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Two-dimensional neutral donors in electric fields

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Abstract

We present numerical data for energies and widths of energy levels of a two-dimensional neutral donor in an electric field. The problem, formally coinciding with that of a two-dimensional hydrogen atom, is solved by a two-dimensional finite-difference method. The data are obtained for a broad range of electric field strengths and are an essential supplement and refinement to existing theoretical investigations, carried out for weak fields.

The properties of both neutral and charged donors in narrow quantum wells are a subject of a large amount of both theoretical and experimental investigation [1–8]. In very narrow wells a neutral donor can be considered as a two-dimensional counterpart of the hydrogen atom. Frequently used compounds for current experimental investigations (see for example [7, 8]) of such systems are layers of GaAs/AlGaAs. The high mobility, i.e. small effective mass, of the electrons and the comparatively large dielectricity constant of this and many other semiconductor materials facilitate study of strong electric field effects in the laboratory.

The simplest theoretical problem in this context is that of the Stark effect and the corresponding broadening of the spectral lines for the two-dimensional hydrogen atom. These effects can be directly observable in optical spectra of semiconductors and also can affect other physical properties of thin films. There are several works in the literature directly addressing this problem [1–4, 9, 10], but, nevertheless, there are no numerical data for a broad range of the electric field strengths published. The goal of this communication consists in filling this gap.

The Schrödinger equation for an electron confined in the plane (x, y) and moving in the field of a Coulomb centre and a constant uniform electric field F pointing along the x direction is given by

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-\frac{1}{r}-Fx\right]\psi = E\psi \tag{1}$$

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Table 1. Energies and half-widths of the ground state level of a neutral donor in two dimensions. (Effective atomic units.)

F	E_0	E_0 [1]	$\Gamma/2$	$\Gamma/2$ [1]
0.0	−2.000 00	−2.000 00		
0.2	−2.003 31	−2.003 28	6.639(−11)	7.4879(−11)
0.3	−2.007 55	−2.007 38	3.679(−7)	4.4331(−7)
0.4	−2.013 81	−2.013 13	2.5233(−5)	3.2692(−5)
0.5	−2.022 45	−2.020 51	2.9888(−4)	4.2082(−4)
0.6	−2.033 78	−2.029 53	1.4696(−3)	2.2729(−3)
0.7	−2.047 63	−2.040 20	4.3871(−3)	7.4921(−3)
0.8	−2.063 39	−2.052 50	9.6579(−3)	1.8164(−2)
1.0	−2.097 76	−2.082 03	2.7792(−2)	6.1634(−2)
1.2	−2.132 59	−2.118 13	5.4838(−2)	1.3686(−1)
1.5	−2.181 63	−2.184 57	1.07587(−1)	2.9775(−1)
2.0	−2.251 39	−2.328 12	2.15454(−1)	6.2723(−1)
3.0	−2.352 24	−2.738 28	4.65656(−1)	1.2457
4.0	−2.417 43	−3.312 50	7.3311(−1)	1.6826
5.0	−2.459 21	−4.050 78	1.0057	1.9648
7.0	−2.497 97	−6.019 53	1.55077	2.2523
10.0	−2.489 55	−10.20 31	2.35289	2.3683

where $r = (x^2 + y^2)^{1/2}$. We use here effective atomic units. The units of energy, length, field strength, and time are $\mu\kappa^{-2}$ (27.2) eV, $\kappa\mu^{-1}$ (5.29×10^{-9}) cm, $\mu^2\kappa^{-3}$ (5.14×10^9) V cm^{-1}, and $\kappa^2\mu^{-1}$ (2.42×10^{-17}) s, where μ is the effective mass of the electron in m_0 units, κ is the dielectric constant, and e is the charge of the electron. The positions E_0 and half-widths $\Gamma/2$ of resonances can be obtained from the complex eigenvalues of the energy $E = E_0 - i\Gamma/2$. These eigenvalues have to correspond to solutions of equation (1) having the asymptotic behaviour of an outgoing wave. The value $1/\Gamma$ gives the average lifetime of corresponding quasi-steady states.

Analytical solutions of equation (1) for the case $F = 0$ are presented in detail in [1, 11]. We recall here that in this case the energy levels form a 2D Coulomb series with energies

$$E_n = -\frac{1}{2(n - 1/2)^2} \tag{2}$$

where $n = 1, 2, 3, \ldots$. The nth level is $2n - 1$ times degenerate. At $F \neq 0$ the corresponding multiplets contain n states of positive parity with respect to the x axis and $n-1$ states of negative parity. In the notation of states we follow [1]. This notation is derived from a representation of equation (1) in terms of parabolic coordinates. It includes two parabolic quantum numbers n_1 and n_2 and an additional quantum number, which was introduced in [1] as m_{3D}. When following this notation, the states of the $n = 2$ triplet get indices $(n_1, n_2, m_{3D}) = (0, 0, \frac{1}{2})$ for the state with the negative parity with respect to the x axis, and $(1, 0, -\frac{1}{2})$ and $(0, 1, -\frac{1}{2})$ for the two other states of positive parity.

We solved equation (1) numerically in Cartesian coordinates. The method is described in detail both for bound states [12] and for quasi-stationary states in external electric fields [13–16]. In particular, our numerical method allowed us to get a solution for the problem concerning the number of bound states of a 2D negative donor in magnetic fields [17]. The applications to electric fields include the first calculation of energies and half-widths of levels of the H_2^+ molecular ion [13] and detailed calculations for the hydrogen atom in parallel electric and magnetic fields [15]. In [13–15] we have developed three different approaches for calculations of wavefunctions with the asymptotics of an outgoing wave. All these approaches

Table 2. Energies and half-widths of the levels for the triplet of lowest excited states of a neutral donor in two dimensions. (Effective atomic units.)

	$(0, 1, -\frac{1}{2})$			$(0, 0, \frac{1}{2})$			$(1, 0, -\frac{1}{2})$		
F	E_0	$\Gamma/2$	$\Gamma/2$ [1]	E_0	$\Gamma/2$	$\Gamma/2$ [1]	E_0	$\Gamma/2$	$\Gamma/2$ [1]
0.000	−0.222 222			−0.222 222			−0.222 222		
0.004	−0.231 491	4.0(−18)	4.5(−18)	−0.222 502	2.0(−19)	3.0(−19)	−0.213 473		
0.005	−0.233 903	3.81(−14)	5.0(−14)	−0.222 662	3.288 2(−15)	4.2(−15)	−0.211 366		
0.006	−0.236 354	1.646(−11)	2.3(−11)	−0.222 858	1.715(−12)	2.3(−12)	−0.209 287		
0.007	−0.238 848	1.160 0(−9)	1.7(−9)	−0.223 092	1.420 3(−10)	2.0(−10)	−0.207 243	5.0(−12)	1.2(−11)
0.008	−0.241 388	2.646 7(−8)	4.2(−8)	−0.223 366	3.737 3(−9)	5.7(−9)	−0.205 225	1.8(−10)	3.9(−10)
0.009	−0.243 979	2.859 3(−7)	4.9(−7)	−0.223 682	4.589 7(−8)	7.4(−8)	−0.203 238	3.8(−9)	5.7(−9)
0.010	−0.246 627	1.832 5(−6)	3.4(−6)	−0.224 042	3.309 9(−7)	5.7(−7)	−0.201 282	3.1(−8)	4.8(−8)
0.012	−0.252 129	2.648 1(−5)	5.7(−5)	−0.224 910	5.940 7(−6)	1.2(−5)	−0.197 467	6.9(−7)	1.2(−6)
0.015	−0.260 996	3.016 7(−4)	8.8(−4)	−0.226 658	9.097 4(−5)	2.2(−4)	−0.192 009	1.141(−5)	2.8(−5)
0.02	−0.276 971	2.325 8(−3)	1.2(−2)	−0.230 780	1.018 8(−3)	3.9(−3)	−0.183 705	2.431(−4)	6.6(−4)
0.03	−0.308 627	1.214 3(−2)	0.11	−0.240 498	7.356 6(−3)	5.7(−2)	−0.169 235	2.8670(−3)	1.5(−2)
0.04	−0.337 521	2.597 6(−2)	0.29	−0.249 060	1.766 4(−2)	0.19	−0.155 216	8.3494(−3)	6.5(−2)
0.05	−0.363 930	4.154 8(−2)	0.44	−0.256 011	2.988 8(−2)	0.37	−0.140 601	1.5422(−2)	0.16
0.07	−0.411 388	7.480 4(−2)		−0.266 171	5.684 2(−2)		−0.109 536	3.1479(−2)	
0.10	−0.473 878	0.126 235		−0.275 297	9.940 8(−2)				
0.15	−0.564 660	0.211 850		−0.281 407	0.170 84				
0.20	−0.645 63	0.296 148		−0.281 225	0.240 93				
0.30	−0.790 53	0.461 52		−0.271 104	0.375 90				

are applicable for a one-centre problem, which we consider here. Most of the results presented below are obtained by means of smooth exterior complex scaling [15].

A specific feature of the present 2D calculations is their slower convergence comparing with calculations for 3D systems [13–15]. This requires one to perform all the calculations on denser grids. Nevertheless, our method allows obtaining precise results with a reliable estimation of numerical errors. These errors do not exceed 1–2 units of the last decimal digit of the results presented in tables 1 and 2. (In these tables the powers of ten for $\Gamma/2$ are given in brackets.) Many of results had higher precision and were truncated for presentation reasons.

Our numerical results in tables 1 and 2 can be compared with those of Tanaka *et al* [1]. The work of Tanaka *et al* provides formulae for the real and imaginary parts of the energy of the ground and lowest excited states obtained for weak electric fields by means of Rayleigh–Schrödinger perturbation theory. For the real part of the energy they present terms linear and quadratic with respect to the field strength. More complicated are the formulae for the imaginary part of the energy. The numerical values obtained from these formulae, which are the leading terms of asymptotic series for $\Gamma/2$, are also presented in our tables. One can see that these approximate $\Gamma/2$ values are larger than the results of our numerical calculations. This difference exists for all the field strengths. Its minimal values are about 20–30% for the ground state at low field strengths. Nearly the same level of overestimation is observable when comparing the calculations for the 3D hydrogen atom of [18] (leading terms of asymptotic series) with the more precise results of the same work [18] and [15, 19–21]. The calculations of [18] were carried out by the same method and were a basis for the investigation of [1]. Thus, we can state that the analytical estimations [1] give precise results in rather narrow ranges of weak fields and are crude approximations for those lifetimes and resonance widths which have prospects for experimental investigation.

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