PULSED POWER PHYSICS TECHNOTE NO. 2019-xx

TITLE: **Notes on running UKRmol+ on Naval Research Laboratory (NRL) workstations, NRL High Performance Computers (HPCs), and Air Force Research Laboratory (AFRL) HPCs***

AUTHORS: P. E. Adamson
Code 6770, Plasma Physics Division, Naval Research Laboratory

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ABSTRACT: The B-spline R-matrix code UKRmol+[1] is used to compute electron scattering cross-sections to complement data available in the literature.

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1 Introduction

The UK-molecular *R*-matrix code suite (UKRmol)[1] is well-established in the domain of electron—molecule scattering using the R-matrix method. In the region of the molecular target, UKRmol uses Gaussian type orbitals (GTOs) to represent the target and the continuum wavefunction. (See ref [2] for a comprehensive review article on electron–molecule collision calculations using the *R*-matrix method.)
In order to compute accurate electron-atom and electron-molecule scattering cross sections, one must include many excited states in the quantum mechanical description (i.e. wavefunction) of the target (atom or molecule), and the underlying quantum chemistry calculations used to compute the target wavefunctions must employ large basis sets with very diffuse orbitals. The inclusion of the diffuse basis functions ensures an accurate description of the electronic spectrum of the molecule and of the scattering observables.[3]
The inclusion of diffuse electronic states was challenging, if not impossible, in traditional *R*-matrix scattering calculations due to numerical problems that arose when a large GTO-only continuum basis was combined with a large *R*-matrix sphere containing the target wavefunction. The UK-molecular *R*-matrix code suite+ (UKRmol+) bypasses this shortfall by representing the continuum with *B*-spline type orbital (BTO) basis functions, maintaining numerical stability with much larger *R*-matrix spheres than UKRmol and other *R*-matrixmethods.[1]

1.1 A subsection

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2 Acknowledgments

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References

[1] J. M. Carr, P. G. Galiatsatos, J. D. Gorfinkiel, A. G. Harvey, M. A. Lysaght, D. Madden, Z. Mašín, M. Plummer, J. Tennyson, and H. N. Varambhia. Ukrmol: a low-energy electron- and positron-molecule scattering suite. *The European Physical Journal D*, 66(3):58, Mar 2012.

[2] Jonathan Tennyson. Electron–molecule collision calculations using the r-matrix method. *Physics Reports*, 491(2):29 – 76, 2010.

[3] Daniel Darby-Lewis, Zdeněk Mašín, and Jonathan Tennyson. R-matrix calculations of electron impact electronic excitation of BeH. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 50(17):175201, aug 2017.

[1] Zatsarinny's *B*-spline *R*-matrix-with-pseudostates (BSR) method achieves similar results for atomic systems. See ref [4] for an excellent example of state-of-the-art calculations of elastic scattering, excitation, and ionization cross sections for all transitions between the lowest 21 states of nitrogen in the electron energy range from threshold to 120 eV.

[4] Yang Wang, Oleg Zatsarinny, and Klaus Bartschat. *b*-spline *r*-matrix-with-pseudostates calculations for electron-impact excitation and ionization of nitrogen. *Phys. Rev. A*, 89:062714, Jun 2014.