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LIBRARY OF PROBLEM-ORIENTED PROGRAMS FOR SOLVING PROBLEMS OF ATOMIC AND NUCLEAR PHYSICS

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The Data Centre of the Leningrad Institute of Nuclear Physics (LIYaF) is continuing work on the establishment of a library of problem-oriented programs for solving problems of atomic and nuclear physics. The programs at present available to the Data Centre are listed and described briefly below. Before giving the list, however, we would recall some general facts about the functioning of the library. ALGOL-60 [1] and FORTRAN-CERN [2] have been adopted as the official algorithmic languages. All the programs at present in the library are written for the BESM-6 computer, with the BESM-ALGOL (Computer Centre of the USSR Academy of Sciences) [3] and ALGOL-GDR [4] translators being used for ALGOL problems and one FORTRAN-DUBNA translator for FORTRAN problems. The two last-mentioned translators form part of the "Dubna" monitor system [5]. Besides its designation and the names of the authors, we give for each of the programs below a brief description and certain cataloguing data, including:

1. The program cipher, consisting of three letters and three digits. The first two letters of the cipher indicate the subject-matter of the problem to be solved, while the third letter indicates the language in which the program is written; the three digits constitute a serial number. The subject breakdown is as follows: AP - atomic physics; NP - nuclear physics; QM - quantum mechanics; CT - the purely mathematical methods used most often in physics calculations;
2. The language in which the program is written;
3. The translator for which the program is designed;
4. The program scope. When the FORTRAN-DUBNA and ALGOL-GDR translators are used, the program scope is determined on the basis of the loading instructions [5] - i.e. with allowance for all duty sub-programs of the "Dubna" monitor system. When the BESM-ALGOL translator is used, the program scope is indicated without allowance for duty sub-programs;

5. A description of the program - i.e. the literature source which describes or will describe the formulation of the problem, the method of solving it, the structure of the program, the rules for data input and the print-out text.

All programs in the Data Centre's library can be supplied on request in the form of a listing and a set of punched cards.

REFERENCES

[1] The algorithmic language ALGOL-60, revised report (in Russian), Mir, Moscow (1965).

[2] The FORTRAN language (in Russian), edited by SHIRIKOV, V.P., Dubna (1970).

[3] KUROCHKIN, V.M. et al., The BESM-6-ALGOL system (in Russian), Computer Centre of Moscow State University, Moscow (1969).

[4] HIRR, R., STROBEL, R., ALGOL in the "Dubna" monitor system (in Russian), translated from German by B.P. Primochkin, I.V. Kurchatov Institute of Atomic Energy, Moscow (1972).

[5] MAZNY, G.L., Guide for working with the "Dubna" monitor system (in Russian), Joint Nuclear Research Institute, Dubna (1972).

I. A T O M I C P H Y S I C S

The "ATOM" system of mathematical aids for atomic calculations

I. PROGRAM FOR SOLVING HARTREE-FOCK SELF-CONSISTENT FIELD EQUATIONS FOR ATOMS

Cipher:	APA001
Language:	ALGOL-60
Translator:	BESM-ALGOL
Program scope:	10110_8 cells
Description:	L.V. Chernysheva, N.A. Cherepkov, V. Radoevich Preprint FTI-486, Leningrad (1975)

The program calculates wave functions of the ground state of an atom or ion in the Hartree-Fock non-relativistic approximation. The system of self-consistent equations is solved by the method of successive refinements of functions. The solution is sought in the form of one Slater determinant or a linear combination of several determinants corresponding to a certain configuration and term.

The "ATOM" system of mathematical aids for atomic calculations

II. PROGRAM FOR CALCULATING THE HARTREE-FOCK WAVE FUNCTIONS OF DISCRETE AND CONTINUOUS SPECTRA IN THE FIELD OF A "FROZEN" ATOMIC CORE

Cipher:	APA002
Language:	ALGOL-60
Translator:	BESM-ALGOL
Program scope:	13001_8 cells
Description:	L.V. Chernysheva, N. Cherepkov, V. Radoevich Preprint FTI-487, Leningrad (1975)

The program calculates Hartree-Fock excited electron wave functions of discrete or continuous spectra in the field of a "frozen" atomic core - i.e. without self-consistency with the functions of the occupied states. The core + electron system can be characterized by a term or merely by the values of the projections of orbital moments and spins of electrons. The wave functions thus found are orthogonal to the occupied states. The phase is calculated for functions of the continuous spectrum.

The "ATOM" system of mathematical aids for atomic calculations

III. PROGRAM FOR CALCULATING GENERALIZED OSCILLATOR STRENGTHS OF ATOMS WITH WAVE FUNCTIONS IN THE HARTREE-FOCK APPROXIMATION AND WITH ALLOWANCE FOR MULTI-ELECTRON CORRELATIONS IN ONE TRANSITION

Cipher:	APA003
Language:	ALGOL-60
Translator:	BESM-ALGOL
Program scope:	15347_8 cells
Description:	L.V. Chernysheva, M.Ya. Amusya, S.I. Sheftel Preprint FTI-493, Leningrad (1975)

The program calculates generalized oscillator strengths of atoms with wave functions in the Hartree-Fock approximation (single-particle calculation) and with allowance for multi-electron correlations in the approximation of random phases with exchange. It enables one to take into account correlations only within the framework of one transition.

The "ATOM" system of mathematical aids for atomic calculations

IV. PROGRAM FOR CALCULATING GENERALIZED OSCILLATOR STRENGTHS OF ATOMS WITH ALLOWANCE FOR MULTI-ELECTRON CORRELATIONS IN TWO TRANSITIONS

Cipher:	APA004
Language:	ALGOL-60
Translator:	BESM-ALGOL
Program scope:	20277_8 cells
Description:	L.V. Chernysheva, M.Ya. Amusya, S.I. Sheftel Preprint FTI-495, Leningrad (1975)

The program calculates generalized oscillator strengths of atoms with wave functions in the Hartree-Fock approximation (single-particle calculation) and with allowance for multi-electron correlations in the approximation of random phases with exchange. It finds generalized oscillator strengths with allowance for correlations in two transitions simultaneously.

The system of programs entitled "The atom in the relativistic approximation.

THE INTERACTION OF GAMMA RADIATION AND OF THE NUCLEUS WITH THE ELECTRONS OF THE ATOM"

Cipher:	APF005-012
Language:	FORTRAN-CERN
Translator:	FORTRAN-DUBNA
System scope:	40000_8 cells
Description:	I.M. Band, M.B. Trzhaskovskaya, M.A. Listengarten (in press)

The proposed system of programs is designed for studying atomic structures by the Hartree-Fock method in the relativistic approximation and for investigating the processes involved in the interaction of gamma radiation and of the nucleus with the electrons of the atomic shell. At present, the system comprises the following programs:

APF005: Program for calculating the self-consistency of a field of an atom in accordance with Hartree-Fock with statistical allowance for exchange in accordance with Slater in the (HFSD) relativistic approximation;

APF006: Program for making the field of an atom self-consistent in the condensed state with boundary conditions of the Wigner-Seitz type in the (HFSD) approximation;

APF007: Calculation of radial wave functions of an electron in a discrete spectrum for any set of arguments;

APF008: Calculation of radial wave functions of an electron with boundary conditions of the Wigner-Seitz type for any set of arguments;

APF009: Calculation of radial wave functions of an electron in a continuous spectrum with definite orbital and total angular moments for any set of arguments;

APF010: Calculation of amplitudes at zero and phase differences at infinity of wave functions of continuous-spectrum electrons in the self-consistent field of an atom;

APF011: Calculation of coefficients of internal conversion of gamma radiation and of conversion matrix elements in any atomic shell with the "no penetration" and "surface currents" models;

APF012: Calculation of photo-effect cross-sections in the relativistic cross-section in any atomic shell.

Within the above range of problems the system of programs will be added to and expanded. Beside the programs enumerated, each of which has an independent field of application, the system includes a number of duty programs. The system is a closed one - i.e. it does not require the use of programs not forming part of it.

II. NUCLEAR PHYSICS

PROGRAM FOR CALCULATING PAIR MATRIX ELEMENTS FOR VELOCITY-INDEPENDENT NUCLEAR FORCES AND THE COULOMB INTERACTION IN A SPHERICALLY SYMMETRIC OSCILLATOR BASE (jj COUPLING SCHEME)

Cipher:	NPA001
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	12332_8 cells
Description:	V.I. Isakov, Yu.I. Kharitonov
	Preprint LIYaF-47, Leningrad (1973)

The program calculates pair matrix elements of Wigner, singlet, tensor and Coulomb forces. The base consists of two-particle wave vectors with a definite total angular momentum which are derived from single-particle wave functions of a spherically symmetric harmonic oscillator in accordance with the jj coupling scheme. The radial dependence of the forces can be in the form either of a δ-function or of a Gaussian well; in the latter case, there is provision for changing the interaction radius. The program enables one to calculate pair matrix elements for any single-particle states within the limits of the shell model. The Pauli principle is not taken into account in the variant of the program.

PROGRAM FOR CALCULATING ANTISYMMETRIC PAIR MATRIX ELEMENTS FOR VELOCITY-INDEPENDENT NUCLEAR FORCES AND THE COULOMB INTERACTION IN A SPHERICALLY SYMMETRIC OSCILLATOR BASE (jj COUPLING SCHEME)

Cipher:	NPA002
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	12722_8 cells
Description:	V.I. Isakov, Yu.I. Kharitonov
	Preprint LIYaF-47, Leningrad (1973)

This program is a variant of program NPA001, in which the same matrix elements are calculated with respect to antisymmetric two-particle wave functions.

PROGRAM FOR CALCULATING PAIR MATRIX ELEMENTS OF CENTRAL FORCES WITH SINGLE-PARTICLE WAVE FUNCTIONS IN SAXON-WOODS POTENTIALS AND A HARMONIC OSCILLATOR

Cipher:	NPFO03
Language:	FORTRAN-CERN
Translator:	FORTRAN-DUBNA
Program scope:	26210_8 cells
Description:	S.A. Artamonov, Yu.I. Kharitonov
	Preprint LIYaF-69, Leningrad (1973)

The first part of this program solves the single-particle Schrödinger equation with a Saxon-Woods potential, in which spin-orbit interaction and Coulomb potential are also taken into account. With the help of the single-particle wave functions obtained, the second part of the program constructs two-particle wave functions with a definite total angular momentum and calculates pair matrix elements of Wigner, spin-spin, singlet, triplet and Coulomb forces. The radial dependence of the forces can be in the form of a Gauss or a Yukawa potential, for which the action radius can be changed, and also in the form of a δ-function. For a given set of single-particle quantum numbers the matrix elements are calculated either for a given value of the total angular momentum or for all its possible values.

PROGRAM FOR CALCULATING PAIR MATRIX ELEMENTS OF THE n-p INTERACTION PRODUCED BY CENTRAL FORCES IN DEFORMED ODD-ODD NUCLEI

Cipher:	NPA004
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	12406_8 cells
Description:	I.S. Guseva, Yu.I. Kharitonov
	Preprint LIYaF-112, Leningrad (1974)

The program calculates pair matrix elements of Wigner and spin-spin forces. Functions describing the motion of a particle in a Nilsson potential are used as single-particle wave functions. The radial dependence of the forces can be in the form either of a Gaussian well, for which the action radius can be changed, or of a δ-function. For the program to function, one must introduce as numerical material the expansion coefficients of a single-particle wave function in a deformed potential with respect to wave functions of a spherically symmetric harmonic potential.

THE "DEPTH" PROGRAM FOR DETERMINING THE DEPTH OF A SPHERICALLY SYMMETRIC POTENTIAL FOR THE WAVE FUNCTION OF A NEUTRON WITH GIVEN QUANTUM NUMBERS

Cipher:	NPF005
Language:	FORTRAN-CERN
Translator:	FORTRAN-DUBNA
Program scope:	13504_8 cells
Description:	S.G. Ogloblin
	Preprint LIYaF-118, Leningrad (1974)

The "DEPTH" program determines the depth of a spherically symmetric Saxon-Woods potential at which a neutron - in a certain discrete state or near a single-particle resonance - has a given energy E. For a discrete spectrum, the state of the neutron is defined by specifying the main quantum number N, the orbital angular momentum ℓ and the total angular momentum j. For a continuous spectrum, near the single-particle resonance the state of the neutron is also defined by, in addition to the above quantum numbers, the scattering phase δ - $(45° \leq \delta_{\ell j} \leq 135°)$. Besides the potential well depth, the program gives values of the radial wave function as a function of the radius.

PAIR MATRIX ELEMENTS OF A TWO-PARTICLE SPIN-ORBIT INTERACTION IN A SPHERICALLY SYMMETRIC OSCILLATOR BASE (jj COUPLING SCHEME)

Cipher:	NPA006
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	12250_8 cells
Description:	V.I. Isakov, Yu.I. Kharitonov
	Preprint LIYaF-154, Leningrad (1975)

The program calculates pair matrix elements of a two-particle spin-orbit interaction. The base is comprised of two-particle wave functions with a certain total angular momentum derived from single-particle wave functions of a spherically symmetric harmonic oscillator in accordance with the jj coupling scheme. The radial dependence of the forces is in the form of a Gaussian well with a variable action radius. The program enables one to calculate matrix elements both between non-symmetrized wave functions (neutron-proton interaction) and between antisymmetric wave

functions (identical nucleons). In both cases, the matrix elements can be calculated either for one specified value of the total momentum J or for all its possible values. With this variant of the program one can use single-particle wave functions with a principal oscillator quantum number $N = 2n + l \leq 7$.

RADIAL INTEGRALS OF A PAIR INTERACTION FOR GAUSS, DELTA-SHAPED AND COULOMB POTENTIALS IN AN OSCILLATOR BASE

Cipher:	NPA007
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	10305_8 cells
Description:	V.I. Isakov, Yu.I. Kharitonov, I.V. Nikitina (in press)

The program calculates pair radial integrals for Gauss, delta-shaped and Coulomb potentials in a spherically symmetric oscillator base. For specified single-particle quantum numbers of the four wave functions, the radial integrals are calculated for all possible ranks, which are resolved by the selection rules attributable to the angular parts of the corresponding total matrix elements of the residual interaction. With this program, which is based on program NPA001, one can use single-particle radial functions relating to states with the principal oscillator quantum number $N = 2n + l \leq 7$.

PROBABILITIES OF ELECTROMAGNETIC TRANSITIONS IN ODD DEFORMED NUCLEI

Cipher:	NPA008
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	15000_8 cells
Description:	I.S. Guseva, Yu.I. Kharitonov (in press)

The type and multipolarity (xL) of the most intense gamma transitions (not more than two) are determined on the basis of specified characteristics of the initial and final states of an odd deformed nucleus. On the basis of the Nilsson model, the reduced probabilities B(xL), the probabilities W(xL) and the partial half-lives $T_{\frac{1}{2}}$ are calculated for these electromagnetic transitions. The wave functions of the initial and final states are found by means of a sub-program which solves the Schrödinger equation with a Nilsson potential and which is one of the procedures making up the program.

Consequently, as characteristics of the initial and final states it is enough to specify the level spins, their projections onto the symmetry axis of the nucleus and the asymptotic quantum numbers of the corresponding Nilsson orbitals. Provision is made for varying the deformation parameter and other parameters of the potential.

PROBABILITIES OF ELECTROMAGNETIC TRANSITIONS IN ODD-ODD DEFORMED NUCLEI

Cipher:	NPA009
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	16334_8 cells
Description:	I.S. Guseva (in press)

The type and multipolarity (xL) of the most intense transitions (not more than two) are determined on the basis of specified characteristics of the initial and final states of an odd-odd deformed nucleus. The reduced probabilities B(xL), the probabilities W(xL) and partial half-lives $T_{\frac{1}{2}}$ are calculated for these electromagnetic transitions. The single-particle wave functions of the neutron and proton are calculated by means of a sub-program which solves the Schrödinger equation with a Nilsson potential and which is one of the procedures making up the program. All possible neutron and proton wave function coupling schemes are considered. Provision is made for varying the deformation parameter and other parameters of the Nilsson potential.

PAIR MATRIX ELEMENTS OF A TWO-PARTICLE SPIN-ORBIT NEUTRON-PROTON INTERACTION (OSCILLATOR BASE)

Cipher:	NPA010
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	13251_8 cells
Description:	I.S. Guseva (in press)

The program calculates pair matrix elements of a two-particle spin-orbit interaction. The base is comprised of two-particle wave functions with a certain total angular momentum derived from single-particle wave functions of a spherically symmetric harmonic oscillator in accordance with the jj coupling scheme. The radial dependence of the forces is in the form of a Gaussian well with a variable action radius. The method of calculating pair matrix elements is based on the use of Talmi-Moshinsky coefficients,

which enable one to isolate in a two-particle wave function the movement of the centre of gravity and the relative motion. This program duplicates program NPA006. Hence, the two programs, which calculate the same matrix elements but by completely different methods, can be used for mutual verification of the correctness of the calculations performed.

THE "DISP" PROGRAM FOR CALCULATING THE DISCRETE SPECTRUM OF THE INTRINSIC ENERGIES AND EIGENWAVE FUNCTIONS OF A SINGLE-PARTICLE SCHRÖDINGER EQUATION WITH A SPHERICAL POTENTIAL OF FINITE DEPTH

Cipher:	NPF011
Language:	FORTRAN-CERN
Translator:	FORTRAN-DUBNA
Program scope:	25364_8 cells
Description:	L.P. Lapina (in press)

The "DISP" program solves a radial Schrödinger equation with a Saxon-Woods potential in which Batty-Greenlees parametrization (Nuclear Physics A 133 (1969) 673) is used. The possibility is provided of solving this equation for any other spherically symmetric potential of finite depth. With the "DISP" program it is possible to obtain the whole discrete spectrum of energies, calculate the energies of several levels for specified initial approximations and determine the radial wave function and its derivative with respect to the argument at a specified energy for one level.

THE "ME2P1H" PROGRAM FOR CALCULATING MATRIX ELEMENTS OF A RESIDUAL INTERACTION FOR STATES OF THE TYPE 2p-1h (CENTRAL FORCES)

Cipher:	NPF012
Language:	FORTRAN-CERN
Translator:	FORTRAN-DUBNA
Program scope:	45716_8 cells
Description:	S.A. Artamonov, S.G. Ogloblin (in press)

The "ME2P1H" program is designed for calculating, in spherical nuclei, matrix elements of a residual nucleon-nucleon interaction produced by Wigner and singlet forces for states of the type 2p-1h. The radial dependence of the forces can be in the form either of a δ-potential or of Gauss or Yukawa potentials. Single-particle wave functions are calculated in a Saxon-Woods potential. The wave functions of states of the type 2p-1h are constructed as follows: first the angular momenta of the particles are added, the resulting momentum then being added together with the angular momentum of the hole to the total spin of the state under consideration. There is provision for the transfer of the calculated matrix elements

to external storage (magnetic tape, drum, disk, punched cards) for further processing.

EIGENVALUES AND EIGENFUNCTIONS OF A SINGLE-PARTICLE MODEL OF A NUCLEUS WITH A FINITE DEFORMED POTENTIAL HAVING A BLURRED EDGE; SPECIFICATION OF THE SHAPE OF THE NUCLEAR SURFACE IN THE LEMNISCATE SYSTEM OF CO-ORDINATES

Cipher:	NPFO13
Language:	FORTRAN-CERN
Translator:	FORTRAN-DUBNA
Program scope:	35633_8 cells
Description:	V.V. Pashkevich, V.A. Rubchenya (in press)

The program is designed for calculating the single-particle spectrum and eigenvectors of single-particle states in a nuclear potential of finite depth with a blurred edge. The shape of the nucleus is specified in lemniscate co-ordinates. This enables one to perform calculations for axially symmetric nuclei, the shape of which may vary from oblate to separation of the nucleus into two fragments. The eigenvalue problem is solved by the diagonalization method. Functions of a deformed, axially symmetric, oscillator potential are used as the base set of functions.

III. QUANTUM MECHANICS

PROGRAM FOR CALCULATING CLEBSCH-GORDAN COEFFICIENTS WITH ZERO MAGNETIC QUANTUM NUMBERS

Cipher:	QMA001, QMF001
Language:	ALGOL-60, FORTRAN-CERN
Translator:	ALGOL-GDR, FORTRAN-DUBNA
Program scope:	6735_8 and 6602_8 cells respectively
Description:	S.A. Artamonov, V.I. Isakov, Yu.I. Kharitonov Preprint LIYaF-73, Leningrad (1973)

These programs enable one to calculate the values of individual Clebsch-Gordan coefficients with zero magnetic quantum numbers provided that the arithmetic sum of the angular momenta under consideration does not exceed 43. Print-out both of the initial parameters and of the computational results in tabular form is provided for. The procedures (sub-programs) making up these programs can be used as ready blocks when programming the more complex problems which contain such coefficients as component parts.

PROGRAMS FOR CALCULATING CLEBSCH-GORDAN COEFFICIENTS OF A GENERAL FORM

Cipher:	QMA002, QMF002
Language:	ALGOL-60, FORTRAN-CERN
Translator:	ALGOL-GDR, FORTRAN-DUBNA
Program scope:	7167_8 and 7133_8 cells respectively
Description:	S.A. Artamonov, V.I. Isakov, Yu.I. Kharitonov Preprint LIYaF-73, Leningrad (1973)

The programs enable one to calculate values of individual Clebsch-Gordan coefficients for specified values of three angular momenta and also their projections provided that the arithmetic sum of the angular momenta under consideration does not exceed 43. Print-out both of the initial parameters and of the computational results in tabular form is provided for. The procedures (sub-programs) making up these programs can be used as ready blocks when programming the more complex problems, which contain Clebsch-Gordan coefficients of a general form as component parts.

PROGRAMS FOR CALCULATING RACAH COEFFICIENTS

Cipher:	QMA003, QMF003
Language:	ALGOL-60, FORTRAN-CERN
Translator:	ALGOL-GDR, FORTRAN-DUBNA
Program scope:	7005_8 and 7113_8 cells respectively
Description:	V.N. Guman, S.A. Artamonov, Yu.I. Kharitonov Preprint LIYaF-76, Leningrad (1973)

These programs enable one to calculate the values of individual Racah coefficients provided that the factorals n! encountered in the calculations are limited by the quantity n! = 44. This range of variations of the parameters is quite sufficient for most spectroscopic calculations. Print-out of the initial parameters and of the computational results in tabular form is provided for. The procedures (sub-programs) making up these programs can be used in solving those problems which contain Racah coefficients as component parts.

PROGRAMS FOR CALCULATING 9j-SYMBOLS

Cipher:	QMA004, QMF004
Language:	ALGOL-60, FORTRAN-CERN
Translator:	ALGOL-GDR, FORTRAN-DUBNA
Program scope:	7160_8 and 7364_8 cells respectively
Description:	S.A. Artamonov, Yu.I. Kharitonov Preprint LIYaF-116, Leningrad (1974)

The program enables one to calculate individual values of 9j-symbols provided that the arithmetic sum of the angular momenta in any of the six triads does not exceed 43; this is quite sufficient for most spectroscopic calculations. Print-out of the initial parameters and of the computational results in tabular form is provided for. The procedures (sub-programs) making up these programs can be used in solving those problems which contain 9j-symbols as component parts. There is some limitation to the program for calculating 9j-symbols which forms part of the ALGOL program whose text is presented in Preprint LIYaF-116. In the Comment on the program for calculating 9j-symbols published in the present Bulletin, this question is considered in detail and the text of the corrected procedure is presented.

PROGRAM FOR CALCULATING $d^{I}_{MM'}(\beta)$ WIGNER FUNCTIONS

Cipher:	QMA005
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	7435_8 cells
Description:	I.S. Guseva
	Preprint LIYaF-124, Leningrad (1974)

The program calculates $d^{I}_{MM'}(\beta)$ Wigner functions with given quantum numbers I, M and M' and angle β varying through 5° intervals from 0° to 90°. Quantum numbers I, M and M' can assume whole and semi-whole values. For angles greater than 90°, d-function values are easy to obtain by using the appropriate relation presented in the preprint. Print-out of the initial parameters and of the computational results in tabular form is provided for.

THE "CFP1A" PROGRAM FOR CALCULATING GENEALOGIC COEFFICIENTS OF SEPARATION OF A SINGLE PARTICLE FOR ANTISYMMETRIC STATES OF IDENTICAL FERMIONS (jj COUPLING SCHEME)

Cipher:	QMF006
Language:	FORTRAN-CERN
Translator:	FORTRAN-DUBNA
Program scope:	54727_8 cells
Description:	S.A. Artamonov, Yu.I. Kharitonov (in press)

The "CFP1A" program calculates genealogic coefficients of separation of a single particle (GCl) from antisymmetric states $|j^n s\alpha JM\rangle$ constructed in accordance with the jj coupling scheme and belonging to configurations of the type $\{j^n\}$. For angular momenta j = 5/2, 7/2, 9/2 and 11/2, the GCls are calculated with a number of particles n ranging from 3 to j + 1/2 for j = 13/2 with n = 3, 4 and for j = 15/2 only for three-particle states. At the same time, the GCls are calculated for all possible values of the total angular momentum J, of the seniority quantum number s and the additional quantum number α. The GCls can be calculated either for the whole parameter variation range indicated above or for any part of it. Print-out of the computational results in the form of tables similar to those of Bayman and Lande (Nuclear Physics 77 (1966) 1) is provided for, as is external storage of the results (on magnetic tape, drum, disk, punched cards). The GCls are calculated by diagonalizing matrices of Casimir operators of a special unitary and a symplectic group.

THE "CFP1B" PROGRAM FOR CALCULATING GENEALOGIC COEFFICIENTS OF SEPARATION OF A SINGLE PARTICLE FOR ANTISYMMETRIC STATES OF IDENTICAL FERMIONS (jj COUPLING SCHEME) IN QUANTUM-MECHANICAL COMPUTATIONS

Cipher:	QMF007
Language:	FORTRAN-CERN
Translator:	FORTRAN-DUBNA
Program scope:	10763_8 cells
Description:	S.A. Artamonov, Yu.I. Kharitonov (in press)

The "CFP1B" program is designed for use as a sub-program in the case of quantum-mechanical problems where it is necessary to calculate various quantities which include a GCl. The range of variation of the parameters for which GCls can be calculated is the same as in the case of program "CFP1A" (see above). Program "CFP1B" is used for economizing on internal memory, it transfers the GCls calculated by program "CFP1A" from external storage (magnetic tape, drum, disk, punched cards) into the internal memory. The transfer is effected on the basis of specified parameters which uniquely determine the desired set of GCls. The parallel print-out of GCls in tabular form is provided for.

PROGRAM FOR CALCULATING CLEBSCH-GORDAN COEFFICIENTS IN SIMPLE FRACTIONS

Cipher:	QMA008
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	23462_8 cells
Description:	T.V. Alenicheva (in press)

The program enables one to calculate Clebsch-Gordan coefficients in the form $(a/b)\sqrt{c/d}$, where a is a whole number (with a sign), b, c and d are natural numbers, and a/b and c/d are irreducible fractions. The form $(a/b)\sqrt{c/d}$ is a general one; if the value obtained for the Clebsch-Gordan coefficients has an arithmetically simpler form, the corresponding simplified expression is printed out. Clebsch-Gordan coefficients in a form which is convenient for theoretical calculations by hand should if possible be used before they become cumbersome. This limits the range of variation of the initial parameters and thus determines the possibilities of the program. The present program enables one to calculate Clebsch-Gordan coefficients in the form indicated as long as the arithmetic sum of the

three momenta under consideration does not exceed 36. The values of the initial parameters and the computational results are printed out in the form indicated and also in the form of a decimal fraction.

PROGRAM FOR CALCULATING RACAH COEFFICIENTS IN SIMPLE FRACTIONS

Cipher:	QMA009
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	22512_8 cells
Description:	T.V. Alenicheva (in press)

The program enables one to calculate individual Racah coefficients in the form $(a/b)\sqrt{c/d}$, where a is a whole number (with a sign), b, c and d are natural numbers, and a/b and c/d are irreducible fractions. The program is best used in cases where the arithmetic sum of the angular momenta in any of the four coefficient triads does not exceed 36. With higher triad values, the expressions for the Racah coefficients become very cumbersome and hence inconvenient for calculations by hand. The form of print-out of the initial data and the computational results is the same as in the case of program QMA008.

TALMI-MOSHINSKY TRANSFORMATION COEFFICIENTS

Cipher:	QMA010
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	10358_8 cells
Description:	I.S. Guseva (in press)

This program calculates Talmi-Moshinsky transformation coefficients, which enable one to go from a description of the independent motion of two particles in the field of a three-dimensional spherically symmetric harmonic oscillator to a description of the movement of the centre of gravity of these particles and of their relative motion. Print-out of the initial parameters and of the computational results in tabular form is provided for. The program is based on a procedure-function which can be used in more complex calculations involving Talmi-Moshinsky coefficients.

PROGRAMS FOR CALCULATING 12j-SYMBOLS OF THE FIRST AND SECOND KIND

Cipher:	QMA011, QMF011
Language:	ALGOL-60, FORTRAN-CERN
Translator:	ALGOL-GDR, FORTRAN-DUBNA
Program scope:	10427_8 and 11023_8 cells respectively
Description:	B.F. Gerasimenko, V.K. Khersonsky (in press)

These programs enable one to calculate the values of individual 12j-symbols of both the first and the second kind provided that the sum of the elements in any of the eight triads which can be constructed from the parameters of a 12j-symbol does not exceed 48. The same condition must be fulfilled for a minimum value of the doubled sums of pairs of corresponding parameters of the upper and lower lines in a 12j-symbol of the first kind - or only of the lower line for a 12j-symbol of the second kind. Such a range of variation of the parameters of 12j-symbols is quite sufficient for most spectroscopic calculations. The programs can be used as sub-programs in solving problems which involve 12j-symbols. Print-out of the initial parameters and of the computational results in tabular form is provided for.

PROGRAM FOR CALCULATING $d^{I}_{MM'}(\beta)$ WIGNER FUNCTIONS

Cipher:	QMA012
Language:	ALGOL-60
Translator:	ALGOL-GDR
Program scope:	7160_8 cells
Description:	I.S. Guseva Preprint LIYaF-124, Leningrad (1974)

The program calculates $d^{I}_{MM'}(\beta)$ Wigner functions with given quantum numbers I, M and M' for any range of variation of the angle β between 0° and 90° with any given increment (or step). Quantum numbers I, M and M' can assume whole and semi-whole values. Print-out of the initial data and computational results in tabular form is provided for.