

# TRANSITION PROBABILITIES FOR $^1\text{H}$ IN STRONG MAGNETIC FIELDS

J. M. BENKŐ

*Konkoly Observatory of the Hungarian Academy of Sciences,  
P. O. Box 67, 1525 Budapest, Hungary,<sup>†</sup>*

AND

K. BALLA

*Computer and Automation Institute, Hungarian Academy of  
Sciences, P. O. Box 63, 1518 Budapest, Hungary,<sup>§</sup>*

When computing synthetic spectra we have to be aware of the strength of the lines. The determination of the required dipole strengths, oscillator strengths and transition probabilities is based on the evaluation of the dipole matrix elements. These quadratic functionals are defined by integrals over the whole space composed of the eigenfunctions  $\Psi$  of the atomic system belonging to the eigenvalues  $E_m$  and  $E_n$ , respectively:

$$\int \Psi^*(E_m) \mathbf{r} \Psi(E_n) d\mathbf{r} = \mathbf{p}. \quad (1)$$

The traditional way of computing (1) blocks the practical error estimates. An inaccuracy in the eigenfunctions of the time-dependent Schrödinger equation appears typically and it is amplified afterwards by both the weight function  $\mathbf{r}$  and the numerical integration algorithm.

We describe here the general framework of an alternative method that works in a wide class of non-separable cases. Splitting the improper integral over the halfspace into two parts by fixing a plane at  $z = z_c$ , we assume

$$\int_0^{z_c} \int \int \Psi^*(E_m) \mathbf{r} \Psi(E_n) dx dy dz = \mathbf{c}_m^{liT}(z_c) K_{mn}^1(z_c) \mathbf{c}_n^{lj}(z_c) \quad (2)$$

<sup>†</sup>e-mail: benko@buda.konkoly.hu. JMB acknowledges the support of the LOC of the 23rd General Assembly of IAU and that of PhD School of L. Eötvös University.

<sup>§</sup>e-mail: balla@sztaki.hu. The work of KB was partially supported by Hungarian Scientific Foundation, Grant No. T019460

$$\int_{z_c}^{\infty} \int \int \Psi^*(E_m) \mathbf{r} \Psi(E_n) dx dy dz = -\mathbf{c}_m^{\text{rT}}(z_c) K_{mn}^{\text{r}}(z_c) \mathbf{c}_n^{\text{r}}(z_c) \tag{3}$$

where  $i, j$  refer to the  $z$ -parities, l (left) or r (right) refer to the directions of the integrations of the equation

$$\frac{dK_{mn}^p}{dz} - K_{mn}^p (Y_m^{\text{T}} Y_m)^{-1} Y_m^{\text{T}} \mathcal{P}_m Y_m - Y_n^{\text{T}} \mathcal{P}_n^{\text{T}} Y_n (Y_n^{\text{T}} Y_n)^{-1} K_{mn}^p - Y_n^{\text{T}} \mathcal{S}_2 Y_m = 0. \tag{4}$$

with initial values  $K_{mn}^{\text{l}}(0) = 0$  and  $K_{mn}^{\text{r}}(\infty) = 0$ , respectively. That is, we get  $\mathbf{p}$  by the solution of initial value problems for ODEs. In (4), the matrices  $\mathcal{P}(E, z)$  and  $\mathcal{S}_2(z)$  depend on the concrete pseudo-basis functions, T denotes the transposed of a matrix. With  $q = \text{li}$  or  $q = \text{r}$ ,  $Y^q(z)$ -s are the solutions of the initial value problems

$$\frac{dY^q}{dz} + [I_{2N} - Y^q (Y^{q\text{T}} Y^q)^{-1} Y^{q\text{T}}] \mathcal{P} Y^q = 0 \tag{5}$$

with initial values  $Y^{\text{li}}(0)$  and  $Y^{\text{r}}(\infty)$  and for both  $E_m$  and  $E_n$ , respectively. Next, for each eigenfunction, the normalization is taken into account by a splitting similar to (2), (3). The change consists in setting  $m = n$ ,  $i = j$  and replacing  $K_{m,m}^p$  by  $H^q$ . The initial value problems for  $H^q$  are only slightly different from those for  $K_{m,m}^p$ . Then

$$(\mathbf{c}^{\text{li}}(z_c), \mathbf{c}^{\text{r}}(z_c)) = (V_1^{\text{T}} H^{\text{li}}(z_c) V_1 - V_2^{\text{T}} H^{\text{r}}(z_c) V_2)^{-\frac{1}{2}} \cdot (V_1, V_2) \tag{6}$$

where  $V_1$  and  $V_2$  are nontrivial solutions of the system of linear algebraic equations  $(Y^{\text{liT}}(z_c) Y^{\text{r}}(z_c) Y^{\text{rT}}(z_c) Y^{\text{li}}(z_c) - I) V_1 = 0, V_2 = Y^{\text{rT}}(z_c) \dot{Y}^{\text{li}}(z_c) V_1$ .

Together with the method of getting the pseudo-basis functions, the main point of the approach is that the truncated one-dimensional non-adjoint eigenvalue problem (5) replaces the original one. In fact, (5) realizes a transfer of boundary conditions due to Bakhvalov <sup>1</sup>.

The advantages of both this and a similar treatment together with the proper handling of singularities has been discussed in our recent papers where the method was applied to and discussed for the diamagnetic Coulomb problem (hydrogen atom in strong magnetic field) <sup>2</sup> related to the model-spectra of magnetized white dwarfs and neutron stars.

When computing the quadratic functional (1) by this process, the most important gain is that we do not need the eigenfuntions  $\Psi$  to be computed! Thus, their non-uniform accuracy disappears, too. The computational errors can be kept under control. The qualitative theory of singular ODEs and that of singular boundary value problems allow us to reduce the problem to regular and stable initial value problems.

<sup>1</sup>Bakhvalov, N. S.: 1973, Numerical Methods, Nauka, Moscow, (in Russian)

<sup>2</sup>Balla K. and Benkő J. M.: 1996, *J. Phys. A: Math. Gen.* **29**, 6747 and 1997, *J. Phys. A: Math. Gen.* (to be submitted)