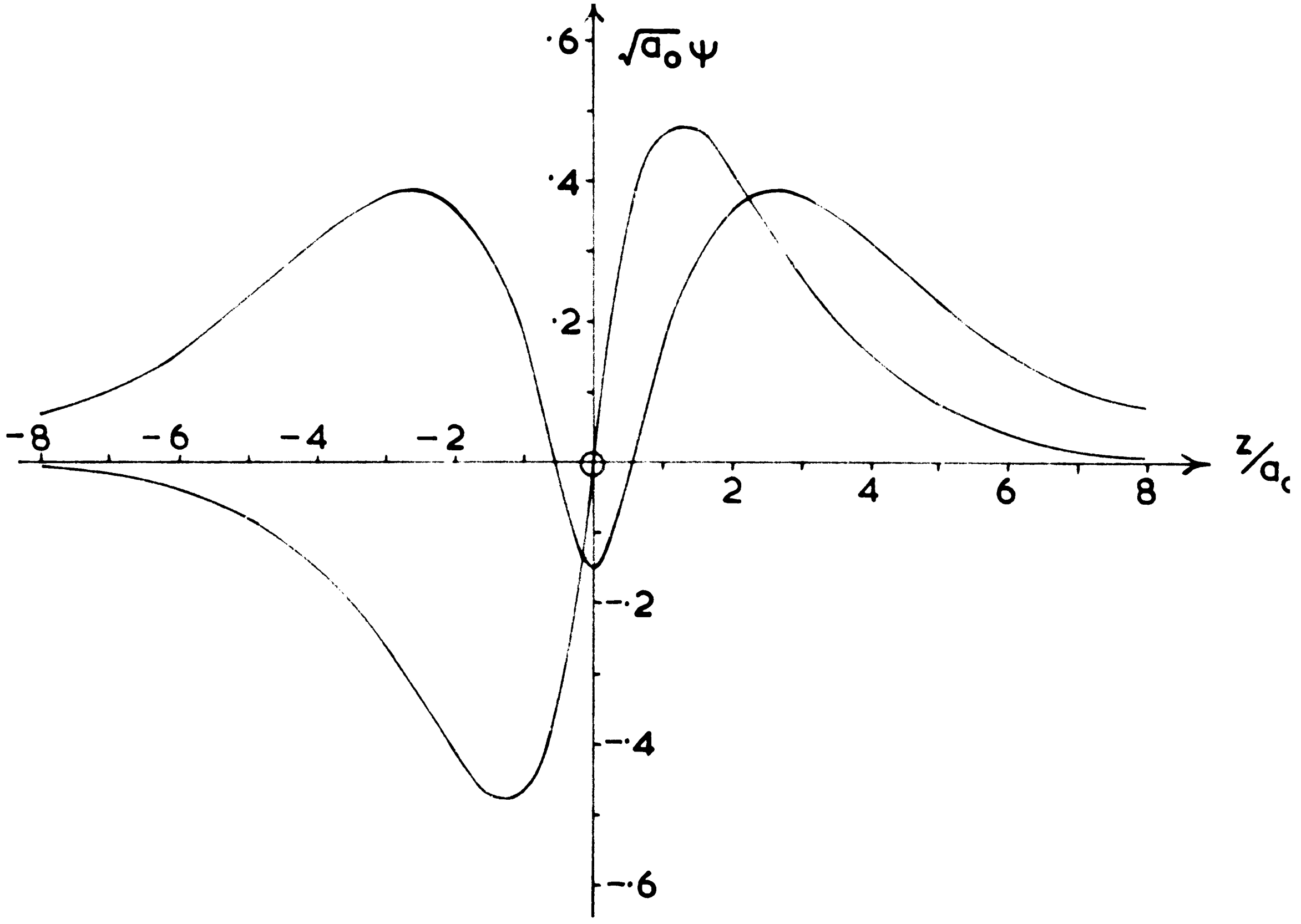


FIGURE 13

for which $\alpha \longrightarrow 1$ as $\frac{a}{a_0} \longrightarrow 0$, for the particular value $\frac{a}{a_0} = \cdot 1$. A rather large value of $\frac{a}{a_0}$ has been chosen so as to shew clearly the shape of the even wave-function in the region of the origin. The quantum defects for the odd and even states are .14 and .50 respectively.

We now wish to obtain the solution to the one-dimensional hydrogen atom problem by taking the limit $a \longrightarrow 0$. We observe that however small a value of a we may choose, it is still possible to find values of α such that (A4.15) and (A4.16) are satisfied, the required values of α tending to the positive integers as $a \longrightarrow 0$. Hence in the limit $a = 0$ there exist pairs of degenerate odd and even states having the Balmer energies, whose wave-functions for positive and negative z are given by the expressions (A4.8) and (A4.9) respectively, joined together at z = 0 to form a function of the correct parity. Figure 14 shews the pair of wave-functions having the Balmer energy corresponding to $\alpha = 1$. For positive z the wave-functions are superimposed. The two wave-functions in figure 13 transform continuously into those of figure 14 as $\frac{a}{a_0}$ changes from .1 to zero.

The final normalised expressions for the wave-functions are:

Odd states: $$\psi = \sqrt{\frac{2}{a_0^3 \alpha^5 (\lfloor \alpha)^2}}\, e^{-\frac{|z|}{\alpha a_0}}\, z\, L^1_\alpha\left(\frac{2|z|}{\alpha a_0}\right) \qquad (A4.22)$$

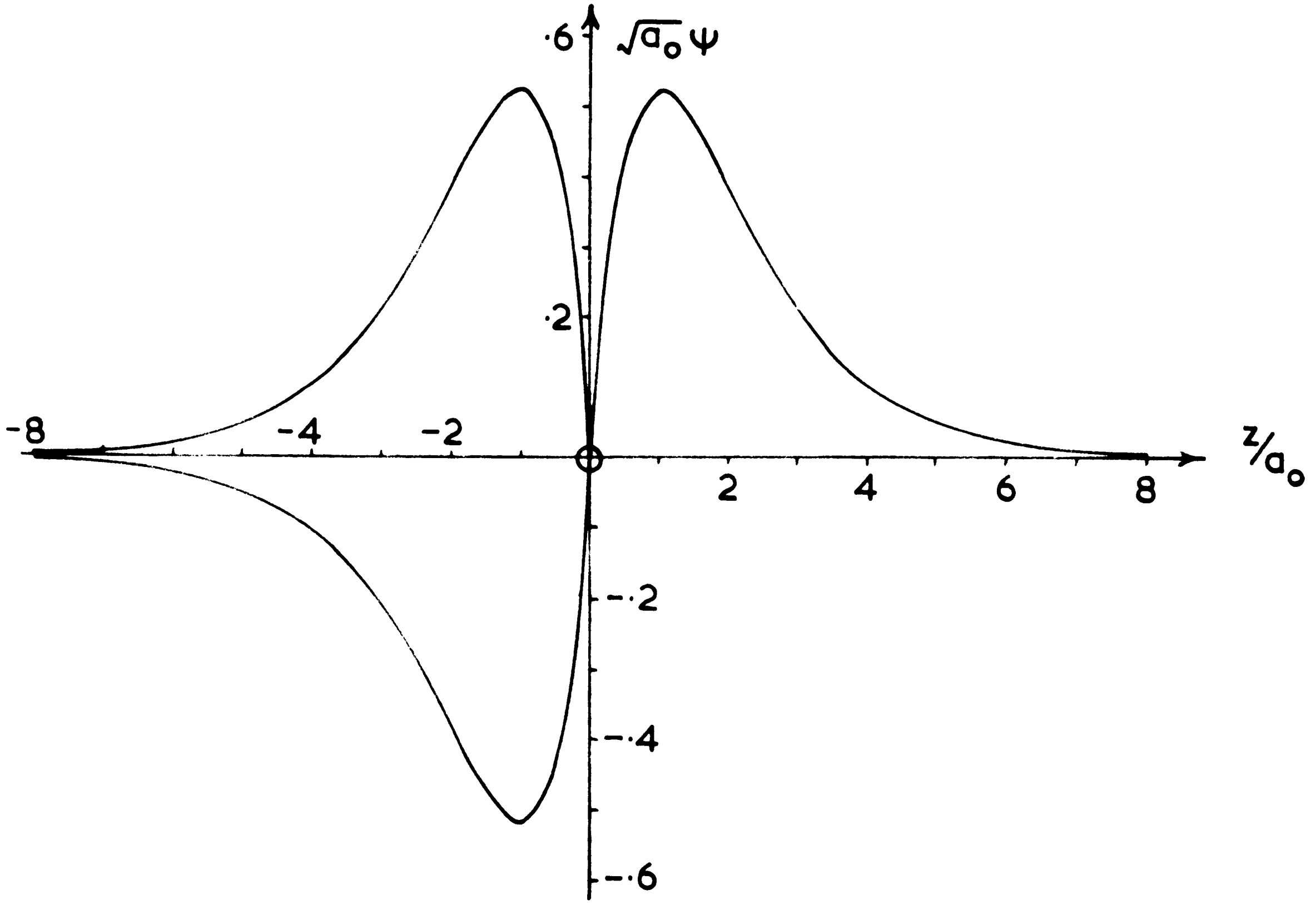


FIGURE 14

Even states: $$\psi = \sqrt{\frac{2}{a_0^3 \alpha^5 (\lfloor \alpha)^2}}\, e^{-\frac{|z|}{\alpha a_0}} |z| L_\alpha^1 \left(\frac{2|z|}{\alpha a_0}\right) \qquad (A4.23)$$

Remarks similar to the above apply also in the case of the ground state. As $a \longrightarrow 0$, $\alpha \longrightarrow 0$ so that in the limit $a = 0$ the ground state has infinite binding energy. This state was missed in our original solution of the wave-equation (A4.1). It is seen by inspection of (A4.5) that the ground state wave-function is $e^{-\frac{1}{i}x}$. The normalised ground state wave-function is therefore:

Ground state: $$\psi = \lim_{\alpha \to 0} \frac{1}{\sqrt{\alpha a_0}}\, e^{-\frac{|z|}{\alpha a_0}} \qquad (A4.24)$$

We note that $|\psi|^2 = \delta(z)$ so that the ground state wave-function is localised at the origin.

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