README file for 'Dalgarno-Lewis equation and two-photon processes'

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1 Numeric and model calculations

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1.1 Files

1. rho_H_1s_to_0.04eV_p_states.dat

2. rho_H_1s_to_3.00eV_p_states.dat

3. rho_H_1s_to_15.00eV_p_states.dat

4. rho_H_1s_to_40.00eV_p_states.dat

5. rho_H_1s_to_150.00eV_p_states.dat

6. rho_H_1s_to_300.00eV_p_states.dat

7. rho_H_2s_to_0.04eV_p_states.dat

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1.2   Description

Files with name pattern $rho\_H\_\$1\_to\_\varepsilon_\kappa\_\$2\_states.dat$ contain different solutions to the Dalgarno-Lewis differential equation

$$[\mathcal{H}_\lambda - \varepsilon_\kappa]\rho_{\varepsilon_\kappa,\lambda}^{l_i} = -rR_{\varepsilon_i,l_i}, \tag{1}$$

for some hydrogen atom initial states. The wildcard $1 indicates the initial state $1= 1s, 2s, 2p and 3p. $\varepsilon_\kappa = \kappa^2/2$ is the energy (in eV) of the intermediate state, whose angular quantum number λ is codified into the wildcard $2= s, p, d.

The structure of files is as follows: the first column indicates the electron position variable r in atomic units. The following six columns display the real and imaginary parts for three different methods of solution, namely: Dahlström *et al.* asymptotic solutions [1, 2], the approximate analytic method in Ref. [3], and the 'exact' numeric solution of Eq. (1) through a Numerov algorithm (see for instance, [4]). The eigth column contains a model ingredient [3]. Additionally, for initial 1s states, we add a semi-analytic solution to Eq. (1) derived from Ref. [5].

1.3 Method

Numerical solutions to the Dalgarno-Lewis differential equation (1) were obtained from a backpropagation starting at asymptotic ($\kappa r \gg 1$) space regions through the Numerov method. The simulation box size was set to $r_{max} > 300|(\lambda + 1 - i/\kappa)(-\lambda - i/\kappa)|/(2\kappa)$ guaranteeing that solutions reached the asymptotic limit. The number of grid points was set to about 600 points per asymptotic cycle of the solution. Solutions were printed to files with a smaller grid density.

Approximate solutions based on the asymptotic expression [1, 2], analytic solution in Ref. [3], and the semi-analytic solution from Ref. [5] were obtained by direct implementation of the corresponding expressions. Bound-Continuum matrix elements can be obtained from different sources, one of them is [6].

1.4 Observations

None.

2 Radial matrix elements. Second-order perturbation theory (SOPT) calculations (length gauge).

Author(s): D.I.R. Boll

2.1 Files

1. RadMatEl_SOPT_single_color_100_Omega_abs.dat

2. RadMatEl_SOPT_single_color_100_Omega_abs.dat

3. RadMatEl_SOPT_single_color_210_Omega_abs.dat

4. RadMatEl_SOPT_single_color_310_Omega_abs.dat

5. RadMatEl_SOPT_two_color_100_1.55_abs.dat

6. RadMatEl_SOPT_two_color_100_1.55_emi.dat

7. RadMatEl_SOPT_two_color_200_1.55_abs.dat

8. RadMatEl_SOPT_two_color_200_1.55_emi.dat

9. RadMatEl_SOPT_two_color_210_1.55_abs.dat

10. RadMatEl_SOPT_two_color_210_1.55_emi.dat

11. RadMatEl_SOPT_two_color_310_1.55_abs.dat

12. RadMatEl_SOPT_two_color_310_1.55_emi.dat

2.2 Description

Files with name pattern *RadMatEl_SOPT_$1_color_nlm_$2_$3.dat* contain the radial matrix elements for two-photon ionization process of hydrogen atoms with initial state quantum numbers *nlm*. The wildcard $1 indicates whether the calculation corresponds to single or two color case. The wildcard $2 informs the second photon frequency. $2=Omega indicates that second-photon frequency is identical to first-photon frequency (single-color). For two color setups it indicates the photon energy in eV. The last wildcard $3=abs,emi, indicates if the final state of the system is arrived after absorption or emission of the second photon.

The structure of the files is as follows: the first column indicates the first photon energy (in eV). Subsequent columns show the real and imaginary parts of the radial matrix elements $T_{L,\lambda}^{l_i}$ (superscript omitted in column headers).

2.3 Method

Radial matrix elements in the above files were obtained by a custom implementation of the explicit method described in Ref. [7]. The results are in the length gauge.

2.4 Observations

None.

3 Radial matrix elements. Second-order perturbation theory (SOPT) calculations (velocity gauge)

Author(s): D.I.R. Boll

3.1 Files

1. RadMatEl_Krylovetsky_single_color_100_Omega_abs.dat

2. RadMatEl_Krylovetsky_single_color_100_Omega_abs.dat

3. RadMatEl_Krylovetsky_single_color_210_Omega_abs.dat

4. RadMatEl_Krylovetsky_single_color_310_Omega_abs.dat

5. RadMatEl_Krylovetsky_two_color_100_1.550_abs.dat

6. RadMatEl_Krylovetsky_two_color_100_1.550_emi.dat

7. RadMatEl_Krylovetsky_two_color_200_1.550_abs.dat

8. RadMatEl_Krylovetsky_two_color_200_1.550_emi.dat

9. RadMatEl_Krylovetsky_two_color_210_1.550_abs.dat

10. RadMatEl_Krylovetsky_two_color_210_1.550_emi.dat

11. RadMatEl_Krylovetsky_two_color_310_1.550_abs.dat

12. RadMatEl_Krylovetsky_two_color_310_1.550_emi.dat

3.2 Description

Files with name pattern *RadMatEl_Krylovetsky_$1_color_nlm_$2_$3.dat* contain the radial matrix elements for two-photon ionization process of hydrogen atoms with initial state quantum numbers *nlm*. The wildcard $1 indicates whether the calculation corresponds to single or two color case. The wildcard $2 informs the second photon frequency. $2=Omega indicates that second-photon frequency is identical to first-photon frequency (single-color). For two color setups it indicates the photon energy in eV. The last wildcard $3=abs,emi, indicates if the final state of the system is arrived after absorption or emission of the second photon.

The structure of the files is as follows: the first column indicates the first photon energy (in eV). Subsequent columns show the real and imaginary parts of the radial matrix elements $T_{L,\lambda}^{l_i}$ (superscript omitted in column headers).

3.3 Method

Radial matrix elements in the above files were obtained by a direct implementation of the analytic method described in Ref. [8]. The results were obtained in the velocity gauge and further converted into the length gauge by applying the results from Ref. [9].

3.4 Observations

None.

4 Changelog

References

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