GECCCOS – a code performing evaluations of observables in reactions with exotic nuclei

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Executive Summary
The construction of an easy-to-use code package for the evaluation of observables of nuclear reactions measurable at radioactive ion-beam facilities has been the goal of this task. Emphasis is given on the general outline to allow reaction calculations in a wide field of applications. An essential element is the inclusion of up-to-date library information and the definition of default values which should enable so-called blind calculations. Emphasis is given on well-defined interfaces in order to allow straightforward extensions with new code modules. Because part of the envisaged developments on breakup reactions led to unprecedented problems, the presented code package represents a skeleton which requires still extensions. In this report a write-up of the basic structure of the code and the underlying theory background is given. Further work towards a full operational system is going on.

1. Introduction

In this report a first description of the code package GECCCOS is provided which is a **GE**neral **C**oupled-**C**hannel **CO**de **S**ystem focussed on nuclear reaction calculations. The basic idea is to develop an easy-to-use code for practitioners working in the field of nuclear studies by means of nuclear reactions. With regard to an easy use the code is self-contained and contains data libraries and does not require links to common libraries. In addition default values for different structure properties and technical parameters are provided which should enable the program to perform blind calculations with a minimum of input information. On the long term this part will contain also a learning option, i.e. the code will store new information which will be available for future applications. In order to guarantee easy extensions of the program package, emphasis is given on well-defined interfaces between the different modules and a flexible structure of the input information.

In section 2 we present the structure of the code and explain the main purpose of the various modules. Section 3 gives a short introduction into the theory background of reaction calculations. Section 4 gives an overview of the activities focussed on inclusion of breakup channels. Finally a summary is given and an outlook for further development is provided in section 5.

2. The Structure of GECCCOS

The GECCCOS program package is constructed around a general core program GECCOS, which is controlling the whole reaction calculations. This core is surrounded by a group of suites which contain one or more modules with specific purpose routines to accomplish well defined operations in the process of the calculation. The general structure of the code package `GECCCOS` is displayed in Fig. 1. The program package `GECCCOS` is structured in 7 suites.

Suite **Input**: Performs the whole input operations into the code `GECCCOS`. It contains two components. The standard input *mod_input*, which reads the standard input information from the file `GECCCOS.in`. The information comprises the information about the entrance channel, the exit channels, the type of calculation and the used techniques, the interactions and the technical parameters. The second component are external files provided by the user to import specific information to the code.

Suite **Tables**: This part consists of several files in the folder *tables* with data libraries including e.g. default values, nuclear matter densities, optical parameters etc.

Suite **Partition**: This suite contains all information about the particles and the reaction channels considered. It provides input and derived information about the reaction channels at all stages of the calculation. Therefore it is the central storage of information necessary to control the calculation.

Suite **Reaction**: This is the central part of the program package, where the modules for different reaction mechanisms and models are implemented. Here, the scattering amplitudes are calculated starting from the basic equation, in general the Schrödinger equation. At the moment the possibilities are limited. For the inclusion of further reaction mechanism modules must be entered into this suite.

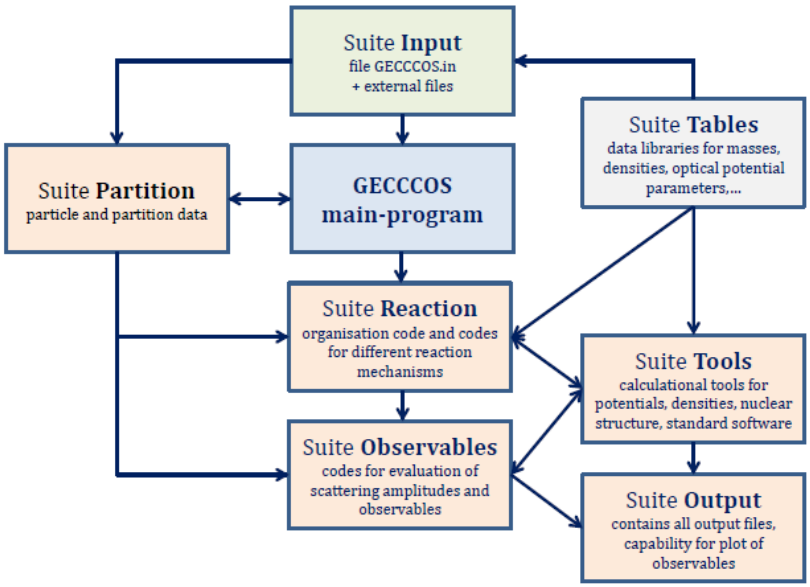

Fig. 1 Schematic view of the structure of the GECCCOS code package

Suite **Observables**: This contains programs to evaluate scattering amplitudes as well as observables from transition matrix elements provided via the suite *Reaction*.

Suite **Tools**: This contains calculations tools for the evaluation of nuclear matter densities, potentials, coupling interactions. In addition it contains standard software for special functions (factorials, Coulomb function, Legendre polynomials, …), angular momentum coupling tools (Clebsch-Gordan coefficients, 6j-symbols, …), as well as standard tools (Fourier transformation, linear algebra,…).

Suite **Output**: This contains the standard GECCCOS output, files used for plots and tables with information on observables and requested intermediate results.

3. Theory Background

3.1 Reaction Channels

The structure of the code GECCCOS deals with two-body channels, where the incoming projectile may be composed of two constituents which may experience breakup during the collision process. In this general description we restrict ourselves to two-body reactions,

$a + B \rightarrow c_i + D_i$,

where a is the incident projectile and B is the target at rest in the entrance channel. In the exit channel we may have various ejectiles c and residual nuclei D which may be excited to the i-th state with excitation energy $E_x^i(D)$. We do not assume an excitation of the ejectile c. In order to clarify the notation used in the code the composition *(c+D)* represents a partition {xpt}, while the index *i* refers to a channel.

Channel Energies

Since reaction experiments at radioactive ion beam facilities are usually fixed target experiments, the projectile a has the kinetic energy E_{Lab} while the target nucleus B is at rest. The calculations are usually performed in the center-of-mass system (cms) at the corresponding cms energy $E_{cm}(aB)$. In the preparatory part of the suite reaction the code calculates for all channels the reduced mass, the channel cms energy and the corresponding Sommerfeld parameter.

Spin Basis

In general the collision partners in a nuclear reaction will have a definite spin I_c and I_D. Between the collision partners there is an orbital angular momentum L. Two alternatives for the coupling to the total angular momentum exist,

S-basis scheme: $\vec{I} = \vec{I}_c + \vec{I}_D$, $\vec{J}_{tot} = \vec{L} + \vec{I}$,

J-basis scheme: $\vec{J}_c = \vec{L} + \vec{I}_c$, $\vec{J}_{tot} = J_c + \vec{I}_D$.

The choice of the basis depends on the problem considered, e.g. the *J*-basis has the advantage that spin-orbit forces of the projectile are diagonal. In the program both schemes are implemented.

3.2 *Optical Potentials*

Optical Potentials are basic ingredients for most reaction calculations. In practice either phenomenological optical potentials determined from elastic scattering or semi-

microscopic optical potentials are used. In the current version of the code two possibilities are implemented:

(i) phenomenological potentials as given in the RIPL3-data base [1]. The corresponding library is included in the folder table.

(ii) semi-microscopic single and double folding potentials. The nucleon densities $\rho(r)$ are taken from the RIPL3 library [1] section *Masses*. Especially, with regard exotic nuclei, the nucleon density functions generated by HFB calculations [2] are included in the program package. The effective nucleon-target or effective nucleon-nucleon interaction is provided. The program includes the M3Y nucleon-nucleon interaction which is suited for nucleus-nucleus scattering, but provides only real-valued optical potentials. The imaginary part has to be adjusted which is not a severe problem as coupled-channel calculations require anyway an adjustment of the imaginary part. The single folding potential makes use of the nuclear matter optical potential for nucleon scattering as developed by Bauge et al. [3]. Codes for the calculation of proton- and neutron-nucleus optical potentials are provided in the RIPL-3 data base [1] and are included in the program package. The nuclear matter approach yields an imaginary part which must be slightly scaled for composite particles.

Coulomb potential

If both collision partners in a partition {xpt} are electrically charged, a Coulomb potential must be added to the optical potential. There are two alternatives included in the code: (i) Coulomb potential of a homogenously charged sphere, (ii) double folding potential

3.3 The Coupled-Channel Equations

A partial wave expansion of the multi-channel wave function can be given for the J- and S-basis scheme (see e.g. Ref [5]). The wave function $\Psi_x^{J_{tot}M_{tot}}\left(R_x,\xi_p,\xi_t\right)$ is a solution of the microscopic Schrödinger equation,

$$\sum_\alpha \left[H-E\right]\left|\alpha;J_{tot}M_{tot}\right\rangle\frac{\psi_\alpha^{J_{tot}}\left(R_x\right)}{R_x}=0\ ,$$

with the microscopic Hamiltonian

$$H=H_{xp}\left(\xi_p\right)+H_{xt}\left(\xi_t\right)+\hat{T}_x\left(R_x\right)+V_x\left(R_x,\xi_p,\xi_t\right).$$

Here $\hat{T}_x$ is the kinetic energy of the relative motion, V_x is the interaction potential between the two collision partners and H_{xp}, H_{xt} are the internal Hamiltonians of the two colliding nuclei. Projecting the Schrödinger equation on a basis state yields a system of coupled differential equations for the relative motion wave function

$$\sum_\alpha R_{x'}\left\langle\alpha'\left|H-E\right|\alpha\right\rangle\frac{1}{R_x}\psi_\alpha\left(R_x\right)=\sum_\alpha R_{x'}\left\langle\alpha'\left|\left[\hat{T}_x+V_x-E_{xpt}\right]\right|\alpha\right\rangle\frac{1}{R_x}\psi_\alpha\left(R_x\right)$$

$$=\sum_\alpha\left\{\hat{N}_{\alpha'\alpha}\left[\hat{T}_{xL}\left(R_x\right)-E_{xpt}\right]+\hat{V}_{\alpha'\alpha}^{prior}\left(R_x\right)\right\}\psi_\alpha\left(R_x\right)=0$$

with the following matrix elements

$$\hat{T}_{xL}\left(R_x\right)=-\frac{\hbar^2}{2\mu_x}\left[\frac{d^2}{dR_x^2}-\frac{L_x\left(L_x+1\right)}{R_x^2}\right],\qquad E_{xpt}=E-\varepsilon_{xp}-\varepsilon_{xt}$$

$$V^{prior}_{\alpha'\alpha} = R_{x'}\left\langle \alpha' \middle| V_x \middle| \alpha \right\rangle R_x^{-1} \quad \text{or} \quad V^{post}_{\alpha'\alpha} = R_{x'}\left\langle \alpha' \middle| V_{x'} \middle| \alpha \right\rangle R_x^{-1}\ , \qquad \widehat{N}_{\alpha'\alpha} = R_{x'}\left\langle \alpha' \middle| \alpha \right\rangle R_x^{-1}.$$

This system of coupled differential equations must be solved for the determination of the relative motion wave function.

3.4 Coupling Potentials

Nuclei with strong collective excitations must be treated within a coupled-channel approach. These collective excitations are related with nuclear deformation. Only the deformation of the target is taken into account. Following standard techniques (see e.g. [4]), the surface of a deformed nucleus is described by spherical harmonics,

$$R = R_0\left[1+\sum_{\lambda\mu}\alpha_{\lambda,\mu}Y^{\mu}_{\lambda}\right] \quad \text{with deformation parameter } \alpha_{\lambda,\mu} = (-1)^{\mu}\,\alpha^{*}_{\lambda,-\mu}\,.$$

The present code must deal with a variety of potential shapes. For short range potentials we consider the above relation as a direction dependent scaling of the r-value. Performing a first order expansion with regard to the deformation parameters yields the coupling potential

$$V^{nuc}_{coupl}\left(\vec{r},\alpha\right) = v^{nuc}_{coupl}(r)\sum_{\lambda\mu}\alpha_{\lambda\mu}Y^{\mu}_{\lambda}\left(\Omega\right) \quad \text{with} \quad v^{nuc}_{coupl}(r) = r\frac{d}{dr}V_{nuc}\left(r\right)\ .$$

This differs slightly from the standard expression obtained for a Woods Saxon potential. In order to account for this difference an effective half-density radius $R_{0.5}$ is determined and used in the corresponding relations for the coupling potential.

For the long-ranged Coulomb potential an effective Coulomb radius R^{eff}_{cou} is determined from the derivative of the given Coulomb potential. The coupling potential is taken as that of a homogenous charged sphere with Coulomb radius R^{eff}_{cou} (see e.g. [4])

At present it is assumed that the same deformation parameters apply for the nuclear and the Coulomb part. Following Ref [4] the evaluation of the coupling matrix elements in the coupled channel equation is straightforward. Thus coupling to rotational states can be included knowing the deformation parameter β_2. Vibrational states can also be included using the reduced matrix elements B(EI; 0→ I).

3.5 Scattering Amplitudes and Observables

The scattering amplitudes can be calculated with the transition matrix elements $\tilde{T}^{J_{tot\pi}}_{\beta\alpha}$, calculated in the suite reaction. In a multi-channel problem the scattering amplitudes are defined in the spin space of the two colliding partners. Consequently they are represented as matrices in the spin space of the involved particles. Hence the final expressions depend on the spin basis scheme applied. Following [5] the expressions for both spin basis schemes are used.

The scattering amplitudes are the basis for the determination of the observables [5]. For unpolarised incident beam the evaluation of the angle differential cross section, angle integrated cross section, the total reaction and the absorption cross section are onsidered. The evaluation of reaction cross sections and analysing powers is also straightforward.

4 Activities to Further Modules

Much effort has been devoted to the inclusion breakup channels. The scientific interest of the work was focused on methodologies for the evaluation of breakup reactions. In particular we have studied two methods:

Eikonal Approach for Breakup of Halo Nuclei
Frequently higher energies are used to study exotic nuclei. Therefore we studied the description of breakup reactions in the eikonal approach developed by D. Brink and A. Bonaccorso [6]. In particular this offers the possibility of an extension to projectiles of effective three-body nature, e.g. ^{6}He, which would be of great interest for studies at future radioactive ion beam facilities. Before taking effort to extend the formalism we checked first whether we can reproduce existing breakup calculations. Considering the example of ^{17}F collision at 72 MeV we evaluated the full breakup amplitude numerically exactly and do not apply any further approximation as done in the original literature. We obtained similar contributions for the pure Coulomb and nuclear breakup as in the original literature, but we also found additional interference terms not considered so far which showed some impact in the forward momentum distributions of the neutrons. The gross structure of the momentum distribution could be reproduced, but looking into more detail we found some systematic deviations from previous results in the literature. Despite great efforts we could not identify its origin and settle the problems in due time.

Lorentz Integral Transformation as tool for breakup reactions
The explicit treatment of continuum states is one of the major problems in breakup reactions. It leads to large dimensions of the coupled-channel system and questions of convergence arise. In principle the Lorentz Integral Transformation technique [7] provides a way to treat the coupling to the continuum globally, but still exact. Therefore we adapted the formalism of the Lorentz Integral Transformation Method to breakup reactions. As a first example we checked the feasibility of the approach on a deuteron-nucleus scattering system. The key problem in this method is the inversion of the transformation. We succeeded to perform the calculation, but we could not achieve proper convergence. Unfortunately the involved PhD student, M. Gal, left suddenly without completing the work. We recovered the essentials of his results, but it was obvious that new ideas are required to solve the problem. Only recently, we could restart this effort with a new concept, i.e. combining the LIT-Technique with an eikonal approach. Comparing with different applications of the LIT technique it seems very promising that the convergence problems should be reduced.

5 Summary and Outlook

We have constructed the skeleton of a general code for reaction calculations, whose structure is generated to allow for general calculations, especially for reactions with exotic nuclei. The code written in `fortran95` contains the essential elements for a reaction calculation. However, it is at the moment only a skeleton which requires input about specific reaction mechanisms. In this write-up we have presented the basic layout of the code. However, not all key words are operational at the moment as details of their implementation can only be fixed when the corresponding modules are introduced. Developments of further modules for GECCCOS are part of current Master and PhD theses and will lead to a continuous progress of the code package.

As outlined in Section 6 major effort has been devoted to the evaluation of breakup reactions by new techniques. Especially, the eikonal approach of Margueron et al. [6] has been numerically implemented using Monte Carlo techniques, which provided proper momentum distributions. The implementation into GECCCOS could not been achieved within the project. The second developments regarding breakup was the attempt to use the Lorentz-Integral-Transformation Technique [7] to account for the breakup of the projectile. The latest attempts to combine the eikonal approach with the Lorentz-Integral-Transformation-Techniques are very promising and we are working to make it operational for GECCCOS in the near future.

The code GECCCOS is far from being complete and many important elements are still missing. However, the project enabled us to generate a numerically convenient environment which allows for extensions towards a general reaction code. Continuous progress on the code package is envisaged in order to become a future standard tool of the community.

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Appendix A: Personnel (on ENSAR Funds)

Bernhard BRUMEC, employed on ENSAR funds at TU Wien, 1.5.-30.6.2012
Main topic: construction of basic modules for code GECCCOS

Martin GAL, PhD student employed on ENSAR funds from 1.7.2012-28.2.2013
Main topics: Lorentz Integral Transform for Breakup Reactions, extension to breakup; Unfortunately he quitted the job and his PhD without delivering a final result

Thomas SRDINKO, PhD student employed on ENSAR funds from 18.9.2013-31.10.2013,1.3.2014-31.8.2014
Main topic: Eikonal approach of neutron-halo nuclei, Optical Potentials, construction of code GECCCOS

Georg SCHNABEL, PhD student employed on ENSAR funds from 1.10.2013-28.2.2014
Main topic: Test and development of tools for GECCCOS.

Appendix B: Presentations/Publications

J. Haidvogl, D.M. Warjri, H. Leeb, *Nuclear matter approach for nucleon optical potential of exotic nuclei*, Poster at the 2nd European Nuclear Physics Conference, Bucharest, Romania, September 17- 21,2012

M. Gal, H. Leeb, Towards LIT Approach for breakup reactions, 2nd THEXO Collaboration Meeting, ECT* Trento, October, 22-24, 2012

D. Kagerbauer, D. Bader, Eikonal approach to ^{17}F-^{208}Pb breakup in forward direction, Bachelor thesis, 09/2013