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A computer code for calculations in the algebraic collective model of the atomic nucleus☆

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ABSTRACT

A Maple code is presented for algebraic collective model (ACM) calculations. The ACM is an algebraic version of the Bohr model of the atomic nucleus, in which all required matrix elements are derived by exploiting the model's SU(1, 1) × SO(5) dynamical group. This paper reviews the mathematical formulation of the ACM, and serves as a manual for the code.

The code enables a wide range of model Hamiltonians to be analysed. This range includes essentially all Hamiltonians that are rational functions of the model's quadrupole moments $\hat{q}_M$ and are at most quadratic in the corresponding conjugate momenta $\hat{\pi}_N$ ($-2 \leq M, N \leq 2$). The code makes use of expressions for matrix elements derived elsewhere and newly derived matrix elements of the operators $[\hat{\pi} \otimes \hat{q} \otimes \hat{\pi}]_0$ and $[\hat{\pi} \otimes \hat{\pi}]_{LM}$. The code is made efficient by use of an analytical expression for the needed SO(5)-reduced matrix elements, and use of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients obtained from precomputed data files provided with the code.

Program summary

Program title: ACM

Catalogue identifier: AEYO_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEYO_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html

No. of lines in distributed program, including test data, etc.: 3873526

No. of bytes in distributed program, including test data, etc.: 46345414

Distribution format: tar.gz

Programming language: Maple 18 (or versions 17, 16, 15).

Computer: Any.

Operating system: Any which supports Maple; tested under Linux, Max OSX, Windows 7.

RAM: 500Mb

Classification: 17.20.

Nature of problem: The calculation of energy eigenvalues, transition rates and amplitudes of user specified Hamiltonians in the Bohr model of the atomic nucleus.

Solution method: Exploit the model's SU(1, 1) × SO(5) dynamical group to calculate analytic (as far as possible) expressions for matrix elements, making use of extensive files (supplied) of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients. Diagonalisation of the resulting matrices (once the entries are converted to floating point) is carried out using the Maple library procedure `Eigenvectors`. (Maple [1] makes use of the NAG [2] and CLAPACK [3] linear algebra libraries.)

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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URLs: http://www.physics.utoronto.ca/~twelsh (T.A. Welsh), http://www.physics.utoronto.ca/~rowe (D.J. Rowe).

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Additional comments:

1. The dimension of the Hilbert space that can be handled is limited only by the available computer memory and the available SO(5) ⊃ SO(3) Clebsch–Gordan coefficients $(v_1\alpha_1 L_1 v_2\alpha_2 L_2 \| v_3\alpha_3 L_3)$.
2. The supplied data files provide coefficients $(v_1\alpha_1 L_1 v_2\alpha_2 L_2 \| v_3\alpha_3 L_3)$ for $1 \leq v_2 \leq 6$, and contain all non-zero coefficients for $v_1 < v_3 \leq 50$ when $v_2 \in 1, 3$, for $v_1 \leq v_3 \leq 30$ when $v_2 \in 2, 4$, and for $v_1 \leq v_3 \leq 25$ when $v_2 \in 5, 6$. (Once calculated, further coefficients can be readily made available to the code without changing the code.) Thus, depending on the model Hamiltonian being analysed, the states in the Hilbert space used are limited in their seniority. For analysis of the more typical types of model Hamiltonian, only the coefficients with $v_2 \in \{1, 3\}$ are required, and therefore, with the supplied files, the seniority limit is 50. More exotic Hamiltonians having terms with seniority $v_2 \in \{2, 4, 5, 6\}$ would have the seniority limited to 30 or 25 accordingly.
3. The code provides lower level procedures that give ready access to the Clebsch–Gordan coefficients and the SU(1, 1) and SO(5) matrix elements. These procedures are described in the manuscript and enable extensions to the code and model to be made easily.
4. The accuracy to which Maple performs numerical calculations is determined by the Maple parameter Digits, which specifies the number of significant decimal digits used. The default value of 10 is more than adequate for most ACM calculations. Note, however, that if Digits is increased beyond a certain value (obtained from the Maple command `evalhf(Digits)`, and usually 15 on modern computers) then the code can no longer take advantage of hardware mathematical operations, and is significantly slower.

Documents included

1. The code makes use of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients which are supplied in zip files, and must be installed by the user.
2. A Maple worksheet that gives various example calculations and tests carried out using procedures from the code is provided.
3. A 162 page PDF file containing everything displayed in the worksheet (input, output and comments, and making use of colour) is also provided.

!!!!! The distribution file for this program is over 46 Mbytes and therefore is not delivered directly when download or Email is requested. Instead a html file giving details of how the program can be obtained is sent. !!!!!

Running time: For a fixed value of the parameter Digits, the running time depends on the dimension of the Hilbert space on which the diagonalisation is performed, and this in turn is governed by the number of eigenvalues required and the accuracy required. Note that diagonalisation is performed separately in each L-space. For typical ACM calculations (such as those carried out in [4]), the matrices being diagonalised are usually of dimension at most a few hundred, and often much smaller. On a modest personal computer, the computation for the smallest cases takes at most a few seconds. The worksheet contains a range of examples for which the calculation time varies between a few seconds and 750s. In the latter case, diagonalisation is performed on L-spaces for $0 \leq L \leq 8$, the dimensions of these spaces being between 154 and 616.

References:

[1] Maplesoft, Waterloo Maple Inc., Waterloo, ON, Canada.
[2] NAG, www.nag.com.
[3] CLAPACK, www.netlib.org/clapack.
[4] D. J. Rowe, T. A. Welsh, M. A. Caprio, Phys. Rev. C 79(2009) 054304.

1. Introduction

The ACM (algebraic collective model) [1–4] is an algebraic version of the Bohr model [5] based on a dynamical group SU(1, 1) × SO(5) for which all the matrix elements needed in applications of the model are calculated analytically. It is a development of the *computationally tractable version of the collective model* [1] that enables collective model calculations to be carried out efficiently by use of wave functions that span modified oscillator series of SU(1, 1) irreps (irreducible representations) [6,7] and complementary SO(5) wave functions. The availability of analytic SU(1, 1) matrix elements and SO(5) Clebsch–Gordan coefficients enable the calculations to bypass expressions for the wave functions entirely, avoiding, in particular, numerical integration. A pedagogical treatment of the geometrical and algebraic foundations of the ACM is given in the recent book by Rowe and Wood [8].

Earlier computer programs that implemented the Bohr model utilised an U(5) ⊃ O(5) ⊃ SO(3) ⊃ SO(2) basis [9–11]. The basis was constructed by starting with a basis of SO(3) coupled polynomials of a given degree in the quadrupole coordinates and diagonalising the O(5) Casimir operator in this basis. The computer program developed by Gneuss and Greiner [12] additionally employed a U(5) ⊃ Sp(4) ⊃ SO(3) × SO(3) ⊃ SO(2) × SO(2) basis, with transformations between the two bases carried out using the methods of [13]. On being further developed, the calculations could be carried out fully in the U(5) ⊃ O(5) ⊃ SO(3) ⊃ SO(2) basis, culminating in the Frankfurt code [14–16]. This was able to analyse model SO(3)-invariant Hamiltonians obtained from three kinetic energy terms and potential energy obtained from various polynomials in β and $\cos 3\gamma$ (the collective model coordinates β and γ are described in Section 2). In the Frankfurt