Chapter 4

Theoretical Details and Estimations

4.1 Introduction

The theoretical calculations are crucial for evaluations of cross section and accurately extrapolate the data to energy ranges, where no data exist, or situations where the measurement is either impossible or impractical. It is generally understood that the main sources of uncertainty in calculations are uncertainties in input nuclear structure parameters used as input in theoretical calculations. These input parameters are nuclear masses, deformations, nuclear levels and their decay characteristics, γ-strength functions, neutron resonances and level densities, optical model parameters, fission barriers, *etc*. The computer programming is used to generate the statistical nuclear reaction codes by using the different reaction models as given by the authors [1]. There are several nuclear codes like TALYS, EMPIRE, COH3 and ALICE and these codes can predict nuclear data such cross section, reaction rates, particle production yields and angular distribution of outgoing particles, *etc*. The Weisskopf-Ewing formalism, which accounts for the conservation of energy, charge, and mass, and the Hauser-Feshbach formalism, which additionally accounts for angular momentum and parity are the two most common approaches in all statistical codes. Accurate calculations of nuclear reaction cross sections are in high demand in different areas including basic nuclear physics, medical isotopes production, astrophysics, shielding, Accelerator Driven Systems, and design of advanced reactor technology [2]. In the present work, the theoretical calculations were performed using two nuclear reaction statistical open source codes the EMPIRE (ver. 3.2.2) [3] and TALYS (ver. 1.9) [4]. Moreover, the optimum input parameters and different level density, preequilibrium and optical model potential of both the codes were used to investigate the neutron induced $(n, 2n)$ and (n, p) reactions cross sections.

4.2 Types of nuclear reactions mechanism

Basically, when an energetic incident particle hits an atomic nucleus, a nuclear reaction takes place. The incident particle is called projectile ‘a’ and the fixed target nucleus is ‘A’, the

nuclear reaction is given by $a + A \rightarrow [C^*] \rightarrow B + b$ or $A(a,b)B$, where b and B are outgoing particles and the products of reaction respectively. The cross section is a measurement of the probability that a reaction will occur, it is typically used to explain how the projectile interacts with the target nucleus. The cross section is often expressed in the barn ($1\text{b} = 10^{-28}\ m^2$) and depends on the incoming particle energy. The excitation function is the plot of $\sigma(E)$ against incoming particle energy. There are three main categories into which the nuclear reactions on a specific mass region can be divided: (i) compound nucleus (ii) pre-equilibrium and (iii) direct reactions. In terms of time scales, direct reactions are categorized as having short reaction times (10^{-22} to 10^{-21} sec) and compound nucleus processes as having lengthy reaction times (10^{-18} to 10^{-16} sec), whereas pre-equilibrium events take place at intermediate time scales. Similarly, in terms of the number of intranuclear collisions, which is one or two for direct reactions, a few for pre-equilibrium processes, and many for compound reactions [5]. These three different reaction categories as a function of energy are shown in Fig. 4.1.

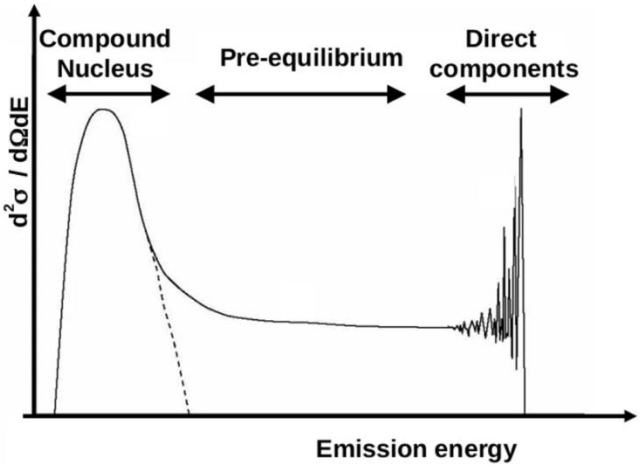

Fig. 4.1 *Nuclear reaction cross section for the three reaction mechanisms with emission energy.*

4.2.1 Compound nucleus reactions

The incident particle is captured, and a compound nucleus is formed, which is either stable or radioactive. The compound nucleus is the intermediate state formed in a compound nucleus reaction. It is normally one of the excited states of the nucleus formed by the combination of the incident particle and target nucleus. However, the mass of this compound nucleus is smaller than the sum of the masses of the original nucleus and the incident particle. Hence photons (prompt gammas) are emitted with energy, determined by this mass difference,

by the kinetic energy of the incident particle and by the excitation levels of the compound nucleus. This phenomenon is usually called radiative capture, represented by the (n,γ) symbol, *i.e.*, the (n,γ) reaction. The incident particle is captured, and another elementary particle is emitted, *e.g.*, a proton, α-particle, neutron, etc. i.e., (n,p), (n,α) and $(n,2n)$, (n,n') reactions. If a target nucleus X is bombarded with particle a, it is sometimes observed that the ensuing nuclear reaction takes place with appreciable probability only if the energy of particle a is in the neighbourhood of certain definite energy values. These energy values are referred to as resonance energies. The compound nuclei of these certain energies are referred to as nuclear resonances. Resonances are usually found only at relatively low energies of the projectile. The widths of the resonances increase in general with increasing energies. At higher energies the widths may reach the order of the distances between resonances and then no resonances can be observed. The narrowest resonances are usually the compound states of heavy nuclei (such as fissionable nuclei) and thermal neutrons (usually in (n,γ) capture reactions). The observation of resonances is by no means restricted to neutron nuclear reactions. In the CN mechanism, Hauser-Feshbach theory based on the Bohr independent theory is applied to calculate the cross section of the CN emission in the centre of the mass frame. The compound nucleus model (the idea of compound nucleus formation) was introduced by Danish physicist Niels Bohr in 1936. In addition to this equation, it is mentioned that the CN cross section has a dependence on the LD model and the OMPs. This model assumes that the incident particle and the target nucleus become indistinguishable after the collision and together constitute the excited state of the nucleus the compound nucleus. To become indistinguishable the projectile must suffer collisions with constituent nucleons of the target nucleus until it has lost its incident energy. In fact, many of these collisions lead to a complete thermal equilibrium inside the compound nucleus [6]. The schematic representation of the formation of compound nucleus C is shown in Fig. 4.2. The compound nucleus is excited by both the kinetic energy of the projectile and by the binding nuclear energy.

$$\sigma_{\alpha\alpha'} = \sigma_C * \frac{\Gamma_{\alpha'}}{\Gamma_{\alpha''}}$$

Where σ_C expresses the cross section for the formation of the compound nucleus, $\Gamma_{\alpha'}$ corresponds to the decay width for the emission of the α' particle and $\Gamma_{\alpha''}$ is the decay width for all possible decay channels. This ratio expresses the probability that the compound

nucleus will decay through the emission of the α' particle against all the other possible output channels.

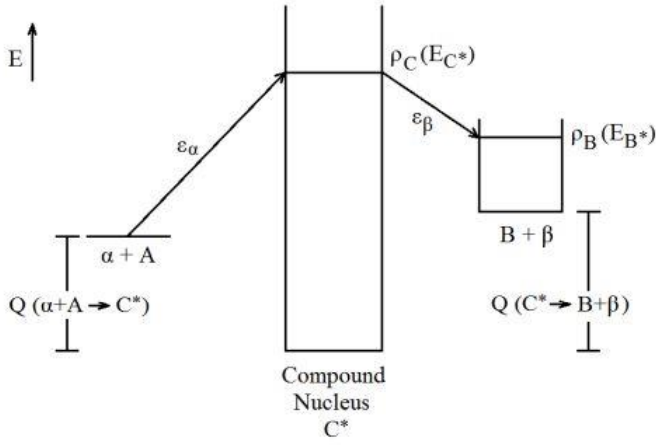

Fig. 4.2 *Schematic representation of the $a + A \rightarrow [C^*] \rightarrow B + b$ via the formation of the compound nucleus C^*.*

4.2.2 Preequilibrium reactions

The pre-equilibrium reactions have occurred at intermediate energies, where the projectile and target nucleus formed a complex system that decays before the system reached the thermodynamic equilibrium. The pre-equilibrium mechanism is vital in calculating the reaction cross section for the projectile energy between 10 to 200 MeV. The incident particle creates more complex states through the step by step stages and gradually loses its memory of the first direction and energy. One of the most widespread models for describing this mechanism is the exciton model. The characterization of the nuclear state in this model is implemented by excitation energy and the total number (n) of particles and holes (exciton) above and below the Fermi surface, respectively [7].

4.2.3 Direct reactions

Nuclear reactions, which occur in a time comparable to the time of transit of an incident particle across the nucleus (10^{-22} sec), are called direct nuclear reactions. Interaction time is critical for defining the reaction mechanism. The very short interaction time allows for an interaction of a single nucleon only (in extreme cases). There is always some non-direct (multiple internuclear interactions) component in all reactions, but the direct reactions have this component limited. To limit the time available for multiple internuclear interactions, the reaction must occur at high energy. Direct reactions have another very important property, the

products of a direct reaction are not distributed isotropically in angle, but they are forward focused. This reflects the fact that the projectiles make only one, or very few, collisions with nucleons in the target nucleus and its forward momentum is not transferred to an entire compound state. The cross sections for direct reactions vary smoothly and slowly with energy in contrast to the compound nucleus reactions and these cross sections are comparable to the geometrical cross sections of target nuclei [8]. The schematic energy diagram of the direct reaction is shown in Fig. 4.3.

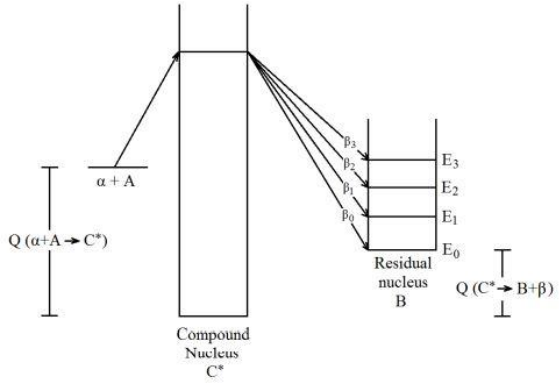

Fig. 4.3 *Schematic representation of the way that the low-lying states of the residual nucleus B can be excited in a direct reaction* $a + A \rightarrow B + b$.

4.3 Theoretical models for nuclear reactions

One of the main components in nuclear reaction cross section calculations is level densities. Over the last fifty years, the statistical properties of excited nuclear levels have been a subject of concern and study. Their density is one of the fundamental statistical properties of nuclear levels. The Fermi-gas and constant temperature models are used to describe the level densities with parameters obtained from the fitting of some experimental results. It is very important to obtain parameters from the description of level density from reliable experimental data for practical applications of statistical models. The cumulative numbers of low-lying levels and the average spacing between neutron resonance data are usually used. Other data such as shell effects, pairing correlations and collective phenomena include some of the most relevant principles on which the current understanding of the structure of low-lying nuclear levels is focused. The Generalized Superfluid Model (GSM) developed by many authors over the last 20 years, all these concepts have been implemented. Changing the default options may considerably improve the comparison with experimental data [9]. However, this approach may

still not be sufficient in some cases, and the next step would be to determine which reaction mechanism is most likely to be responsible for the disagreement, remembering that neutron capture below 10 MeV and the low energy part of the particle spectra are essentially due to compound nucleus decay process. The high energy part of particle spectra is dominated by the pre-equilibrium emission, and the population of the collective discrete levels in inelastic scattering arises mainly from the direct reactions. We also note that at incident energies below 50 MeV the multiple-chance pre-equilibrium emission is rather small and multiple particle emission is governed by the statistical decay. Similarly, the capture cross sections below 10 MeV underestimated (overestimated) as mentioned before, the compound nucleus is responsible for this process. The discrepancy might be traced to the γ-ray strength function being too low being too low (too high) or to the ratio of level densities in the daughter nuclei and the compound nucleus being too low (too high) [10].

4.3.1 The Hauser-Feshbach theory

In a nuclear reaction, the Hauser-Feshbach theory is used to calculate the cross sections which proceed via the formation of a compound nucleus. The cross section of the reaction is given by:

$$\sigma(\alpha + A \rightarrow B + \beta) = \sigma(\alpha + A \rightarrow C^*)P(C^* \rightarrow B + \beta) \qquad \sigma_{\alpha\beta} = \sigma_\alpha P_\beta$$

Where σ_α is the compound nucleus formation cross section and P_β is the compound nucleus decay probability to channel β. The binary cross section for the compound nucleus is calculated using the formula given by:

$$\sigma_{\alpha\alpha'}^{comp} = D^{comp} \frac{\pi}{k^2} \sum_{J=mod(I+s,1)}^{l_{max}+I+s} \sum_{\Pi=-1}^{1} \frac{2J+1}{(2I+1)(2s+1)} \sum_{j=|J-I|}^{J+I} \sum_{l=|j-s|}^{j+s} \sum_{j'=|J-I'|}^{J+I} \sum_{l'=|j'-s'|}^{j+s} \times$$

$$\delta_\pi(\alpha)\, \delta_\pi(\alpha') \frac{T_{\alpha l j}^{J}(E_a) \langle T_{\alpha' l' j'}^{J}(E_{a'}) \rangle}{\sum_{\alpha'',l'',j''} \delta_\pi(\alpha'') \langle T_{\alpha'' l'' j''}^{J}(E_{a''}) \rangle} W_{\alpha l\, j \alpha' l' j'}^{J}$$

In the above equations, the symbols have the meaning mentioned in the TALYS code. The width fluctuation correction (WFC) factor 'W' includes the correlations between the input and output channels. At low incident energy, this factor enhances the elastic channel, but at energies over a certain MeV, it is meaningless [11].

4.3.2 The optical potential models

The optical model describes the nuclear reactions using a mean nucleus potential. The optical model potential parameters given by Koning and Bechetti for neutron and proton were used from the Reference Input Parameters Library (RIPL-3.0) [12]. There are local and global phenomenological optical model potentials (OMPs) for neutrons and protons with incident energies from 1 keV up to 200 MeV, for near spherical nuclides in the mass range $24 \leq A \leq 209$. Based on detailed fits of neutron total and nucleon elastic cross sections and angular distributions with the ECISVIEW interactive code. The optical model is used to calculate the transmission coefficients, which is important in the Hauser-Feshbach theory, as they are utilized in the estimations of the compound nucleus formation and decay. The elastic scattering in the presence of absorbing effects was described using the optical model. The calculation approaches that of light striking a relatively opaque glass sphere. The complex potential $U(r)$ is used to represent the scattering and which is given by the following relation:

$$U(r) = V(r) + i\,W(r)$$

Where the real part $V(r)$ describes the nuclear interaction of scattering between target and projectile and the imaginary part $W(r)$ is responsible for the absorption [13]. The standard optical model potential is given as follows:

$$U(r, E) = -V_V(r, E) - iW_V(r, E) - iW_D(r, E) + V_{SO}(r, E) \cdot l \cdot \sigma + iW_{SO}(r, E) \cdot l \cdot \sigma + V_C(r)$$

In the above equation, 1st term is a real volume, 2nd term is an imaginary volume, 3rd term is an imaginary surface, 4th term is a real spin-orbit, 5th term is an imaginary spin-orbit and 6th term is a Coulomb.

4.3.3 The pre-equilibrium models

The quantum mechanical approach of pre-equilibrium reactions is the multistep theory, in which it is assumed that the interaction between the incident nucleon and the target nucleus takes place in several stages of increasing complexity. The projectile enters the nucleus and collides with a nucleon, producing a two particle one hole excitation. The secondary particles can themselves interact, producing three particles two hole excitations and so on. At each stage, there is a finite probability that the reaction proceeds to the next stage, returns to a previous stage or goes directly to the continuum. The latter possibility corresponds to pre-equilibrium

reactions. A distinction is made for them, in the theory of H. Feshbach *et al.*, between multistep compound and multistep direct reactions.

- Multistep Compound (MSC)

In a multistep compound reaction, all the particles remain bound during the equilibration cascade. The phases of the matrix elements (J, parity etc.) which are required to specify a channel, are assumed to be random so that no interference terms remain after averaging. Thus, the energy averaged cross sections are symmetric at about 90^o in the multistep compound.

- Multistep Direct (MSD)

A multistep direct reaction occurs as the incident energy increases and is more likely that one particle remains in the continuum and therefore retains a strong memory of the original direction of the projectile. In this case, there is constructive interference between matrix elements involving the same change in the momentum of the particle in the continuum and so the cross sections are forward peaked in multistep direct.

- Exciton model

The simplest pre-equilibrium model is given by the Griffin's, and it is known as the exciton model. According to the exciton model, once the projectile enters the target nucleus, the system gets excited with a series of stages and different angular momenta. Before it goes to the final stage of equilibrium, it emits the particles and residue. The energy transferred by the projectile in the target nucleus decides the complexity of the stage, which can be estimated with the number of particles and holes excited. These excited particles p, and holes h are called excitons and the number of excitons is $n = (p + h)$. By solving the dynamical equations of these exciton one can calculate the resultant stage and products from the reaction. This pre-equilibrium reaction mechanism is based on the two particles' one hole $(2p - 1h)$ state and three particles two holes $(3p - 2h)$ state as shown in Fig 4.4.

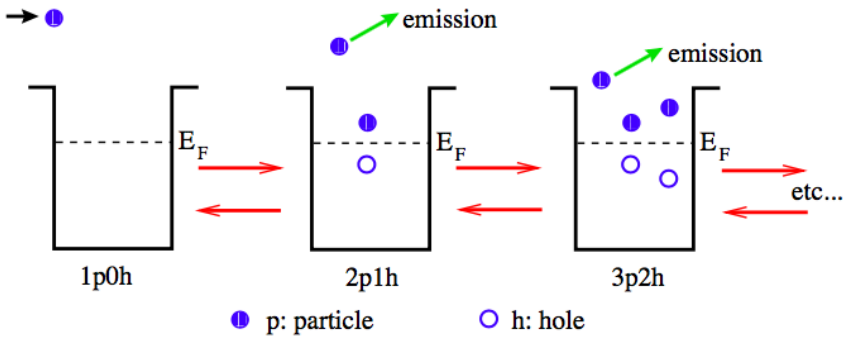

Fig. 4.4 *The pre-equilibrium mechanism based on the exciton model.*

4.3.4 The γ-ray strength functions

The γ-ray emission is a universal channel that can accompany the emission of any other particle. Therefore, the γ-ray transmission coefficients are entered in the Hauser-Feshbach calculations to consider the competition of the γ emission with other particles. The transmission coefficient of a γ-ray with multipolarity l and energy E_γ is given by the following relation:

$$T_{Xl}(E_\gamma) = 2\pi f_{Xl}(E_\gamma) E_\gamma^{2l+1}$$

Where $f_{Xl}(E_\gamma)$ represent the γ-ray strength functions. The calculations of capture cross sections, γ-ray production spectra, isomeric state populations, and competition between γ-ray and particle emission in the compound nucleus model depend heavily on γ-ray strength functions. The γ-ray strength functions contain information on nuclear structure and are usually applied to research both nuclear structure and the mechanisms behind nuclear reactions [14].

4.3.5 Nuclear level density (NLD) models

The level density $\rho(E_x, J, \Pi)$ corresponds to the number of nuclear levels per MeV around an excitation energy E_x, for a certain spin J and parity Π. The total level density $\rho^{tot}(E_x)$ corresponds to the total number of levels per MeV around E_x, and is obtained by summing the level density over spin and parity as given as follows:

$$\rho^{tot}(E_x) = \sum_J \sum_\Pi \rho(E\_x, J, \Pi)$$

The single particle level density of the atomic nucleus consisting of Z protons and N neutrons with the total angular momentum J and the excitation energy U has the following form:

$$\rho_0(U,Z,N,J) = \frac{(2J+1)\sqrt{a}}{24\left(U-\Delta-\frac{\hbar^2 J(J+1)}{2\Im_\perp}\right)^2}\left(\frac{\hbar^2}{\Im_\perp}\right)^{3/2} exp\left(2\sqrt{a\left(U-\Delta-\frac{\hbar^2 J(J+1)}{2\Im_\perp}\right)}\right)$$

Where a is the level density parameter, $\Im_\perp$ is the moment of inertia of the nucleus about the axis perpendicular to its axis of symmetry, and Δ is the pairing energy which is given by the following relation:

$$\Delta = \chi\frac{12}{\sqrt{A}}$$

Where A is the mass number of the nucleus, and χ is the parameter equal to 0, 1 or 2 for odd-odd, odd and even-even nuclei, respectively [15]. The energy dependent level density parameter in the presence of shell effect can be written as:

$$a(E_x) = \tilde{a}\left(1 + \delta W\frac{1-exp[-\gamma U]}{U}\right)$$

In the above equation, δW is the shell correction energy and $U = (E_x - \Delta)$ is the excitation energy, where this energy shift Δ adjustable empirical parameter closely related to the pairing energy and includes odd-even effects in nuclei. The asymptotic value $\tilde{a}$ is given by the smooth form:

$$\tilde{a} = \alpha A + \beta A^{2/3}$$

Where A is the mass number α, β and γ are the coefficients with the default values 0.073 MeV^{-1}, 0.095 MeV^{-1} and 0.061 MeV^{-1}, respectively. The value of $\tilde{a}$ is obtained in the absence of any shell effects. the damping parameter γ is given by following systematic formulae:

$$\gamma = \frac{\gamma_1}{A^{1/3}} + \gamma_2$$

Where, A is the mass number, γ_1 and γ_2 are global parameters that have been determined to give the best average level density description over a whole range of nuclides [16].

4.3.5.1 The phenomenological level density models

- **Fermi gas model (FGM)**

This model is based on the assumption of equally spaced single particle states which construct the exciting levels of the nucleus. It's considering the non-interacting nucleons in the absence of collective levels. The Fermi gas model gives the best expression for nuclear level density and the pairing energy is treated as an adjustable parameter in this model. The Fermi gas level density is given as follows:

$$\rho_F(E_x, J, \pi) = \frac{1}{2}\frac{2J+1}{2\sqrt{2\pi}\sigma^3}\exp\left[-\frac{\left(J+\frac{1}{2}\right)^2}{2\sigma^2}\right]\frac{\sqrt{\pi}}{12}\frac{\exp\left(2\sqrt{aU}\right)}{a^{1/4}U^{5/4}}$$

Where is a is the level density parameter, σ the square root of the spin cut-off parameter and U is the effective excitation energy. The total Fermi gas level density by summing over all spins and parities is given as follows:

$$\rho_F^{tot}(E_x) = \frac{1}{\sqrt{2\pi}\sigma}\frac{\sqrt{\pi}}{12}\frac{\exp\left(2\sqrt{aU}\right)}{a^{1/4}U^{5/4}}$$

Where, σ^2 is called the spin cut-off parameter and it refers to the width of the angular momentum distribution of the level density and a is the level density parameter.

- **Gilbert-Cameron model (GCM)**

In the Gilbert-Cameron level density model these level density parameters were obtained by fitting the Fermi-gas model formula to the recommended spacing of s-wave neutron resonances and matching the corresponding level density to discrete levels. Two parts are considered for a range of excitation energy in the constant temperature model; a low energy part from 0 to a matching energy E_M; which in its the adjustable parameters E_0 and the nuclear temperature T called the constant temperature law is applied for low energy region, whereas the higher energies region above E_M is described by the Fermi gas model. The constant temperature level density formula was modified by Gilbert Cameron in 1965 and is given as follows:

$$\rho_T^{tot}(E_x) = \frac{1}{T}exp\left(\frac{E_x - E_0}{T}\right)$$

Here, the effective excitation energy is $U = (E_x - \Delta^{CTM})$, T is the nuclear temperature, E is the excitation energy, Δ is the pairing energy, E_0 is the adjustable energy shift.

$$\Delta^{CTM} = \chi \frac{12}{\sqrt{A}}$$

Where χ = 0, 1 and 2 for odd-odd, odd-even and even-even nuclei respectively.

• Back Shifted Fermi gas model (BSFGM)

In the Back shifted Fermi gas model, the expression of the Fermi gas model is applied in all energy domains, and the pairing energy is considered as the adjustable parameter. The level density parameters for the Back shifted Fermi gas model are obtained by fitting the Fermi gas model formula both to the recommended spacing of s-wave neutron resonances and to the cumulative number of low-lying levels evaluated from the analysis of nuclear levels. The total level density for Back shifted Fermi gas model is given as follows:

$$\rho_{BSFM}^{tot}(E_x) = \left(\frac{1}{\rho_F^{tot}(E_x)} + \frac{1}{\rho_0(t)}\right)$$

Where,

$$\rho_0^{tot}(t) = \frac{e}{24\sigma} \frac{\left(\alpha_n + \alpha_p\right)^2}{\sqrt{\alpha_n \alpha_p}} e^{4\alpha_n \alpha_p t^2}$$

In the given equation $\alpha_n = \alpha_p = \frac{\alpha}{2}$ and t is so called thermodynamics temperature and it is equal to $= \sqrt{\frac{U}{\alpha}}$.

• Generalized superfluid model (GSM)

The Generalized Superfluid Model (GSM) considers collective enhancement of the nuclear level density in addition to shell and superfluid effects. The level density parameters for the Generalized Superfluid model were obtained by fitting the corresponding model formulas to the recommended spacing of s-wave neutron resonances and matching level densities to discrete levels. This model includes the superconductive pairing energy correlation in terms of the Bardeen-Cooper-Schrieffer theory at low excitation energies, which cause superfluid behavior. As the Generalized Superfluid Model (GSM), The Enhanced Generalized Superfluid Model (EGSM) also contains two parts, in the first part below the critical excitation

energy U_C the superfluid model uses, while the Fermi gas model is employed for the above critical excitation energy U_C.

$$\rho(E_x, J, \Pi) = \frac{1}{2} R_F(E_x, J) \rho_{GSM}^{tot}(E_x) U' \leq U_C$$

$$\rho(E_x, J, \Pi) = \frac{1}{2} R_F(E_x, J) \rho_{GSM}^{tot}(E_x) U' \geq U_C$$

Where,

$$\rho_{GSM}^{tot}(E_x) = \frac{1}{\sqrt{2\pi\sigma}} \frac{e^S}{\sqrt{D}}$$

$$\sigma^2 = \sigma_C^2 \frac{U'}{U_C}$$

where σ^2 is the spin cut-off parameter at the critical energy.

4.3.5.2 Microscopic level densities

Since these available microscopic level densities, which we will call ρ_{HFM}, have not been adjusted to experimental data, we add adjustment flexibility through a scaling function, *i.e.*

$$\rho(E_x, J, \pi) = exp\left(c\sqrt{E_x - \delta}\right) \rho_{HFM}((E_x - \delta), J, \pi)$$

Where by default $c = 0$ and $\delta = 0$ (*i.e.*, unaltered values from the tables). The "pairing shift" δ simply implies obtaining the level density from the table at different energy. The constant c plays a role like that of the level density parameter a of phenomenological models. Adjusting c and δ together gives adjustment flexibility at both low and higher energies. The microscopic level density models are as follows:

- **Microscopic NLD (Skyrme force) – Goriely's tables**

In this model, the NLD calculation in terms of Hartree–Fock's calculation by Goriely (Goriely *et al.*, 2001) for the RIPL database is used for excitation energy up to 150 MeV and spin value up to 30.

- **Microscopic NLD (Skyrme force) – Helaire's combinatorial tables**

Helaire has considered NLD dependence on energy, spin and parity and Goriely's approach based on the microscopic combinatorial model is employed in this model (Goriely *et al.,* 2008).

- **Microscopic NLD (temperature-dependent HFB, Gogny force) – Helaire's combinatorial tables**

This model is based on the temperature-dependent on Hartree–Fock-Bogolyubov's calculations using Gogny force (Hilaire *et al.,* 2012).

4.4 Nuclear reaction simulation codes

4.4.1 TALYS (ver. 1.9) code

A computer software called TALYS is used to analyze and estimate nuclear reactions. The primary goal of code is to simulate nuclear reactions involving neutrons, photons, protons, deuterons, tritons, ^{3}He and α-particles in the energy range of eV to 200 MeV, for target nuclides with a mass of 12 and heavier. There are two main purposes of the Talys code, (i) analysis of the nuclear reaction experiments and (ii) generated the nuclear data where no measurements are available. The conventional and innovative nuclear power reactors, transmutation of radioactive waste, fusion reactors, accelerator applications, homeland security, and medical isotope production, and radiotherapy, single-event upsets in microprocessors, oil-well logging, geophysics, and astrophysics are important applications that rely directly or indirectly on data generated by nuclear reaction simulation codes like TALYS.

The calculation of cross sections using TALYS code contributes to the compound nucleus by the Hauser-Feshbach theory. In the direct reaction calculation, the default option used is the coupled-channels model. There are four models for width fluctuation corrections in compound nucleus calculations in TALYS code as follows [17-21]:

- **Hauser-Feshbach model** (TALYS input keyword “widthmode 0”)
- **Moldauer model** (TALYS input keyword “widthmode 1”) **(default)**
- **Hofmann-Richert-Tepel-Weidenmüller model** (TALYS input keyword “widthmode 2”)
- **GOE triple integral model** (TALYS input keyword “widthmode 3”)

There are 9 possibilities for the γ-ray strength function model in TALYS code as follows [22-29]:

- **Kopecky-Uhl generalized Lorentzian** (TALYS input keyword "strength 1") **(default)**
- **Brink-Axel Lorentzian** (TALYS input keyword "strength 2")
- **Hartree-Fock BCS tables** (TALYS input keyword "strength 3")
- **Hartree-Fock-Bogoliubov tables** (TALYS input keyword "strength 4")
- **Goriely's hybrid model** (TALYS input keyword "strength 5")
- **Goriely T-dependent HFB** (TALYS input keyword "strength 6")
- **T-dependent RMF** (TALYS input keyword "strength 7")
- **Gogny D1M HFB+QRPA** (TALYS input keyword "strength 8")
- **SMLO** (TALYS input keyword "strength 9")

The four optical potentials proposed by Koning-Delaroche and Bauge-Delaroche were used to obtain optical model parameters for neutrons and protons from the RIPL-3.0 database. These models are mentioned in the TALYS code as follows [30-31]:

- **dispersive optical model potential** (TALYS input keyword "dispersion y")
- **local optical model potential** (TALYS input keyword "localomp y") **(default)**
- **global optical model potential** (TALYS input keyword "localomp n")
- **JLM microscopic optical model potential** (TALYS input keyword "jlmomp y")

The pre-equilibrium mechanism is important to describe the higher energy region above 10 MeV and the TALYS code includes the following four pre-equilibrium reaction models as follows [32-35]:

- **Exciton model:** Analytical transition rates with energy-dependent matrix element (TALYS input keyword "preeqmode 1")
- **Exciton model:** Numerical transition rates with energy-dependent matrix element (TALYS input keyword "preeqmode 2") **(default)**
- **Exciton model:** Numerical transition rates with the optical model for collision probability (TALYS input keyword "preeqmode 3")
- **Multi-step direct/compound model:** (TALYS input keyword "preeqmode 4")

The six different nuclear level density models are mentioned for predicting cross section at excitation energies where discrete level information is not available or incomplete. These models range from phenomenological analytical expressions to tabulated level densities

derived from microscopic models. These three phenomenological and three microscopic level density models of the TALYS code are as follows [36-41]:

- **Constant Temperature (CTM)** (TALYS input keyword "ldmodel 1") **(default)**
- **Back-shifted Fermi Gas Model (BFM)** (TALYS input keyword "ldmodel 2")
- **Generalized Superfluid Model (GSM)** (TALYS input keyword "ldmodel 3")
- **S. Goriely (microscopic)** (TALYS input keyword "ldmodel 4")
- **S. Hilaire (microscopic)** (TALYS input keyword "ldmodel 5")
- **Hartree-Fock-Bogoliubov (microscopic)** (TALYS input keyword "ldmodel 6")

A simplified representation of the function and incorporated different theoretical models of the TALYS code are mentioned in Fig. 4.5.

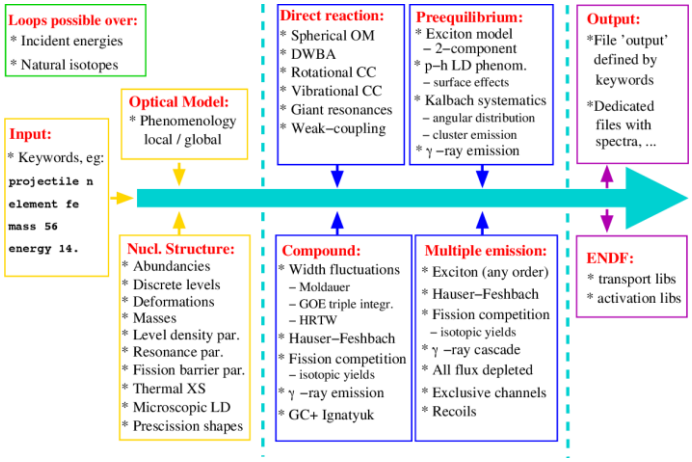

Fig. 4.5 *A simplified representation of the function and incorporated models of the TALYS code.*

https://tendl.web.psi.ch/tendl_2019/talys.html

4.4.2 EMPIRE (ver. 3.2.3) code

This is the modular system of nuclear reaction codes for advanced modelling of nuclear reactions using various theoretical models. It consists of several FORTRAN codes, input parameter libraries, and an experimental data library (EXFOR/CSISRS) operated through the Graphic User Interface (GUI). EMPIRE is intended to be a general, flexible, and easy to use tool for basic research and evaluation of nuclear data. It offers the possibility of combining several theoretical approaches, choosing among alternative input parameters, and calculating an extended set of observables in a single run. Nuclear data evaluation is facilitated by the

ENDF-6 formatting, file verification and graphical comparison with experimental data. EMPIRE code is distributed as a complete, self-contained, and install-free package ready to run when unpacked. It comes with executables, data libraries, sources, the FORTRAN compiler (gfortran), and local implementation of Tcl/Tk-8.4 to be used if needed. The code can be placed anywhere including the home directory or an external device (e.g., flash drive or external drive). It is provided for the three most popular operating systems (Linux/Unix, Mac and MS Windows). The schematic picture of the graphical user interface (GUI) of the EMPIRE code is shown in Fig. 4.6.

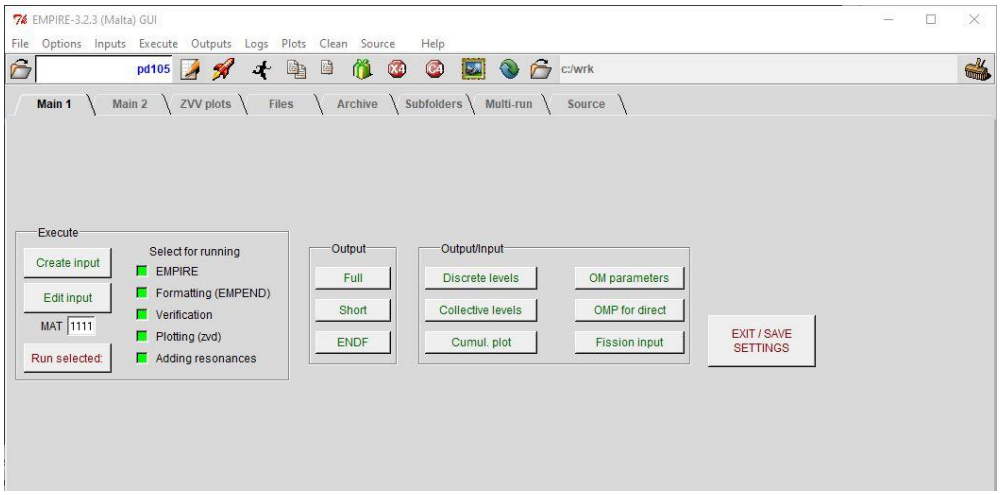

Fig. 4.6 *The GUI of the EMPIRE code.*

In addition, the theoretical calculations were also performed using the EMPIRE (ver. 3.2.3) code. In the EMPIRE code, the compound nucleus (CN) reaction cross section was calculated in the framework of the Hauser-Feshbach theory. The calculation of the direct reaction was considered using the ECIS06 code [42]. The width fluctuation corrections were considered using the Hofmann, Richert, Tepel, and Weidenmuller model (HRTW) up to an incident neutron energy of 3 MeV. The optical potential model parameters for the outgoing protons were also taken from the RIPL-3 database using Koning and Delaroche *et al*. The γ-ray strength function was described via the modified Lorentzian model available in the RIPL-3 database. This code includes six closed forms for the E1 strength function (selected by keyword GSTRFN) as follows [43-49]:

- **GSTRFN = 0** EGLO enhanced generalized Lorentzian (Uhl-Kopecki)
- **GSTRFN = 1** MLO1 modified Lorentzian version 1 (Plujko, RIPL) **(default)**
- **GSTRFN = 2** MLO2 modified Lorentzian version 2 (Plujko, RIPL)

- **GSTRFN = 3** MLO3 modified Lorentzian version 3 (Plujko, RIPL)
- **GSTRFN = 4** EGLO enhanced generalized Lorentzian (RIPL)
- **GSTRFN = 5** GFL (Mughabghab)
- **GSTRFN = 6** SLO standard Lorentzian

There are four different level density models are mentioned for estimating the cross sections in EMPIRE code as follows [50-52]:

- **LEVDEN = 0** EMPIRE-specific level densities, adjusted to RIPL-3 experimental D_{obs} and to discrete levels **(default)**,
- **LEVDEN = 1** Generalized Superfluid Model (GSM, Ignatyuk et al.), adjusted to RIPL experimental D_{obs} and to discrete levels,
- **LEVDEN = 2** Gilbert-Cameron level densities (parameterized by Ijinov et al.), adjusted to RIPL experimental D_{obs} and to discrete levels,
- **LEVDEN = 3** RIPL-3 microscopic HFB level densities.

Moreover, the two quantum mechanical and two phenomenological pre-equilibrium models are implemented in EMPIRE code to consider the pre-equilibrium emission at higher energies as follows [53-56]:

- **MSC = 1** Multi-Step-Compound
- **MSD = 0** Multi-Step-Direct model
- **PCROSS=1.5** Exciton model with default mean free path multiplier (MFP) **(default)**
- **HMS = 1** Monte Carlo Hybrid (DDHMS)

https://www-nds.iaea.org/empire/index.html

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