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Strong-perturbation theory for a surface hydrogen-like impurity in a magnetic field of arbitrary strength

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Abstract. The strong-perturbation theory is employed to calculate the energy levels of a hydrogen-like system at the surface in a constant magnetic field of arbitrary strength. The applied magnetic field is taken to be normal to the boundary surface. Using the parabolic coordinate system, we obtain the analytic expression of levels depending on the parameter η which represents the magnetic field strength. The numerical results are given.

1. Introduction

The problem of the energy levels of a hydrogen-like system in a constant magnetic field has been a topic of interest for many years. It has become of increasing relevance in astrophysics; it is also of interest in semiconductor physics where typical values of the effective mass m^* and dielectric constant ϵ make the effective Rydberg constant R^* about 10^4 times smaller than for the free hydrogen atom. In particular, the magneto-absorption of semiconductors has received great attention because it can provide important information about the electronic band structure of these materials. This problem has been investigated by numerous workers. In the high-field limit the adiabatic approximation has been found appropriate (Boyle and Howard 1961, Elliott and Loudon 1960, Simola and Virtamo 1978, Friedrich 1982, Hasegawa and Howard 1961, Wunner *et al* 1981, Rösner *et al* 1981). Other researchers have favoured the use of the variational method and the perturbation theory (Yafet *et al* 1956, Calib *et al* 1971, Cohen and Herman 1981, Ruder *et al* 1981, Aldrich and Greene 1979, Hylton and Rau 1980, Praddaude 1972, Makado 1985, Makado and McGill 1986).

Recently, a strong-perturbation theory has been proposed by Jiang (1987). This method has been shown to be effective for any strength of perturbation. We use this method to study the ground state of a hydrogen-like atom at the surface of semi-infinite crystal in a uniform magnetic field of arbitrary strength. We obtain an analytic expression and numerical results.

2. Theory and results

Consider a semi-infinite isotropic crystal occupying the $z \geq 0$ half-space and with a surface coincident with the xy plane. Let a donor impurity be at the origin with an extra positive charge in the nucleus. An extra electron is at an arbitrary point \mathbf{r} in the $z \geq 0$ half-space. Let this system be placed in a constant magnetic field of arbitrary strength. In the isotropic effective-mass approximation the Hamiltonian for the hydrogen atom located at the surface of a semi-infinite crystal in the presence of a constant magnetic field is

$$H = (1/2m^*)[\mathbf{p} + (e/c)\mathbf{A}]^2 - e^2/\epsilon r \quad z \geq 0 \quad (1)$$

where \mathbf{A} is the vector potential, $-e$ and m^* are the electronic charge and effective mass respectively, and ϵ is the isotropic static dielectric constant inside the isotropic crystal. We assume that the potential function is infinite for $z < 0$. If we choose as usual the cylindrical gauge,

$$\mathbf{A} = \frac{1}{2}(\mathbf{B} \times \mathbf{r}) \quad (2)$$

where \mathbf{B} is the applied magnetic field, and using a cylindrical coordinate system (ρ, φ, z) where the magnetic field is applied along the z direction, the Hamiltonian can be expressed as

$$H = -\nabla^2 - 2/r - i\eta\partial/\partial\varphi + \frac{1}{4}\eta^2\rho^2. \quad (3)$$

Here we have used the effective Bohr radius $a^* = a_0\epsilon m_0/m^*$ as our unit of length and the effective Rydberg constant $R^* = R_0 m^*/m_0\epsilon^2$ as our unit of energy, where m_0 is the free-electron mass, and R_0 and a_0 are the hydrogen Rydberg constant and the Bohr radius, respectively. For a typical semiconductor such as GaAs ($\epsilon = 12.5$; $m^* = 0.067m_0$), we have $a^* = 98.7 \text{ \AA}$ and $R^* = 5.83 \text{ meV}$. η is a dimensionless parameter which is a measure of magnetic field:

$$\eta = \hbar\omega_c/2R^* \quad (4)$$

where $\omega_c = Be/m^*c$ is the cyclotron frequency of a free carrier in the field B . We can rewrite the Hamiltonian as

$$H = H_1 + V' \quad (5)$$

where

$$H_1 = -\nabla^2 - 2/r - i\eta\partial/\partial\varphi, \quad (6)$$

$$V' = \eta^2\rho^2/4 \quad (7)$$

and $r = (\rho^2 + z^2)^{1/2}$, $\rho = (x^2 + y^2)^{1/2}$, ρ being the distance in the xy plane.

The Schrödinger equation of the system is

$$H\psi = E\psi. \quad (8)$$

We shall use the strong-perturbation theory proposed by Jiang (1987) to solve the Schrödinger equation. Because H_1 commutes with $H_0 = -\nabla^2 - 2/r$, i.e. $[H_1, H_0] = 0$, they have simultaneous functions. For the hydrogen-like atom at the surface of a semi-infinite crystal, their simultaneous function is

$$\phi^0 = \phi_{nlm}(r, \theta, \varphi) \quad l + m = \text{odd} \quad (9)$$

and is called the Levine (1965) wavefunction.

We introduce a factor

$$f = \exp(-g) \tag{10}$$

into the wavefunction and assume that

$$\psi = Nf\phi^0, \tag{11}$$

where N is a normalisation constant. Substituting equation (11) into (8), we obtain

$$H\psi = Nf[(H_1 + \eta)\phi^0 + \phi^0(V' - |\nabla g|^2 + \nabla^2 g - \eta) + 2\nabla g \cdot \nabla \phi^0]. \tag{12}$$

We chose g in such way that

$$|\nabla g|^2 - \nabla^2 g = V' - \eta = \frac{1}{4}\eta^2\rho^2 - \eta. \tag{13}$$

Then, from equations (9)–(12), we have

$$f\tilde{H}\phi^0 = Ef\phi^0 \tag{14}$$

where

$$\tilde{H} = H_1 + \eta + H' \tag{15}$$

and

$$H_1^0 = H_1 + \eta = -\nabla^2 - 2/r + \eta - i\eta \partial/\partial\varphi \tag{16}$$

$$H' = 2\nabla g \cdot \nabla. \tag{17}$$

We can use equation (14) to solve the energy E . Note that H_1^0 and H' only operate on ϕ^0 ; the function g can be solved from equation (13) with the initial conditions

$$V' = 0 \quad g = 0 \quad \nabla g = \mathbf{0}. \tag{18}$$

Equation (18) is deduced from the condition that $H\psi = fH_1^0\phi^0$ when $V' = 0$ ($\eta = 0$). The wavefunction ψ already includes the term $f = \exp(-g)$ which connects it to V' through equation (13); after this transformation, the perturbation theory is applicable even if the perturbation is very large.

In the non-degenerate case, we have

$$E_{nlm}^{(0)} = \int \phi^{0*} H_1^0 \phi^0 \, d\tau \tag{19}$$

$$E_{nlm}^{(1)} = N^2 \int |f|^2 \phi^{0*} H' \phi^0 \, d\tau \tag{20}$$

$$N^{-2} = \int |f|^2 |\phi^0|^2 \, d\tau \tag{21}$$

where $E_{nlm}^{(0)}$ is the zeroth-order energy and $E_{nlm}^{(1)}$ is the first-order perturbation energy. Combining equation (13) with the initial conditions $\eta = 0$, $g = 0$ and $\nabla g = \mathbf{0}$, we have $g = \eta\rho^2/4$ and

$$f = \exp(-\eta\rho^2/4). \tag{22}$$

The wavefunction ψ and H' are given by

$$\psi = N \exp(-\eta\rho^2/4) \phi^0 \tag{23}$$

and

$$H' = 2\nabla g \cdot \nabla = \eta\rho \partial/\partial\rho. \quad (24)$$

From equations (19) and (16), we can obtain

$$E_{nlm}^{(0)} = \langle \phi_{nlm} | H_1^0 | \phi_{nlm} \rangle = -1/n^2 + \eta + m\eta. \quad (25)$$

We discuss the results for only the ground state here. For the ground state,

$$\phi_{210} = (1/32\pi)^{1/2} r \cos \theta \exp(-r/2) \quad (26)$$

$$\psi_{210} = N \exp(-\eta\rho^2/4 - r/2)(1/32\pi)^{1/2} r \cos \theta \quad (27)$$

$$N^{-2} = \frac{1}{16} \int_0^\infty \int_0^{\pi/2} \exp\left(-\frac{\eta\rho^2}{2} - r\right) r^4 (\sin \theta - \sin^3 \theta) dr d\theta. \quad (28)$$

To perform the integration, we change to the parabolic coordinates α_1 and α_2 ; let

$$\alpha_1 = r + z = (1 + \cos \theta)r \quad (29a)$$

$$\alpha_2 = r - z = (1 - \cos \theta)r \quad (29b)$$

and we have

$$d\alpha_1 d\alpha_2 = 2r \sin \theta dr d\theta \quad (30)$$

$$\alpha_1 \alpha_2 = r^2 \sin^2 \theta \quad (31)$$

$$(\alpha_1 + \alpha_2)/2 = r. \quad (32)$$

Substituting (29)–(31) into (28), we obtain

$$N^{-2} = \frac{1}{64} \int_0^\infty \int_0^\infty \exp\left(-\frac{\eta}{2} \alpha_1 \alpha_2 - \frac{\alpha_1 + \alpha_2}{2}\right) \times \left[\left(\frac{\alpha_1 + \alpha_2}{2}\right)^3 - \alpha_1 \alpha_2 \frac{\alpha_1 + \alpha_2}{2} \right] d\alpha_1 d\alpha_2. \quad (33)$$

Using (24) and (26), we obtain

$$H' \phi_{210} = -\frac{1}{2}(1/32\pi)^{1/2} \eta(\rho^2/r)z \exp(-r/2). \quad (34)$$

Substituting (22), (26), (33) and (34) into (20), we find that

$$E_{210}^{(1)} = -\frac{N^2}{64} \eta \int_0^\infty \int_0^\infty \exp\left(-\frac{\eta}{2} \alpha_1 \alpha_2 - \frac{\alpha_1 + \alpha_2}{2}\right) \times \left[\left(\frac{\alpha_1 + \alpha_2}{2}\right)^2 \alpha_1 \alpha_2 - (\alpha_1 \alpha_2)^2 \right] d\alpha_1 d\alpha_2. \quad (35)$$

If we let

$$X(\eta, \tau) = \int_0^\infty \int_0^\infty \exp\left(-\frac{\eta}{2} \alpha_1 \alpha_2 - \frac{\tau}{2}(\alpha_1 + \alpha_2)\right) d\alpha_1 d\alpha_2 \\ = \frac{2}{\eta} \exp\left(\frac{\tau^1}{2\eta}\right) E_1\left(\frac{\tau^2}{2\eta}\right) \quad (36)$$

Table 1. Energies of the hydrogen-like atom at the surface of a semi-infinite crystal in a uniform magnetic field.

η	N^{-2}	$E_{210}^{(1)}$	$E_{210}^{(0)} = -\frac{1}{4} + \eta$	$E^0 = E_{210}^{(0)} + E_{210}^{(1)}$
0.05	0.3395	-0.13617	-0.20	-0.336
0.1	0.6510	-0.02884	-0.15	-0.179
0.2	0.4963	-0.02647	-0.05	-0.076
0.3	0.4045	-0.02227	0.05	0.028
0.4	0.3428	-0.01863	0.15	0.131
0.5	0.2982	-0.01573	0.25	0.234
0.7	0.2375	-0.01160	0.45	0.438
0.9	0.1978	-0.00891	0.65	0.641
1.0	0.1827	-0.00791	0.75	0.742
1.5	0.1325	-0.00479	1.25	1.245
2.0	0.1042	-0.00323	1.75	1.747
3.0	0.7320	-0.00177	2.75	2.748
4.0	0.5648	-0.00172	3.75	3.748
5.0	0.4601	-0.00078	4.75	4.749
10.0	0.2391	-0.00023	9.75	9.750
20.0	0.1221	-0.00007	19.75	19.750
30.0	0.8203	-0.00003	29.75	29.750
40.0	0.6176	-0.00002	39.75	39.750
50.0	0.4952	-0.00001	49.75	49.750
100.0	0.2488	-0.00001	99.75	99.750

where

$$E_1(\theta) = \int_0^\infty \frac{\exp(-t)}{t} dt = -\gamma - \ln \theta - \sum_{n=1}^\infty \frac{(-1)^n \theta^n}{nn!} \tag{37}$$

$$\gamma = 0.5772157 \tag{38}$$

then we obtain

$$N^{-2} = -[\frac{1}{84} f_3(\eta) + \frac{1}{32} df_1(\eta)/d\eta] \tag{39}$$

$$E^{(1)} = -N^2 \frac{1}{128} \eta [-2df_2(\eta)/d\eta - 4d^2f_0(\eta)/d\eta^2], \tag{40}$$

where

$$f_0(\eta) = X(\eta, \tau)|_{\tau=1} = (2/\eta) \exp(1/2\eta) E_1(1/2\eta) \tag{41}$$

$$f_1(\eta) = (\partial X/\partial \eta)|_{\tau=1} = (2/\eta^2) \exp(1/2\eta) E_1(1/2\eta) - 4/\eta \tag{42}$$

$$f_2(\eta) = (\partial^2 X/\partial \tau^2)|_{\tau=1} = 2(1/\eta + 1/\eta^2) \exp(1/2\eta) E_1(1/2\eta) + 4(1 - 1/\eta) \tag{43}$$

$$f_3(\eta) = (\partial^3 X/\partial \tau^3)|_{\tau=1} = (2/\eta) \exp(1/2\eta) (3/\eta + 1/\eta^2) E_1(1/2\eta) - 4(1/\eta^3 + 1/\eta^2 + 2/\eta) \tag{44}$$

$$N^{-2} = -\frac{1}{32} [(1/\eta^3) \exp(1/2\eta) E_1(1/2\eta) - 2/\eta + 4/\eta] \tag{45}$$

$$E_{210}^{(1)} = N^2 \frac{1}{84} [(-3/\eta + 4/\eta^2 + 8/\eta^3 + 1/\eta^4) \exp(1/2\eta) E_1(1/2\eta) + 6/\eta - 10/\eta^2 - 2/\eta^3]. \tag{46}$$

In table 1, we list the results of our calculation. The ground-state energies of a

hydrogen-like system at the surface of semi-infinite semiconductor in a constant magnetic field of arbitrary strength are obtained for the first time. Here we used a very simple calculation, only to the first order of energy; nevertheless the results are very reasonable. For example, table 1 indicates that, for $\eta > 10$, namely at very high fields, the binding effect of the magnetic field in the xy plane is so large that the energy of the system is determined by the Landau energy nearly totally.

References

- Aldrich C and Greene R L 1979 *Phys. Status Solidi* **93** 343
Boyle W S and Howard R E 1961 *J. Phys. Chem. Solids* **19** 181
Calib D, Fabri E and Fiori G 1971 *Solid State Commun.* **9** 1517
Cohen M and Herman G 1981 *J. Phys. B: At. Mol. Phys.* **14** 2761
Elliott R J and Loudon R 1960 *J. Phys. Chem. Solids* **15** 196
Friedrich H 1982 *Phys. Rev. A* **26** 1827
Hasegawa H and Howard R E 1961 *J. Phys. Chem. Solids* **21** 179
Hylton O J and Rau A R P 1980 *Phys. Rev. A* **22** 321
Jiang H X 1987 *Phys. Rev. B* **35** 9287
Levine J D 1965 *Phys. Rev.* **140** A586
Makado P C 1985 *Physica B* **132** 7
Makado P C and McGill N C 1986 *J. Phys. C: Solid State Phys.* **19** 873
Praddaude H C 1972 *Phys. Rev. A* **6** 1321
Rösner W, Wunner G, Herold H and Reinecke M 1984 *J. Phys. B: At. Mol. Phys.* **17** 29
Ruder H, Wunner G, Herold H and Reinecke M 1981 *J. Phys. B: At. Mol. Phys.* **14** L45
Simola J and Virtamo J 1978 *J. Phys. B: At. Mol. Phys.* **11** 3309
Wunner C, Ruder H and Herold H 1981 *Phys. Lett.* **85A** 430
Yafet Y, Keyer R W and Adams E N 1956 *J. Phys. Chem. Solids* **1** 137