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Ts. Tsogbayar · M. Horbatsch

Calculation of Resonance Parameters for Atomic Hydrogen in a Static Electric Field

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Abstract A mapped Fourier grid method for the Schrödinger equation is implemented in cylindrical coordinates. The complex absorbing potential method with Padé extrapolation and Riss–Meyer iteration is applied to calculate resonance parameters for the ground state of the hydrogen atom in a strong static electric field. The obtained values are compared with known results from the literature.

1 Introduction

The Stark effect in the hydrogen atom has received much attention since the early days of quantum mechanics [1,2]. Various methods of finding resonance parameters for this effect have been developed by many authors [3–7]. A bound state of atomic hydrogen becomes a quasi-bound state under the influence of the external field. The electron can tunnel through the barrier that is created as a result of the combination of the Coulomb potential and the electric field. After choosing the electric field to be along the z-axis, one can solve the problem in cylindrical coordinates. Upon applying the $\Psi(\mathbf{r}) = u(\rho, z)e^{im\varphi}/\sqrt{\rho}$ transformation the Schrödinger equation reads

$$\left[-\frac{1}{2}\frac{d^2}{d\rho^2} + \frac{m^2 - 1/4}{2\rho^2} - \frac{1}{2}\frac{d^2}{dz^2} - \frac{1}{\sqrt{\rho^2 + z^2}} + Fz\right] u(\rho, z) = Eu(\rho, z), \tag{1}$$

where F is the electric field strength.

In this work we attack this resonance problem by the Fourier grid method (FGM) combined with a complex absorbing potential (CAP). The FGM is based on the discrete Fourier transform. From finding the coefficients of the series expansion an ortho-normal sum, called the cardinal function g_{ij} is calculated (in closed form) at chosen grid points. One chooses a computational grid $\{\rho_i, z_j | i = 1 \ldots N, j = 1 \ldots M\}$, and defines the wave function for all ρ, z in terms of coefficients u calculated on the grid:

$$u^{(NM)}(\rho, z) = \sum_{i=1}^{N}\sum_{j=1}^{M} u(\rho_i, z_j) g_{ij}(\rho, z), \tag{2}$$

Ts. Tsogbayar (✉) · M. Horbatsch
Department of Physics and Astronomy, York University, 4700 Keele Street, Toronto M3J 1P3, Canada
E-mail: tsog218@yorku.ca

M. Horbatsch
E-mail: marko@yorku.ca

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where,

$$g_{ij}(\rho, z) = \frac{2}{N+1}\frac{2}{M+1}\sum_{k_\rho=1}^{N}\sum_{k_z=1}^{M}\sin(k_\rho\theta_{\rho i})\sin(k_\rho\theta_\rho)\sin(k_z\theta_{zj})\sin(k_z\theta_z). \tag{3}$$

For singular potentials, such as a Coulomb-type potential, it is advantageous to use a mapping technique for the coordinates. The mapping increases the number of points near the singularity, and a good solution is obtained using fewer grid points. Previously, such mapping techniques were applied to non-relativistic and relativistic wave equations [8,9]. We use here the following mappings for the ρ and z coordinates, in which ρ is mapped to θ_ρ and z to θ_z respectively:

$$\rho(\theta_\rho) = L_\rho\frac{\theta_\rho}{\pi-\theta_\rho}, \quad 0<\theta_\rho<\pi, \;\; z(\theta_z) = z_0 + L_z\tan\left(\frac{\theta_z}{2}\right), \quad -\pi<\theta_z<\pi, \tag{4}$$

where L_ρ and L_z are parameters chosen in some optimal way. Note that in analogy $\rho_i \leftrightarrow \theta_{\rho i}$ and $z_j \leftrightarrow \theta_{zj}$.

To avoid the calculation of outgoing waves we add an artificial complex absorbing potential in the Hamiltonian Eq. (1):

$$H = H_0 - i\eta W, \;\; W(\rho, z) = \Theta(\rho-\rho_c)(\rho-\rho_c)^2 + \Theta(z-z_c)(z-z_c)^2, \tag{5}$$

where Θ is the step function, η is a positive small parameter, and ρ_c, z_c determine the points where the CAP starts to dampen the outgoing wave in the asymptotic region. This means that the eigenfunction of the resonance state can be solved for in a square-integrable basis, that is, one solves a complex matrix problem to find complex energy eigenvalues, whose real part yields the resonance position, and the inverse of the imaginary part is associated with the lifetime of the state:

$$\left[-\frac{1}{2}\frac{d^2}{d\rho^2} + \frac{m^2-1/4}{2\rho^2} - \frac{1}{2}\frac{d^2}{dz^2} - \frac{1}{\sqrt{\rho^2+z^2}} + Fz - i\eta W(\rho, z)\right]u(\rho, z) = Eu(\rho, z). \tag{6}$$

While using a finite basis set to calculate $E_{fb} \approx E$, ideally we want η to be small to have a small artefact. However, when the parameter η tends to zero, the computational representation error increases. Thus, we want η to be not too small to have an easier calculation. Then, we want to remove the artefact due to the CAP. This can be done by an iterative correction method of Riss and Meyer [10], or by an extrapolation method [11,12]. Following [10] we have

$$E^{(n)} = E^{(n)}(\tilde{\eta}) = E_{fb}(\tilde{\eta}) + \sum_{j=1}^{n}\frac{(-\tilde{\eta})^j}{j!}\frac{d^j E_{fb}}{d\eta^j}\Big|_{\eta=\tilde{\eta}}, \tag{7}$$

where $\tilde{\eta}$ is an optimal value found by the condition $\left|\frac{\eta^{n+1}}{(n+1)!}\frac{d^{n+1}E_{fb}}{d\eta^{n+1}}\right|_{\eta=\tilde{\eta}} = \min$, $n = 0, 1, 2, 3$ [10].

2 Results and Discussion

We present resonance parameters for two fields strengths, namely $F = 0.05$ au and $F = 0.10$ au. In Table 1 we display the directly calculated complex eigenenergy and its corrected values from the Riss–Meyer method. The correction scheme leads to convergence of resonance parameters shown for two different values of z_c, where the absorbing potential starts. Using a higher order in the method results in larger optimal $\tilde{\eta}$. For larger z_c, one needs larger $\tilde{\eta}$ values.

Table 2 shows the relative errors of the third-order corrected eigenvalues as a function of basis size N. They do not converge uniformly as N increases. In both tables the primes mean that the calculations are carried out for $F = 0.05$ au.

In Fig. 1 we show the features of the outgoing waves along the z axis for two different values of η, for $F = 0.10$ au. On the left hand side, for a very small value of η, the action of the CAP is practically non-existent, and the resulting outgoing wave shows oscillatory behavior. It has decreasing amplitude due to the FGM. For larger values of η, this oscillatory nature is damped by the CAP. This feature renders the problem to be truly

Table 1 Resonance parameters for the H atom in electric fields $F = 0.05$ au (top half), and $F = 0.1$ au (bottom half) for fixed basis size $N : a'$, for $L_\rho = 1.20$, $L_z = 2.0$, $r_c = 2.2$, $z_c = 3.0$, $z_0 = -1.5$; b', for $L_\rho = 1.20$, $L_z = 2.0$, $r_c = 2.2$, $z_c = 3.5$, $z_0 = -1.5$; a, for $L_\rho = 1.20$, $L_z = 2.0$, $r_c = 2.2$, $z_c = 2.0$, $z_0 = -1.5$; b, for $L_\rho = 1.20$, $L_z = 2.0$, $r_c = 2.2$, $z_c = 2.5$, $z_0 = -1.50$

$N = M$	$\tilde{\eta}^{(0)}$	$\Re(E^{(0)})$	$\Im(E^{(0)})$	$\tilde{\eta}^{(1)}$	$\Re(E^{(1)})$	$\Im(E^{(1)})$	$\tilde{\eta}^{(2)}$	$\Re(E^{(2)})$	$\Im(E^{(2)})$	$\tilde{\eta}^{(3)}$	$\Re(E^{(3)})$	$\Im(E^{(3)})$
$48^{a'}$	0.002	−0.500 891	−0.000 3343	0.006	−0.500 969	−0.000 1314	0.009	−0.500 954	−0.000 0934	0.013	−0.500 943	−0.000 0855
$48^{b'}$	0.002	−0.500 900	−0.000 3040	0.008	−0.500 981	−0.000 1486	0.010	−0.500 959	−0.000 0866	0.015	−0.500 947	−0.000 0818
48^{a}	0.008	−0.520 287	−0.008 115	0.017	−0.521 870	−0.007 017	0.024	−0.522 437	−0.006 765	0.031	−0.522 763	−0.006 645
48^{b}	0.011	−0.520 504	−0.007 850	0.022	−0.522 151	−0.006 875	0.031	−0.522 689	−0.006 654	0.041	−0.522 986	−0.006 540

Table 2 Resonance parameters for the H atom in electric fields $F = 0.05$ au (left half), and $F = 0.1$ au (right half) depending on basis size N : a', for $L_\rho = 1.20, L_z = 2.0, r_c = 2.2, z_c = 3.0, z_0 = -1.5$; b', for $L_\rho = 1.20, L_z = 2.0, r_c = 2.2, z_c = 3.5, z_0 = -1.5$; a, for $L_\rho = 1.20, L_z = 2.0, r_c = 2.2, z_c = 2.0, z_0 = -1.5$; b, for $L_\rho = 1.20, L_z = 2.0, r_c = 2.2, z_c = 2.5, z_0 = -1.50$

$N = M$	$\Re(E^{(3)})$	$\Im(E^{(3)})$	Rel.	Err. (in %)	$N = M$	$\Re(E^{(3)})$	$\Im(E^{(3)})$	Rel.	Err. (in %)
$48^{a'}$	−0.500 943	−0.000 0855	0.010	1.22	48^{a}	−0.522 763	−0.006 645	0.88	8.60
$48^{b'}$	−0.500 947	−0.000 0818	0.010	1.12	48^{b}	−0.522 986	−0.006 540	0.84	10.04
$54^{a'}$	−0.505 580	−0.000 0519	0.001	0.35	54^{a}	−0.527 609	−0.006 729	0.04	7.44
$54^{b'}$	−0.505 581	−0.000 0507	0.001	0.32	54^{b}	−0.527 769	−0.006 732	0.07	7.40
$66^{a'}$	−0.505 716	−0.000 0344	0.001	0.11	66^{a}	−0.527 355	−0.006 656	0.01	8.45
$66^{b'}$	−0.505 717	−0.000 0352	0.001	0.09	66^{b}	−0.527 547	−0.006 666	0.03	8.31
$72^{a'}$	−0.503 622	−0.000 0351	0.005	0.09	72^{a}	−0.526 057	−0.007 129	0.26	1.94
$72^{b'}$	−0.503 621	−0.000 0390	0.005	0.01	72^{b}	−0.526 074	−0.007 129	0.25	1.93
True [7]	−0.506 105	−0.000 0385				−0.527 412	−0.007 270		

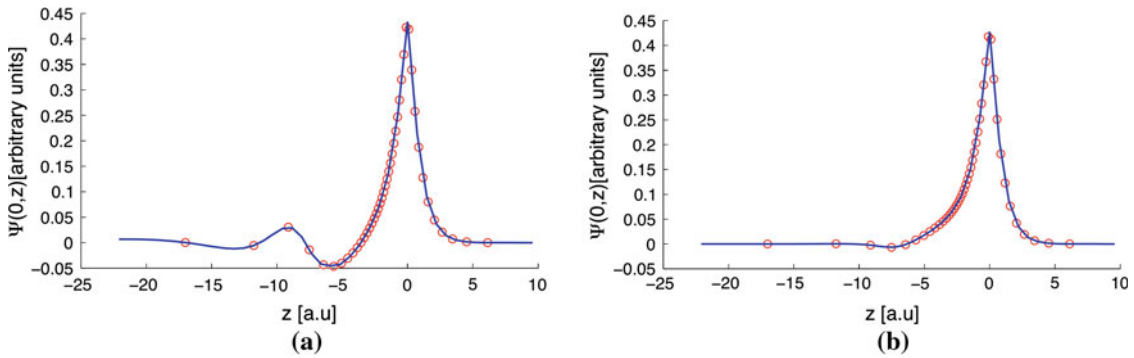

Fig. 1 The outgoing wave functions along the z axis for $F = 0.10$ au: **a** $N = 48$, $E^{(0)} = -0.495 - 0.22 \times 10^{-8}i$, $\eta^{(0)} = 10^{-7}$; **b** $N = 48$, $E^{(0)} = -0.521 - 0.0078i$, $\eta^{(0)} = 0.011$

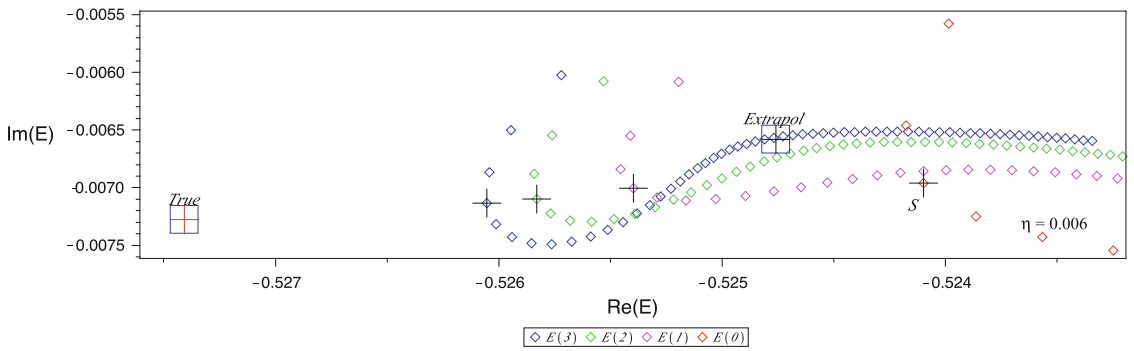

Fig. 2 The η-trajectories of complex eigenvalues and its corrected values for H atom in electric field $F = 0.10$ au, and $N = 72$, $L_r = 1.20$, $L_z = 2.00$, $r_c = 2.20$, $z_c = 2.00$, $z_0 = -1.50$

square-integrable. The red circles in both plots represent the eigenvectors at the grid points, while the blue curves show interpolations carried out by the global cardinal function (cf. Eqs. (2, 3)).

In Fig. 2 we display η trajectories for directly calculated complex eigenvalues and their corrected values, for $F = 0.10$ au. On the zeroth-order matrix eigenvalue trajectory S marks the result of the stabilization method. We also marked an extrapolated value for the originally calculated complex energy trajectory and true converged value from Ref. [7]. Even tough the values of $E^{(0)}$ deviate from the true value, the corrected values are approaching this value. One can argue that a direct Padé extrapolation from the zeroth-order matrix eigenvalues fails in this case. In simpler 1D or 2D calculations we found better convergence for the Riss–Meyer iteration and good agreement with Padé extrapolation. The Padé extrapolation shown in Fig. 2 is based upon points at much larger η than those shown on the graph.

We conclude that the mapped Fourier grid method is successfully employed to a 2D cylindrical problem, in which the interaction potentials are directly calculated at the chosen grid points, and eigenvectors from a matrix problem give exactly calculated values of the eigenfunction. A quadratic CAP combined with a FGM was used to compute the resonance parameters of the Stark effect for atomic hydrogen in a static electric field, and compared with the results in the literature. We have not yet carried out a convergence analysis in terms of the basis size. The next step will be to adjust the grid points such that the outgoing-wave region receives a better representation (cf. Fig. 1).While the results for $F = 0.05$ au are better converged, we focused in Fig. 2 on the more challenging case of $F = 0.1$ au to show that direct multi-dimensional calculations of the FGM/CAP method can be challenging in the strong-field regime. It will be of interest to push the Riss–Meyer iteration to higher order using spline-method based derivatives. One will need to demonstrate the convergence of the numerical calculations in terms of the grid parameters N, M in order to show how the values of Ref. [7] are approached by this direct two-dimensional grid method.

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