J. Phys. Chem. Solids, 1974, Vol. 35, pp. 1429–1431. Pergamon Press. Printed in Great Britain

SEMI-CONDUCTOR IMPURITY AND EXCITON LEVELS IN A MAGNETIC FIELD

K. M. ROUSSEL* and R. F. O'CONNELL

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, U.S.A.

(*Received* 15 *January* 1974; *in revised form* 29 *March* 1974)

Abstract—An accurate multiparameter variational calculation of impurity and exciton levels in a magnetic field is presented. Of particular interest are effects due to screening.

Previous investigations of excitons[1] and semiconductor impurity levels[2] in a magnetic field have been based primarily on the theory of an isolated hydrogen atom in a magnetic field (since in the effective mass approximation the Hamiltonian is similar to that of the hydrogen atom). Van Vleck[3] initially presented a solution for the hydrogen atom spectrum in a magnetic field. This was based on perturbation theory and was valid only for weak magnetic fields $\gamma \ll 1$, where

$$\gamma = B/k^2 B_0, \tag{1}$$

$$k = \mu_c/\mu_0\epsilon, \tag{2}$$

$$B_0 = \mu_0^2 ce^3/\hbar^3 = 2{\cdot}350 \times 10^9 \text{G}, \tag{3}$$

and μ_0, μ_c, and ϵ denote the isolated electron mass, effective electron mass and dielectric constant respectively. Solutions valid in the region of very strong fields ($\gamma \gg 1$) have been presented by numerous authors, notably Yafet, Keyes and Adams[4]. A recent variational calculation[5], valid for all values of the magnetic field, has been particularly successful in the difficult intermediate range of magnetic fields ($\gamma \approx 1$).

In the absence of a magnetic field, exciton theory has been based on the solution for the free hydrogen atom. However, recent experimental data on modulated reflectance[6], exciton photoluminescence[7] and photoconductivity[8] has suggested that a screened Coulomb potential (such as the Debye–Hückel potential) should be used instead of the simple Coulomb potential to describe the binding of the exciton. Various methods for the solution of the Schrödinger equation for the Debye–Hückel potential have been presented[9], in particular a simple multiparameter variational method has been given by the authors[10].

Due to the apparent success of the screened potential in describing the excitons for zero magnetic field, it is of interest to consider the effects of screening on the Coulomb potential in the presence of a magnetic field. Effects due to screening on the ground state have previously been studied by several authors, mainly for the region $\gamma \gg 1$. Most of these calculations have used simple variational functions. Fenton and Haering[11] used a variational function similar to that used by Yafet, Keyes and Adams[4] for the Coulomb potential. Jaskorzynska[12] extented a variational method presented by Wright[13], using linear combinations of his radial exponential trial wave function. Treating the entire potential as a perturbation to the free particle in a magnetic field, Ortenberg and Landwehr[14] used the known solution for a free particle in a magnetic field, with an implied parameter, as a variational function. In a nonvariational calculation, an adiabatic approximation, valid only for $\gamma \gg 1$, was used by D'Yakonov, Mitchell and Efros[15] to reduce Schrödinger's equation to a one dimensional equation. The solution of this reduced equation in particular regimes of the screening length were then found for the very strong magnetic fields.

We present here an accurate multiparameter variational method for the ground state *and excited states* which is valid for *all* values of the magnetic field and screening length. The two limiting cases of this method have previously been presented—a screened Coulomb potential in the absence of a magnetic field[10] and the Coulomb potential in a magnetic field in the absence of screening[5].

To be definitive, let us consider initially the

*In partial fulfillment of the requirement for a Ph.D. Degree.

energy levels of a semi-conductor impurity. In the effective mass approximation, the Hamiltonian for an impurity bound by the Debye–Hückel potential (with $Z = 1$) in a magnetic field may be written as

$$H = P^2 - \frac{2}{r} e^{-r/D} + \gamma L_z + \frac{1}{4}\gamma^2 r^2 \sin^2\theta, \qquad (4)$$

where the unit of length is $a_0/k \equiv a_\epsilon$ (a_0 is the Bohr radius) and the unit of energy is $Ry^* = (k/\epsilon)Ry$, L_z denotes the z-component of angular momentum and D is the screening length. For a non-degenerate gas of electrons at temperature T, with an equal number of neutralizing positively charged particles

$$D = \left\{\frac{4\pi e^2}{\epsilon k_B T}\sum_i Z_i^2 \rho_i\right\}^{-1/2}, \qquad (5)$$

where ρ_i is the number of density of particles of type i with atomic number Z_i. Since only inversion and rotations about the z axis leave the Hamiltonian invariant, the only "good" quantum numbers are the eigenvalues of parity and L_z, which we denote by $\pm$ and m, respectively. Labelling our trial function with these two quantum numbers, its general form is

$$\psi_m^{(\pm)}(r) = \sum_l \sum_{k=1}^{n_{max}} A_{lk} r^k \exp(-\alpha_l r) Y_{lm}(\theta, \phi), \qquad (6)$$

where n_{max} is determined in a manner similar to that for the zero field case[10], α_l are chosen input parameters, and A_{lk} are parameters evaluated numerically in the course of diagonalization of the Hamiltonian. States with even parity are obtained by a summation on l in (6) over even integers, whereas odd parity states are obtained by a summation on l over odd integers. Figure 1 gives the ionization energy as a function of screening length D for various values of γ. A comparison of our results for the ionization energies with estimates from previous calculations indicate that our ionization energies are larger (i.e. closer to the "exact" values, since the variational energy is an upper limit to the true energy) than those of the best previous calculation[14] by about 4% for $\gamma = 10$ and 1·5% for $\gamma = 50$. The binding energies of the first 5 excited states are shown in Fig. 2 and have been labelled with their good quantum numbers, m and parity respectively. One could attempt to label these states with quantum numbers appropriate in the two limiting cases of the Hamiltonian; that is, either by the quantum numbers of the Landau level structure for the case where there is no screened Coulomb potential term or by the quantum numbers of the hydrogen atom for the case of no magnetic field. Since our wavefunction is hydrogen-like we have chosen the latter alternative. For example, for $\gamma = 10$ the most strongly bound state $(-1, -)$ may thus be labelled $2p_{-1}$ for it is an

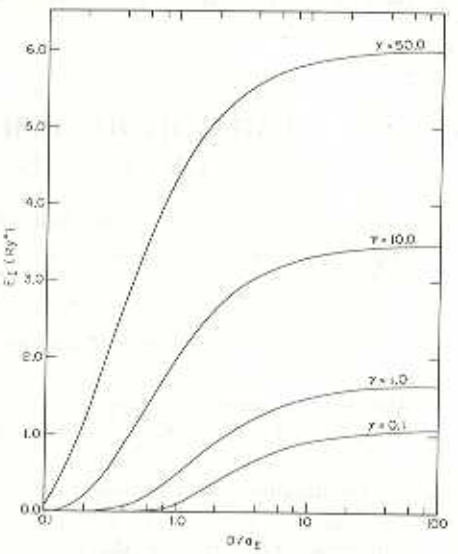

Fig. 1. Ionization energies (in effective Rydbergs) vs screening length (in effective Bohr radii) for various values of the magnetic parameter γ.

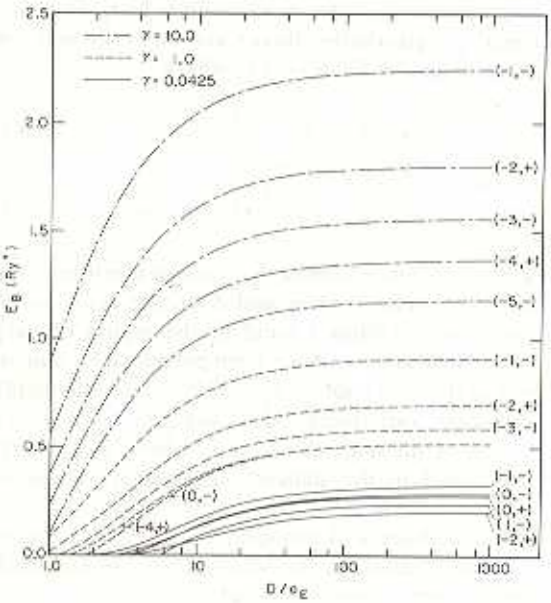

Fig. 2. The binding energies of the five lowest excited states (in effective Rydbergs) vs screening length (in effective Bohr radii) for various values of the magnetic parameter γ. The states are labelled with their quantum numbers of m and parity.

odd-parity state with $m = -1$ and as $B \to 0$ it also has $n = 2$ and $l = 1$. Following this convention, the excited states in Fig. 2 from top to bottom may thus be labelled; for $\gamma = 10$, $2p_{-1}$, $3d_{-2}$, $4f_{-3}$, $5g_{-4}$, $6h_{-5}$; for $\gamma = 1$, $2p_{-1}$, $3d_{-2}$, $4f_{-3}$, $5g_{-4}$, $2p_0$; and for $\gamma = 0{\cdot}0425$, $2p_{-1}$, $2p_0$, $2s_0$, $2p_1$, $3d_{-2}$.

The solution of the exciton problem is identical with the above solution in the case where the mass of the hole is infinite. In general, if μ_e denotes the effective mass of the electron, as before, and if μ_h denotes the effective mass of the hole, then the generalization of equation (4) to the case of the exciton is,

$$H = P^2 - \frac{2}{r}e^{-\mu r D} + \left(\frac{\mu_h - \mu_e}{\mu_h}\right)\gamma L_z + \left(\frac{\mu_h + \mu_e}{\mu_h}\right)\frac{1}{4}\gamma^2 r^2 \sin^2\theta. \quad (7)$$

We see that when μ_h is infinite, equation (7) is the same as equation (4) and the solution to the exciton problem is identical to that of the impurity level problem. In the case where $\mu_e = \mu_h$, the solution to the exciton is identical to that of the impurity problem in the case where $m = 0$ and $B \to (B/\sqrt{2})$. In the more general case, the calculation is similar to that outlined above.

A possible generalization of the above would be to consider an anisotropic screening potential[16] or the possible effect of screening on the central cell correction[17].

REFERENCES

1. Elliott R. J. and Loudon R., *J. Phys. Chem. Solids* **15**, 196 (1960); Fritsche L., *Phys. Status Solidi* **34**, 195 (1969).
2. Keyes R. W. and Sladek R. J., *J. Phys. Chem. Solids* **1**, 143 (1956).
3. Van Vleck J. H., *The Theory of Electric and Magnetic Susceptibilities*, p. 178. Oxford University Press, London.
4. Yafet Y., Keyes R. W. and Adams E. N., *J. Phys. Chem. Solids* **1**, 137 (1956).
5. Smith E. R., Henry R. J. W., Surmelian G. I., O'Connell R. F. and Rajagopal A. K., *Phys Rev.* **D6**, 3700 (1972).
6. Albers, Jr. W. A., *Phys. Rev. Lett.* **23**, 410 (1969).
7. Bleil C. E., Albers, Jr. W. A. and Wang E. Y., *J. Luminescence* **1, 2**, 265 (1970).
8. Albers, Jr. W. A., Bleil C. E. and Wang E. Y., In *Proc. 3rd Photoconductivity Conf.* (Edited by E. M. Pell), (1969).
9. See, for example, Rogers F. J., Graboske, Jr. H. C. and Harwood D. J., *Phys. Rev.* **A1**, 1577 (1970); and references therein.
10. Roussel K. M. and O'Connell R. F., *Phys. Rev.* **A9**, 52 (1974).
11. Fenton E. W. and Haering R. R., *Phys. Rev.* **159**, 593 (1967).
12. Jaskorzynska B., *Solid State Comm.* **11**, 1265 (1972).
13. Wright G. B., *Proc. int. Conf. of Luminescence, Budapest*, p. 1514 (1966).
14. Ortenberg M. V. and Landwehr G., *Phys. Stat. Sol.* **37**, K69 (1970).
15. D'yakonov M. I., Mitchell D. L. and Efros A. L., *Soviet Phys. Solid State* **10**, 2021 (1969).
16. Horing N. J. *Ann. Phys.* **54**, 405 (1969).
17. Fetterman H. R., Larsen D. M., Stillman G. E., Tannerward P. E. and Waldman J., *Phys. Rev. Lett.* **26**, 975 (1971).