A computer program is presented by which one may calculate the multiple electric dipole, electric quadrupole and magnetic dipole Coulomb excitation with relativistic heavy ions. The program applies to an arbitrary nucleus, specified by the spins and energies of the levels and by all E1, E2 and M1 matrix elements. Nuclear excitation is calculated optionally for monopole, dipole and quadrupole excitations and needs inputs of optical potentials. For given bombarding conditions, the differential cross sections and statistical tensors (useful to calculate $\gamma$-ray angular distribution functions) are computed.

1 Introduction

Relativistic Coulomb Excitation (RCE) is a well established tool to unravel interesting aspects of nuclear structure [1, 2]. The RCE induced by large-Z projectiles and/or targets, often yields large cross sections in grazing collisions. This results from the large nuclear response (specially in the region of the giant resonances) to the acting electromagnetic fields. As a consequence, a strong coupling between the excited states is expected. The present report describes a computer program for the calculation of multiple excitation among a finite number of nuclear states. The system of coupled differential equations for the time-dependent amplitudes of the eigenstates of the free nucleus is solved numerically for electric dipole (E1), electric quadrupole (E2), and magnetic dipole (M1) excitations. If the optical potential for the system is given, the program can also calculate the amplitudes for (nuclear) monopole, dipole and quadrupole excitations. All nuclear quantities, either known from experiments or calculated from a model, as well as the conditions realized in the experiment, are explicitly specified as input parameters. The program then computes the Coulomb+nuclear excitation probabilities and cross sections as well as the statistical tensors for the angular distribution of the $\gamma$-quanta.

2 The semiclassical method for the CC-problem

In relativistic heavy ion collisions, the wavelength associated to the projectile-target relative motion is much smaller than the characteristic lengths of the system. It is,

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therefore, a reasonable approximation to treat $r$ as a classical variable $r(t)$, given at each instant by the trajectory followed by the relative motion. At high energies it is also a good approximation to replace this trajectory by a straight line. The intrinsic dynamics can then be handled as a quantum mechanics problem with a time dependent Hamiltonian. This treatment is discussed in full details by Alder and Winther in ref. [3].

The intrinsic state $|\psi(t)\rangle$ satisfies the Schrödinger equation

\[
\{H_0 + V[\mathbf{r}(t)]\} |\psi(t)\rangle = i\hbar \frac{\partial |\psi(t)\rangle}{\partial t}. \tag{1}
\]

Above, $H_0$ is the intrinsic Hamiltonian and $V$ is the channel-coupling interaction.

Expanding the wave function in the set $\{ |k\rangle; \ k = 1, N \}$ of eigenstates of $H_0$, where $N$ is the number states included in the coupled-channels (CC) problem, we obtain a set of coupled equations. Taking the scalar product with each of the states $<j |$, we get

\[
i\hbar \dot{a}_k(t) = \sum_{j=1}^{N} \langle k | V(t) | j \rangle \exp [i(E_k - E_j)t/\hbar] \ a_j(t), \quad k, j = 1 \text{ to } N. \tag{2}
\]

where $E_n$ is the energy of the state $|n\rangle$. It should be remarked that the amplitudes depend also on the impact parameter $b$ specifying the classical trajectory followed by the system. For the sake of keeping the notation simple, we do not indicate this dependence explicitly. We write, therefore, $a_n(t)$ instead of $a_n(b,t)$. Since the interaction $V$ vanishes as $t \to \pm \infty$, the amplitudes have as initial condition $a_n(t \to -\infty) = \delta_{n1}$ and they tend to constant values as $t \to \infty$.

A convenient measure of time is given by the dimensionless quantity $\tau = \gamma vt/b$, where $\gamma = (1 - v^2/c^2)^{-1/2}$ is the Lorentz factor for the projectile velocity $v$. A convenient measure of energy is $E_0 = \gamma \hbar v/b$. In terms of these quantities the CC equations become

\[
\frac{da_k(\tau)}{d\tau} = -i \sum_{j=1}^{N} \langle k | W(\tau) | j \rangle \exp (i\xi_{kj}\tau) \ a_j(\tau); \quad W(\tau) = \frac{V(\tau)}{E_0}; \quad \xi_{kj} = \frac{E_k - E_j}{E_0}. \tag{3}
\]

The nuclear states are specified by the spin quantum numbers $I$ and $M$. Therefore, the excitation probability of an intrinsic state $|n\rangle \equiv |I_n, M_n\rangle$ in a collision with impact parameter $b$ is obtained from an average over the initial orientation $(M_1)$, and a sum over the final orientation of the nucleus, respectively:

\[
P_n(b) = \frac{1}{2I_1 + 1} \sum_{M_1, M_n} |a_{I_n, M_n}(M_1)|^2. \tag{4}
\]

The total cross section for excitation of the state $|n\rangle$ is obtained by the classical expression

\[
\sigma_n = 2\pi \int P_n(b) \, b \, db. \tag{5}
\]
2.1 Coulomb excitation

We consider a nucleus 2 which is at rest and a relativistic nucleus 1 which moves along the z-axis. Nucleus 2 is excited from the initial state $|I_jM_j\rangle$ to the state $|I_kM_k\rangle$ by the electromagnetic field of nucleus 1. The nuclear states are specified by the spin quantum numbers $I_j$, $I_k$ and by the corresponding magnetic quantum numbers $M_j$ and $M_k$. We assume that the relativistic nucleus 1 moves along a straight-line trajectory with impact parameter $b$, which is therefore also the distance of the closest approach between the center of mass of the two nuclei at the time $t = 0$. The interaction, $V_C(t)$, due to the electromagnetic field of the nucleus 1 acting on the charges and currents nucleus 2 can be expanded into multipoles, as explained in ref.\cite{4}. One has

$$W_C(\tau) = \frac{V_C(\tau)}{E_0} = \sum_{\pi\lambda\mu} W_{\pi\lambda\mu}(\tau),$$

where $\pi = E, M$ denotes electric and magnetic interactions, respectively, and (misprints in ref.\cite{4} have been corrected)

$$W_{\pi\lambda\mu}(\tau) = (-1)^{\lambda+1} \frac{Z_1 e \ 1}{\hbar v b^\lambda \lambda} \sqrt{\frac{2\pi}{(2\lambda + 1)!!}} Q_{\pi\lambda\mu}(\xi, \tau) \mathcal{M}(\pi\lambda, \mu),$$

where $\mathcal{M}(\pi\lambda, \mu)$ is the multipole moment of order $\lambda\mu$,

$$\mathcal{M}(E\lambda, \mu) = \int d^3r \rho(r) \ r^\lambda Y_{1\mu}(r),$$

and

$$\mathcal{M}(M1, \mu) = \frac{-i}{2c} \int d^3r \ J(r).L (rY_{1\mu}),$$

$\rho (J)$ being the nuclear charge (current). The quantities $Q_{\pi\lambda\mu}(\tau)$ were calculated in ref.\cite{4}, and for the E1, E2, and M1 multipolarities are given by

$$Q_{E10}(\xi, \tau) = \gamma \sqrt{2} \left[ \tau \phi^3(\tau) - i \xi \left( \frac{V}{c} \right)^2 \phi(\tau) \right]; \quad Q_{E1\pm1}(\xi, \tau) = \mp \phi^3(\tau),$$

$$Q_{M10}(\xi, \tau) = 0; \quad Q_{M1\pm1}(\xi, \tau) = i \left( \frac{V}{c} \right) \phi^3(\tau),$$

and

$$Q_{E20}(\xi, \tau) = \gamma^2 \sqrt{6} \left[ (2\tau^2 - 1) \phi^5(\tau) - i \xi \left( \frac{V}{c} \right)^2 \tau \phi^3(\tau) \right];$$

$$Q_{E2\pm1}(\xi, \tau) = \pm \gamma \left[ 6 \tau \phi^5(\tau) - i \xi \left( \frac{V}{c} \right)^2 \phi^3(\tau) \right]; \quad Q_{E2\pm2}(\tau) = 3 \phi^5(\tau),$$

3
where $\phi(\tau) = (1 + \tau^2)^{-1/2}$.

We use here the notation of Edmonds [5] where the reduced multipole matrix element is defined by

$$M_{kj}(E\lambda, \mu) = (-1)^{I_k-M_k} \left( \begin{array}{ccc} I_k & \lambda & I_j \\ -M_k & \mu & M_j \end{array} \right) < I_k || M(E\lambda) || I_j >$$

To simplify the expression (3) we introduce the dimensionless parameter $\psi_{kj}^{(\lambda)}$ by the relation

$$\psi_{kj}^{(\lambda)} = (-1)^{\lambda+1} \frac{Z_1 e}{h v b^\lambda} \lambda \sqrt{\frac{2\pi}{(2\lambda + 1)!}} M_{kj}(E\lambda)$$

Then we may write eq. 3 in the form

$$\frac{da_k(\tau)}{d\tau} = -i \sum_{r=1}^{N} \sum_{\pi\lambda\mu} Q_{\pi\lambda\mu}(\xi_{kj}, \tau) \psi_{kj}^{(\lambda)} \exp(i\xi_{kj}\tau) a_j(\tau) .$$

The fields $Q_{\pi\lambda\mu}(\xi, \tau)$ peak around $\tau = 0$, and decrease rapidly within an interval $\Delta\tau \simeq 1$, corresponding to a collisional time $\Delta t \simeq b/\gamma v$. This means that numerically one needs to integrate the CC equations in time within an interval of range $n \times \Delta\tau$ around $\tau = 0$, with $n$ equal to a small integer number.

### 2.2 Nuclear excitation

In peripheral collisions the nuclear interaction between the ions can also induce excitations. According to the Bohr-Mottelson particle-vibrator coupling model, the matrix element for the transition $j \rightarrow k$ is given by

$$V_{N(\lambda\mu)}^{(kj)}(r) \equiv < I_k M_k | V_{N(\lambda\mu)} | I_j M_j > = \frac{\delta_\lambda}{\sqrt{2\lambda + 1}} < I_k M_k | Y_{\lambda\mu} | I_j M_j > Y_{\lambda\mu}(\hat{r}) U_\lambda(r)$$

where $\delta_\lambda$ is the vibrational amplitude and $U_\lambda(r)$ is the transition potential.

The transition potentials for nuclear excitations can be related to the optical potential in the elastic channel. This is discussed in details in ref. [6]. The transition potentials for isoscalar excitations are

$$U_0(r) = 3U_{opt}(r) + r \frac{dU_{opt}(r)}{dr} ,$$

for monopole,

$$U_1(r) = \frac{dU_{opt}}{dr} + \frac{1}{3} R_0 \frac{d^2U_{opt}}{dr^2} ,$$

for dipole, and
\[ U_2(r) = \frac{dU_{opt}(r)}{dr}, \]  

(18)

for quadrupole modes.

The time dependence of the matrix elements above can be obtained by making a Lorentz boost. One gets

\[ V_{N\lambda\mu}(r) = \gamma \frac{\delta\lambda}{\sqrt{2\lambda + 1}} < I_k M_k | Y_{\lambda\mu} | I_j M_j > Y_{\lambda\mu}(\theta(t), 0) U_\lambda [r(t)], \]  

(19)

where \( r(t) = \sqrt{b^2 + \gamma^2 v^2 t^2} = \frac{1}{(b \phi(\tau))}, \theta = \tau \phi(\tau), \) and

\[ < I_k M_k | Y_{\lambda\mu} | I_j M_j > = (-1)^{I_k - M_k} \frac{(2I_k + 1)(2\lambda + 1)}{4\pi(2I_j + 1)} \left( \begin{array}{ccc} I_k & \lambda & I_j \\ -M_k & \mu & M_j \end{array} \right) \left( \begin{array}{ccc} I_k & \lambda & I_j \\ 0 & 0 & 0 \end{array} \right). \]  

(20)

To put it in the same notation as in eq. (14), we define \( Q_{N\lambda\mu}(\tau) = V_{N\lambda\mu}(r)/E_0, \) and the coupled-channels equations become

\[ \frac{da_k(\tau)}{d\tau} = -i \sum_{j=1}^{N} \sum_{\lambda\mu} \left[ Q^{(kj)}_{N\lambda\mu}(\tau) + \sum_{\pi} Q_{\pi\lambda\mu}(\kappa(kj), \tau) \psi^{(\pi)}_{kj} \right] \exp(i\kappa_{kj}(\tau)) a_j(\tau). \]  

(21)

### 2.3 Absorption at small impact parameters

If the optical potential \( U_{opt}(r) \) is known, the absorption probability in grazing collisions can be calculated in the eikonal approximation as

\[ A(b) = \exp \left[ \frac{2}{\hbar v} \int_{-\infty}^{\infty} \Im[U_{opt}(r)] \, dz \right], \]  

(22)

where \( r = \sqrt{b^2 + z^2}. \) If the optical potential is not known, the absorption probability can be calculated from the optical limit of the Glauber theory of multiple scattering, which yields:

\[ A(b) = \exp\left\{ -\sigma_{NN} \int_{-\infty}^{\infty} \left[ \int \rho_1(r') \rho_2(r - r') \, d^3r' \right] \, dz \right\}, \]  

(23)

where \( \sigma_{NN} = 40 \text{ mb} \) is the nucleon-nucleon cross section in high energy collisions and \( \rho_i \) is the ground state density of the nucleus \( i. \) These densities are taken from the droplet model densities of Myers and Swiatecki [7], but can be easily replaced by more realistic densities.

Including absorption, the total cross section for excitation of the state \( |n > \) is obtained by

\[ \sigma_n = 2\pi \int A(b) P_n(b) \, b \, db. \]  

(24)
2.4 Coulomb recoil correction

At intermediate bombarding energies a correction of the excitation amplitudes due to Coulomb recoil can be easily introduced. The excitation occurs most probably when the nuclei are closer along the trajectory. But then, due to recoil, they are displaced by an extra distance of order of $a_0/\gamma$, where $a_0 = Z_1 Z_2 e^2 / m_0 v^2$. It is thus expected that one should correct the amplitudes by a rescaling of the impact parameter. In ref. [1] it was shown that a comparison between the Rutherford integrals with large angular momenta for the non-relativistic case with the straight-line integrals for the relativistic case yields a reasonable correction. It amounts in the replacement of $b$ of $P_n(b)$ in equation (24) (and also in $A(b)$ of eq. (22)) by $b' = b + \pi a_0/2 \gamma$, i.e., for a given impact parameter $b$ the excitation amplitudes and probabilities are calculated for $b'$.

2.5 Gamma-ray angular distributions

As for the non-relativistic case [8, 3], the angular distributions of gamma rays following the excitation depend on the frame of reference used. In our notation, the z-axis corresponds to the beam axis, and the statistical tensors are given by

$$A_{k\kappa}(N) = \frac{(2I_N + 1)^{1/2}}{(2I_1 + 1)} \sum_{M_N = -(M'_N + \kappa), M'_N} (-1)^{I_N + M_N} \binom{I_N}{M_N} \binom{I_N}{M'_N} \binom{k}{\kappa} \times \sum_{M_1} a^*_I_{N,M'_N}(M_1) a_{I_N,M_N}(M_1) ,$$

where $N$ is the state from which the gamma ray is emitted, and 0 denotes the initial state of the nucleus, before the excitation. To calculate the angular distributions of the gamma rays one needs the statistical tensors for $k = 0, 2, 4$ and $-k \leq \kappa \leq k$. Since the nuclear levels are not only populated by Coulomb excitation but also by internal conversion and gamma transitions cascading down from higher states, the angular distributions depend not only on the $\gamma$-transition rates, $\delta_{N \rightarrow M}$ (for all $M$'s), but also on the internal conversion coefficients, $\alpha_{N \rightarrow M}$. With those parameters at hand one calculates the angular distributions of gamma rays, $dW_{\gamma N \rightarrow M} / d\Omega_{\gamma}$, by using the equations given in section IV of ref. [8] (also reprinted in [3]).

3 Computer program and user’s manual

The units used in the program are fm (Fermis) for distances and MeV for energies. The output cross sections are given in millibarns.
3.1 Input parameters

To avoid exceeding use of computer’s memory, the file RELEX.DIM contains the dimension of the arrays and sets in the maximum number of levels (NMAX), maximum total number of magnetic substates, (NSTMAX), maximum number of impact parameters (NBMAX), and maximum number of coordinates points used in the optical potentials and absorption factors, (NGRID).

The integrals appearing in eqs. (22-24) are performed by the 1/3-Simpson’s integration rule. It is required that NGRID be a even number, since an extra point (origin) is generated in the program.

The file RELEX.IN contains all other input parameters. These are

1. AP, ZP, AT, ZT, which are the projectile and the target mass and charge numbers, respectively.
2. ECA, the bombarding energy per nucleon in MeV.
3. EX(j) and SPIN(j): the energy and spins of the individual states j.
4. MATE1(j,k), MATE2(j,k), MATM1(j,k), the reduced matrix elements for E1, E2 and M1 excitations, j → k, (as defined in (13)).
5. DELTE(0,j), DELTE(1,j), DELTE(2,j), the deformation parameters for monopole, dipole and quadrupole nuclear excitations, entering eq. (19).

The input cards in file RELEX.IN are organized as following:

1. First data card: AP, ZP, AT, ZT, ECA, IW, IOUT.
   - IW = 0 (or 1) for projectile (or target) excitation
   - IOUT = 0 (or 1) for output (or not) of statistical tensors. The statistical tensors are calculated for each impact parameter, so that one can use them in the computation of \( dP_{\gamma N \rightarrow M}(b)/d\Omega_{\gamma} = P_{N}(b).dW_{\gamma N \rightarrow M}/d\Omega_{\gamma} \).

2. Second data card: NB, ACCUR, BMIN, ITOT
   - NB = number of points in impact parameter mesh.
   - ACCUR = accuracy required for the time integration of the CC-equations for each impact parameter. A reasonable value is ACCUR = 0.001, i.e., 0.1%.
   - BMIN = minimum impact parameter (can be set to zero).
   - ITOT = 1 (0) prints (does not print) out impact parameter probabilities.

3. Third data card: IOPW, IOPNUC
   - IOPW is an option to use (or not) an optical potential: IOPW = 1 (0).
If the optical potential is provided (IOPW = 1), it should be stored in file IOPW.IN in rows of R x Real[U(R)] x Imag[U(R)]. The first row in this file gives the number of rows (maximum = NGRID). The program makes an interpolation to obtain intermediate values.

IOPNUC = 1 (0) is an option to compute (or not) nuclear excitation.

4. Fourth data card: NST
   Number of nuclear levels.

5. Fifth and following data cards: J, EX(J), SPIN(J)
   Input of state labels (J), energy (EX), and angular momentum (SPIN). J ranges from 1 to NST and should be listed in increasing value of energies.

6. Following data cards: J, K, MATE1(J,K), MATE2(J,K), MATM1(J,K)
   Reduced matrix elements for electromagnetic E1, E2 and M1 excitations:
   MATE1(j→k), for electric dipole transitions, MATE2(j→k), for electric quadrupole transitions, MATM1(j→k), for magnetic dipole transitions. Matrices for reorientation effects, i→i, can also be given.
   To end reading the matrix elements add a row of zeros for each column.

7. Following data cards: K, DELTE (0,K), DELTE(1,K), DELTE(2,K)
   If IOPNUC = 1 these rows give the values of deformation parameters for monopole, dipole and quadrupole nuclear excitations, respectively, for each excited state K.

3.2 Computer program

The program starts with a catalogue of the nuclear levels by doing a correspondence of integers to each magnetic substate. J = 1 corresponds to the lowest energy level, with the magnetic quantum number $M_1 = -I_1$. J increases with $M_1$ and so on for the subsequent levels.

A mesh in impact parameter is done, reserving half of the impact parameter points, i.e., $NB/2$, to a finer mesh around the grazing impact parameter, defined as $b_0 = 1.2 \left( A_p^{1/3} + A_T^{1/3} \right)$ fm. The interval $b_0/2 \text{ fm} \leq b \leq 3b_0/2 \text{ fm}$ is covered by this mesh. A second mesh, with the other half of points, extends from $b = 3b_0/2 \text{ fm}$ to $b = 200 \text{ fm}$. Except for the very low excitation energies ($E_j \ll 1 \text{ MeV}$), combined with very large bombarding energies ($\gamma \gg 1$), this upper value of $b$ corresponds to very small excitation probabilities, and the calculation can be safely stopped. The reason for a finer mesh at small impact parameters is to get a good accuracy at the region where both nuclear, Coulomb, and absorption factors play equally important
At large impact parameters the probabilities fall off smoothly with $b$, justifying a wider integration step.

A mesh of NGRID points in polar coordinates is implemented to calculate the nuclear excitation potentials and absorption factors, according to the equations presented in sections 2.2 and 2.3. The first and second derivatives of the optical potentials are calculated by the routine DERIVATIVE. A 6-point formula is used for the purpose. The routines TWOFOLD computes the folding over the densities, as used in eq. (23). Routines RHOPP and RHONP generate the liquid drop densities, and the routine PHNUC computes the eikonal integral appearing in eq. (22).

Repeated factors for the nuclear and for the Coulomb potentials are calculated in the main program and stored in the main program with the arrays PSITOT and PSINUC. These arrays are carried over in a common block to the routine VINT which computes the function $Q^{(k)}_{N\lambda\mu}(\tau) + \sum_{\pi} Q^{(l)}_{\pi\lambda\mu}(\xi_{kj}, \tau) \psi_{kj}^{(\lambda)}$, used in eq. (21).

The time integrals are performed by means of an adaptive Runge-Kutta method. All routines used for this purpose have been taken from the Numerical Recipes Software, described in the book [9]. They are composed by the routines ODEINT, RKQS, RKCK, and RK4. The routine ODEINT varies the time step sizes to achieve the desired accuracy, controlled by the input parameter ACCUR. The right side of (21) is computed in the routine DCADT, used externally by the fourth-order Runge-Kutta routine RK4. RKCK is a driver to increase time steps in RK4, and RKQS is used in ODEINT for the variation of step size and accuracy control. The main program returns a warning if the summed errors for all magnetic substates is larger than $10 \times$ ACCUR.

The routine THREEJ computes Wigner-3J coefficients (and Clebsh-Gordan coefficients), and YLM is used to compute the spherical harmonics.

The routines SPLINE and SPLINT perform a spline interpolation of the excitation amplitudes, before they are used for integration by means of the routines QTRAP and QSIMP. All of them are from Numerical Recipes Software [4].

The program delivers outputs in RELEX.OUT. The statistical tensors are given in RELEX2.OUT for each impact parameter (only if IOUT=1).

The program is available at http://www.if.ufrj.br/~bertu/prog.html.

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