Table of Contents

Volume 103 • Number 1 • January 2025

Bound States and Quantum Correlations — in honour of A. Ravi P. Rau: Part I

Introduction

Bound states and quantum correlations: a special issue in honour of Prof. A.R.P. Rau

Chitra Rangan and Sai Vinjanampathy

Vol. 103 • No. 1 • pp. 1–2

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Note

Second Born electrons, Born again seamen

A.R.P. Rau

Vol. 103 • No. 1 • pp. 3–6

The multiple puns in the title play on a curiosity, that the rescue of a person overboard at sea and the dominance of the second Born term in forward charge transfer in atomic collisions share common elements of physics. Essentials and commonality in the two are explained.

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Research Article

A semi-analytic approximation for a single-particle continuum wavefunction

Robin Shakeshaft

Vol. 103 • No. 1 • pp. 7–20

A moderately simple approximation to the radial wavefunction of an unbound particle which carries arbitrary angular momentum $l(l+1)$ and which scatters from any physical potential, including one with a Coulomb tail, is presented. The approximate wavefunction has the form of a linear combination of short- and long-range analytical functions that satisfies the correct boundary conditions at both the origin and at large distances. The coefficients of the short-range functions are determined by solving a matrix equation whose elements are highly suited to numerical quadrature, and which are hardly more difficult to evaluate for $l \gg 1$ than for $l = 0$. The coefficients of the long-range functions are determined by both the nature of the interaction at large distances and the cusp condition on the wavefunction at the origin. This wavefunction has been tested by application to pure Coulomb scattering and to electron scattering from hydrogen within the 1s–2s–2p close coupling framework.

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Reviews

Interchannel coupling effects on atomic photoionization: correlation in the continuum

Steven T. Manson

Vol. 103 • No. 1 • pp. 21–26

Correlation in the form of interchannel coupling of continuum states is explained in the context of atomic photoionization. A number of examples are presented illustrating some of the qualitative and quantitative effects of this coupling.

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Plasma effects on resonant phenomena

Anil Pradhan

Vol. 103 • No. 1 • pp. 27–33

The effect of autoionizing resonances in atomic systems and processes is reviewed. Theoretical framework for treating resonances in the coupled channel approximation using the R-matrix method, as well as approximations related to plasma applications are described. The former entails large-scale atomic computations, and the latter is based on a new method for including collisional, Stark, thermal, and other broadening mechanisms. We focus particularly on the problem of opacities calculations in high-energy-density plasmas such as stellar interiors and inertial confinement fusion devices. The treatment is generally relevant to radiative and collisional processes as the cross sections become energy-temperature-density dependent. While the computational difficulty increases considerably, the reaction rates are significantly affected. The related issue of the Boltzmann–Saha equation-of-state and its variants in local thermodynamic equilibrium is also explored as the intermediary between atomic data on the one hand and plasma environments on the other.

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Research Articles

Time delays in anisotropic systems

Ulf Saalmann and Jan M. Rost

Vol. 103 • No. 1 • pp. 34–41

Scattering properties and time delays for general (nonsymmetric) potentials in terms of the respective S-matrices are discussed paradigmatically in one dimension and in comparison to symmetric potentials. Only for the latter the Wigner and Smith time delays coincide. Considering asymmetric potentials also reveals that only one version of S-matrices used in the literature (the one with reflection coefficients on the diagonal) generalizes to the asymmetric case. Finally, we give a criterion how to identify a potential with intrinsic symmetry that behaves like an asymmetric one if it is merely offset from the scattering center.

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Measurability of Wigner time delay in a photoionization experiment

Pranawa C. Deshmukh, Sourav Banerjee, and Steven T. Manson

Vol. 103 • No. 1 • pp. 42–50

We visit significant historical steps in quantum collision physics that make photoionization time delay

measurable, especially considering the time-reversal symmetry in related processes. The works of A. Ravi P. Rau and Ugo Fano inspire key ideas presented in this article.

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Wigner time delay and Hartman effect in quantum motion along deformed Riemannian manifolds

Benjamin Schwager, Lars Meschede, and Jamal Berakdar

Vol. 103 • No. 1 • pp. 51–59

Elastic scattering of a wave can be quantified by a shift in the phase with respect to the phase of the incoming wave. A qualitative measure of the time during which the effect occurs is given by the Wigner time delay. The tunneling time is known to saturate with increasing tunneling barrier width (Hartman effect). Here, we analyze the elastic quantum mechanical scattering in a deformed one-dimensional Riemannian manifold, particularly with respect to the Wigner time delay and conclude on the Hartman effect. It is shown that scattering due to local curvature variations results in imperfect conduction and leads to a Wigner time delay that at low energies, is in variance with the classical time delay that is inferred from the arc length. At moderate and high energies, however, classical and quantum time delays coincide.

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Ground-state energy of H^-: a critical test of triple basis sets

E.M.R. Petrimoulx, A.T. Bondy, E.A. Ene, L.A. Sati, and G.W.F. Drake

Vol. 103 • No. 1 • pp. 60–66

We report an improved variational upper bound for the ground state energy of H^- using Hylleraas-like wave functions in the form of a triple basis set having three distinct distance scales. The extended precision DQFUN of Bailey, allowing for 70 decimal digit arithmetic, is implemented to retain sufficient precision. Our result exceeds the previous record [A. M. Frolov, Euro. J. Phys. D 69, 132 (2015)], indicating that the Hylleraas triple basis set exhibits comparable convergence to the widely used pseudorandom all-exponential basis sets, but the numerical stability against roundoff error is much better. It is argued that the three distance scales have a clear physical interpretation. The new variational bound for infinite nuclear mass is –0.527 751 016 544 377 196 590 814 478 a.u. New variational bounds are also presented for the finite mass cases of the hydrogen, deuterium, and tritium negative ions H^-, D^-, and T^-.

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Adiabatic and post-adiabatic hyperspherical treatment of the huge ungerade proton-hydrogen scattering length

Shayamal Singh and Chris H. Greene

Vol. 103 • No. 1 • pp. 67–74

While the hydrogen molecular ion is the simplest molecule in nature and very well studied in all of its properties, it remains an interesting system to use for explorations of fundamental questions. One such question treated in this study relates to finding an optimal adiabatic representation of the physics, i.e., the best adiabatic description that minimizes the role of nonadiabatic effects. As a test case explored here in detail, we consider the ungerade symmetry of H_2^+, which is known to have a huge scattering length of order 750 Bohr radii, and an incredibly weakly bound excited state. We show that a hyperspherical adiabatic description does an excellent job of capturing the main physics. Our calculation yields a competitive scattering length and shows that nonadiabatic corrections are small and can even be adequately captured using the post-adiabatic theory of Klar and Fano.

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The movement of Efimov states in 2n halo nucleus: probing the roles of mass asymmetry and short range of interaction

Indranil Mazumdar

Vol. 103 • No. 1 • pp. 75–80

This brief communication presents the results of our work to study the movement of Efimov states in two-neutron halo nuclei. We discuss the emergence and evolution of Efimov states into resonances beyond the two-body (n–core) breakup threshold and also the movement of the Efimov state in a two-neutron halo nucleus to the region of the so-called Thomas collapse. We especially probe the roles of mass asymmetry of the three-body system (n–n–core) and the short range of the n–core interaction in the movement of the Efimov states. The analysis has been carried out within the framework of a three-body model, assuming two-body, non-local, separable potentials for the binary sub-systems, namely, the n–n and n–core systems. The primary motivation has been to scan the parameter space of the range parameter and determine the value(s) for which the system can support the Efimov states. The analysis shows that the value of the range parameter $\beta = 5.2\alpha$ (α being the energy parameter given in terms of the deuteron binding energy) produces the realistic three-body binding energy for ^{20}C and also generates the excited Efimov states. However, as the value of β is increased corresponding to decrease in the range of the two-body (n–core) interaction the ground and excited state binding energies increase drastically. In other words, as the range of the two-body interaction tends to zero the system enters the Thomas collapse region away from the Efimov region.

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Probability distributions of atomic scattering lengths

John L. Bohn and Reuben R.W. Wang

Vol. 103 • No. 1 • pp. 81–88

The probability distributions of the real and imaginary parts of atomic scattering lengths a are derived, in a two-channel model that allows for inelastic scattering to occur. While the real part of a remains Cauchy-distributed, as predicted for single channel scattering in the classic work of Gribakin and Flambaum, the imaginary part of a is seen to be strongly peaked near zero. Two-body inelastic scattering rates may therefore be smaller in general than a naive estimate would suggest.

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Energy levels and characteristic features in photoionization of Cl III using the R-matrix method

Sultana N. Nahar

Vol. 103 • No. 1 • pp. 89–99

We report study of Cl III for its large number of fine structure bound levels, 890, with $n \leq 10$ and $l \leq 9$, and 1/2

$\leq j \leq$ 19/2 of even and odd parities with spectroscopic designation and photoionization cross sections (σ_{PI}) of the levels revealing various characteristic features. Various resonant structures and the shapes of the background, and their interference in σ_{PI} are illustrated for the ground, excited equivalent electron, low and high lying excited levels with single valence electron, and effects of fine structure couplings. σ_{PI} of the ground level shows Rydberg series of resonances on smooth background, and of equivalent electron levels producing strong closely spaced Rydberg series of resonances belonging to the low lying core ion excitation thresholds. They will impact applications in low temperature plasma. For the single valence electron excited levels, we find that σ_{PI} of low lying excited states are dominated by Rydberg series of resonances and of high lying excited states exhibit prominent broad feature of Seaton resonances. Partial photoionization cross sections of the ground level for leaving the core ion in the ground and various excited levels are also presented for applications in plasma modeling. The study was carried out in relativistic Breit–Pauli R-matrix method using a large close coupling wave function expansion of 45 levels of the core ion configurations $3s^23p^2$, $3s3p^3$, $3s^23p3d$, $3s^23p4s$, $3s3p^23d$, and $3p^4$ with closed 1s, 2s, 2p orbitals. They belong to the optimized set of 13 configurations of Cl IV, $3s^23p^2$, $3s3p^3$, $3s^23p3d$, $3s^23p4s$, $3s^23p4p$, $3s^23p4d$, $3s3p^23d$, $3s3p^24s$, $3s3p^24p$, $3p^4$, $3p^33d$, $3p^34s$, and $3p^34p$. Cl III energies are in good agreement with measured values. σ_{PI} features of low lying levels were benchmark with observation carried out at Advanced Light Source at LBNL with very good agreement. The present set of high accuracy data should complete for any practical applications.

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Spectra of phosphorus ions for astrophysical modeling: P I–P XV

Sultana N. Nahar and Bilal Shafique

Vol. 103 • No. 1 • pp. 100–130

Phosphorus (P), a basic element of life, has been a least studied element due to its poor presence in astrophysical spectra. However, search for the P lines has increased considerably with discoveries of exoplanets and are being detected by high resolution and sophisticated astronomical observatories, e.g., James Webb Space Telescope (JWST). JWST may provide a clue for life with detection of P in its infrared (IR) region. Identification of the element and analysis of the observed spectra will require high accuracy data for atomic processes that produces lines and their predicted features. The present study focuses on these needs and reports systematically regions of wavelengths, from X-ray to IR, that show prominent lines by the 15 individual ionization stages of phosphorus, P I–P XV for the first time. We present large amount of relevant atomic data for energies, transition parameters, and lifetimes obtained in relativistic Breit–Pauli approximation using the R-matrix method and atomic structure program SUPERSTRUCTURE. Our spectral features for the 15 ions, P I–P XV, predict strengths of lines in various wavelength regions. They show dominance of P I and P II in the IR region and other ions in the ultraviolet and optical regions often stretching to IR in the continuum. For determination of accuracy, we have made extensive comparisons of our atomic data with available experimental and theoretical values. Based on these, our results and features are expected to provide precise plasma diagnostics and astrophysical modeling.

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LIST OF ISSUES

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LIST OF ISSUES

Volume 103
Issue 1

January 2025

Volume 102
Issue 12

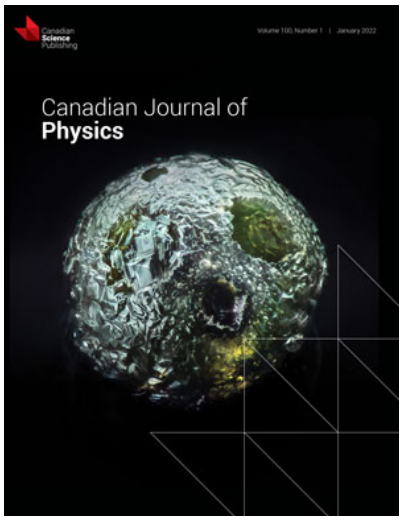
December 2024

Volume 102
Issue 11

November 2024

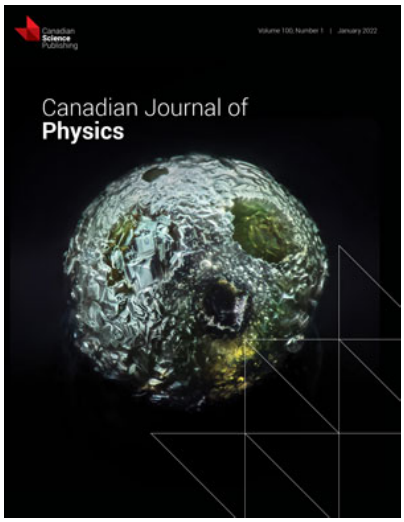
Volume 102
Issue 10

October 2024



Volume 102
Issue 9

September 2024



Volume 102
Issue 8

August 2024

VIEW LIST OF ISSUES