Chapter 2

Brief Survey of Various Transport Models used for Heavy-Ion Collisions

2.1 Introduction

The nuclear collisions in medium energy regime are associated with various phenomena like collective flow [1–3], multi-fragment emission [4,5], and subthreshold particle production [6]. One needs proper transport theories to simulate the HI reactions and understand the reaction dynamics. In the current scenario, theoretical interest lies in the investigation of nuclear equation of state [7,8], dynamics of fragmentation [9,10], and bimodal-distribution of fragments [11,12] etc. Theoretical description of heavy-ion collisions is also important to explain phenomena beyond nuclear physics. For instance, the stability and radius of neutron stars, as well as formation of stars and supernovae explosions strongly depend upon the character of nuclear equation of state.

The main purpose of this chapter is to highlight various important features of commonly used transport models in different incident energy regimes. No single transport model is capable of describing the reaction dynamics for the whole incident energy range. One has to employ a specific theory depending upon the incident energy regime. To interpret the experimental observables, different theoretical efforts have been made in past, which describe the evolution of such non-equilibrium processes. One of the primary microscopic theory to describe the heavy-ion collisions was inter nuclear cascade (INC) model. This type of model has been extensively employed in relativistic HI collisions [13–15], where one assumes that nucleons interact via binary collisions only. With coalescence, it could create fragments upto alpha particles ($^4He$) only. This limits the scope of INC model to study the fragment formation and related observables at intermediate energies.
Molitoris et al. [16] showed that INC approach lacks dynamical flow due to very little intrinsic pressure built up in the cascade model. It reflects the absence of compression energy in the nuclear system.

In the present day scenario, two different semi-classical theoretical approaches, namely Boltzmann-Uehling-Uhlenbeck (BUU) model [17,18] and molecular dynamics approach, the so-called ‘quantum’ molecular dynamics (QMD) model [19–21] are in use. These models include important quantum features viz. Fermi motion of nucleons, stochastic nucleon-nucleon (n-n) scattering and Pauli blocking. At low energies (below 50 AMeV), Pauli principle dominates the physics suppressing the 2-body collisions. In the latter case, mean field approaches like TDHF [22] or its semi classical version (Vlasov equation) [23–25] are suitable candidates. Some attempts have also been made to incorporate residual n-n collisions in extended approach (ETDHF) [26]. In the following sections, we shall be having an overview of these transport models.

2.2 On the derivation of time dependent Hartree-Fock (TDHF) theory

The TDHF theory belongs to the class of microscopic models to describe heavy-ion collisions. In Schrödinger picture, time development of the system is given as:

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle,$$

(2.1)

where $H$ is the many-body Hamiltonian. The one-body density matrix is then given by

$$\rho_{ji}(t) = \langle \psi | c_j^+ c_i | \psi \rangle.$$

(2.2)

Differentiating w.r.t time $t$, we get

$$ih\rho_{ji} = \langle \psi | [c_j^+ c_i, H] | \psi \rangle.$$

(2.3)

The Hamiltonian $H$ is defined as:

$$H = T + V = \sum_{\alpha \beta} T_{\alpha \beta} c_{\alpha}^+ c_{\beta} + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} V_{\alpha \beta \gamma \delta} c_{\alpha}^+ c_{\beta}^+ c_{\gamma} c_{\delta},$$

(2.4)

with $T$ as the single particle kinetic energy operator and $V$ as the two-body interactions. $c_{\alpha}^+$ and $c_{\beta}$ represent the creation and destruction operators, respectively.
Defining Hartree-Fock (HF) potential as:

\[
(j|U|\gamma) = \sum_{ab} [(j\alpha|V|\gamma\delta) - \langle \alpha j|V|\gamma\delta \rangle \rho_{ab}]
\]

and using in Eq. (2.3), we obtain Liouville’s equation for the density matrix in the interaction representations:

\[
\rho_{ji} = \frac{1}{\hbar} [T + U, \rho]_{ji}.
\]

This is familiar TDHF equation with time dependent potential.

The TDHF equations has also been used with Skyrme energy density functional [27, 28]. The main feature of this theory is to ensure antisymmetrized independent particle states so as to simulate the Pauli principle. It has been extensively employed to heavy-ion fusion reactions for last three decades [27–30]. Recently TDHF method predicted that nucleus-nucleus potential becomes energy dependent when center-of-mass energy approaches corresponding Coulomb barrier [30]. Such energy dependence is expected to affect the sub-barrier fusion process.

### 2.3 The intranuclear cascade (INC) model

In contrast to the TDHF theory, the intranuclear cascade model treats the n-n collisions in an explicit way. In this model, no Fermi momenta are assigned to nuclei. Each nucleon is treated as a collection of point nucleons distributed within a sphere. Initial coordinates of nucleons within a sphere are assigned by Monte Carlo procedure. When two nucleons collide, a Monte Carlo sampling decides whether scattering is elastic or inelastic. Cascade is a rapid process that takes place in about \(10^{-22}\) s. The intranuclear cascade models rely on the assumption that incoming particles interact with individual nucleons of the target and not the nucleus as a whole. This assumption is easily justified at higher incident energies since the de Broglie wavelength is much smaller than the average distance between the nucleons in a nucleus. It has been proposed that a sufficient condition for this justification is [31]:

\[
\lambda_B \ll r_o \ll vt_{\text{coll}} \ll d,
\]

where \(\lambda_B\) is the de Broglie wavelength, \(r_o\) is the range of the interaction, \(v\) is the relative speed, \(t_{\text{coll}}\) is the collision time and \(d\) is the average distance between nucleons in a nucleus. For beam energy of 150 AMeV or more, only inelastic channel of importance
is the pion channel. This is commonly included as the \( \Delta \)-formation: \( nn \rightarrow n\Delta \), and \( \Delta \)-absorption: \( n\Delta \rightarrow nn \). For these inelastic and elastic channels (\( nn \rightarrow nn \), \( n\Delta \rightarrow n\Delta \) and \( \Delta\Delta \rightarrow \Delta\Delta \)), the Cugnon parametrization of scattering cross section is employed \([32]\). At the end of multiple collision process, \( \Delta \) particles are allowed to decay isotropically into a pion and a nucleon. In fact, intra-nuclear cascade codes treat the interaction of incident nucleons with a piece of matter providing them with a random mean free path. An excited remnant, the residue, is formed in initial stage which decays through sequential evaporation of nucleons and heavier fragments. It may be worth noticing that INC model neglects the interaction between cascading particles.

Cascade model left a great deal of things to be dealt with. For instance, Fermi momentum should be assigned to nucleons in the initial state. Fermi motion also demands inclusion of potential wells to model the reaction correctly. Some versions of this model have also tried inclusion of Fermi momenta for both target and projectiles \([33]\). However, potential well is not included in these Monte-Carlo calculations. The absence of potential well rules out its applicability in describing the production of composite particles as well as projectile fragmentation. Further possibility of using INC model to study heavy-ion collisions is limited to high-energy regimes, particularly. This is due to the absence of interactions among cascading particles.

The INC calculations can explain the high energy tail of the emitted protons and neutrons energy spectra, but failed to explain the low energy tail and energy spectra of composite particles \textit{i.e.} deuterons, tritons and heavier particles. The cascade model is, therefore, well suited for studying the equation of state (EoS) of an ideal gas only. Now, we shall discuss various transport theories that employ mean field along with \( n-n \) collisions. These theories include one-body approach namely Boltzmann-Uehling-Uhlenbeck (BUU) model \([17,18]\) and many-body approaches such as quantum molecular dynamics (QMD) model \([20]\), antisymmetrized molecular dynamics (AMD) \([34–36]\), and fermionic molecular dynamics (FMD) \([37]\). Also these models include various quantum effects such as Pauli-blocking, Fermi momentum \textit{etc.}\n
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2.4 The Boltzmann-Uehling-Uhlenbeck (BUU) equation

The BUU model can be regarded as an improvisation of the cascade model with inclusion of mean field. Under TDHF scheme, two-body correlations are retained at various levels. BUU equation describes the time evolution of one-body distribution function in six-dimensional phase space. Consider the coordinate space density matrix

\[ \rho_{rr} = \sum_i \psi_i(r)\psi_i^*(r), \quad (2.7) \]

Instead of considering \( \rho_{rr} \), we find the equation of motion of its Fourier transform \( f(r, p) \):

\[ f(r, p) = \frac{1}{(2\pi\hbar)^3} \int e^{-\frac{ip}{\hbar}\cdot r}s d^3s. \quad (2.8) \]

An equivalent definition in momentum representation will be

\[ f(r, p) = \frac{1}{(2\pi\hbar)^3} \int e^{-\frac{ip}{\hbar}\cdot r}g_{r+\frac{p}{2}p-\frac{q}{2}}d^3q. \quad (2.9) \]

The quantity \( f(r, p) \) is the closest analogue to classical phase space density that satisfies following relations:

\[ \int f(r, p)d^3p = \rho(r), \quad (2.10) \]
\[ \int f(r, p)d^3r = g(p), \quad (2.11) \]
\[ \int g(p)\frac{p^2}{2m}d^3p = \langle \psi|T|\psi \rangle. \quad (2.12) \]

From TDHF equation, we have

\[ \dot{\rho}_{ji} = \frac{1}{i\hbar} \sum_\gamma \langle j|T + U|\gamma \rangle \rho_{\gamma i} - \rho_{j\gamma} \langle \gamma|T + U|i \rangle. \quad (2.13) \]

Using Eq. (2.13),(2.9) and (2.8), we calculate \( \frac{df}{dt} \) as

\[ \frac{df(r, p)}{dt} = A + B, \quad (2.14) \]

where

\[ A = \frac{1}{(2\pi\hbar)^3} \frac{1}{i\hbar} \int \left[ e^{-ip\cdot r/\hbar}|(p + q/2)|T|\rho_{p+q/2}\right] \frac{d^3p}{d^3q}, \quad (2.15) \]
\[ B = \frac{1}{(2\pi\hbar)^3} \frac{1}{i\hbar} \int \left[ e^{-ip\cdot r/\hbar}|(r + s/2)|T|\rho_{r+s/2}\right] \frac{d^3r}{d^3s}. \quad (2.16) \]
Here \( 'q' \) is the relative pair momentum \( (= q_1 - q_2) \) between two particles. Similarly \( 's' \) denotes relative distance in coordinate space. Equation (2.14) then reduces to

\[
\frac{\partial f(r, p, t)}{\partial \tau} + v \cdot \nabla_r f(r, p, t) - \nabla_r U(r, p, t) \cdot \nabla_p f(r, p, t) = \frac{\partial f}{\partial \tau}_{\text{coll}} \tag{2.17}
\]

Here \( U(r, p, t) \) is a self-consistent mean field associated with one-body distribution function \( f(r, p, t) \). The term on r.h.s. of Eq. (2.17) is a collision term which shows that \( f(r, p, t) \) will change when there is an interaction among particles. Assuming that only binary collisions dominate and ignoring the possibility that three or more particles collide simultaneously, we have from Eq. (2.17):

\[
\left( \frac{\partial}{\partial \tau} + v_1 \cdot \nabla r_1 - \nabla r_1 U \cdot \nabla v_1 \right) f_1 = \int d\Omega \, d^3 \sigma(\omega) \left| v_1 - v_2 \right| \left( \hat{f}_1 \hat{f}_2 - f_1 f_2 \right) \tag{2.18}
\]

\( \sigma(\omega) \) is the differential cross-section for the collision \( (v_1, v_2) \rightarrow (\hat{v}_1, \hat{v}_2) \). Here, following abbreviations have been used [38]:

\[
\begin{align*}
    f_1 & \equiv f(r, v_1, t), \\
    f_2 & \equiv f(r, v_2, t), \\
    \hat{f}_1 & \equiv f(r, \hat{v}_1, t), \\
    \hat{f}_2 & \equiv f(r, \hat{v}_2, t).
\end{align*}
\]

This is integro-differential equation for \( f(r, p, t) \). Bertsch and Das Gupta have solved this equation for \( A \)-particles [17], where for the general case Eq. (2.18) is replaced by a set of \( A \)-coupled equations.

In the BUU model, particles are point like entities in configuration and momentum space. BUU equation (2.17) describes the time evolution of one body distribution function in six-dimensional phase space using Hamiltonian formulation:

\[
\begin{align*}
    \dot{r}_i &= \{p_i, H\} = \{p_i, T + U\}, \\
    \dot{p}_i &= -\{r_i, H\} = -\{r_i, T + U\}, \tag{2.19}
\end{align*}
\]

where \( T \) and \( U \) represent the total kinetic and potential energies of all nucleons and \( 'i' \) is index of the nucleons. For the mean field, one takes a Skyrme type potential \( U(\rho) \) as has been used in TDHF calculations:

\[
U(\rho) = \alpha \left( \frac{\rho}{\rho_0} \right) + \beta \left( \frac{\rho}{\rho_0} \right)^3. \tag{2.20}
\]

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The density in BUU approach is determined by means of a cubic grid of size ‘a’ in the coordinate space. At each time step, one-particle distribution function \( f^{(1)} \) has to be generated from the pseudo A-particles. Then, one can choose again randomly the test particles according to distribution function \( f^{(1)} \). Therefore, this treatment retains some correlations but destroys all \( n-n \) correlations at each time step. For realistic calculations, one prefers to retain these correlations which would be suitable in many dynamical scenarios like instabilities, fission, multifragmentation and chaos etc. As far as single particles are concerned, BUU theory has been established as one-body approach to HI reactions. The recent advances in the BUU simulation incorporate momentum dependent [39] and isospin dependent potentials as well as isospin dependent \( n-n \) scattering cross section [40]. A good agreement has been found for longitudinal and transfer momenta, particle multiplicities and double differential cross section from the predictions of BUU model. The BUU equation is found suitable for describing the flow angle, which has a relevance to the nuclear EoS. Recently, BUU transport model was applied to calculate the anisotropy ratio \( \langle E^z/E^l \rangle \) for \(^{197}\text{Au}+^{197}\text{Au} \) collisions as a function of impact parameter at incident energies of 100, 250 and 400 AMeV [41]. A better agreement with FOPI data was reached employing a stiff EoS. These predictions on stopping of nuclear matter indicate preferential expansion of nuclear matter into transverse direction rather than longitudinal direction for the head-on \(^{197}\text{Au}+^{197}\text{Au} \) collisions. However, predictive power for the ‘best fit’ equation of state is limited one, since FOPI data can not be used to directly decide on incompressibility due to acceptance cuts. Detector inefficiency naturally, tends to reduce the sensitivity of this ratio towards incompressibility. Therefore, one needs systematic study and reliable information from various transport models rather than immediately running into best choice for EoS.

A covariant description of BUU equation has also been advanced to study the hadron-nucleus and heavy-ion collisions [42]. This relativistic kinetic equation also termed as relativistic Boltzmann-Uehling-Uhlenbeck (RBUU) equation is defined as:

\[
[k^\mu \partial^\nu_n + (k_n^\mu P_{\mu\nu} + M^2(\partial^\nu_n M^\nu_n))\partial^\mu_n]f(x,k^\mu) = \frac{1}{2(2\pi)^7} \int \frac{dk_2}{E_{k_2}} \frac{dk_3}{E_{k_3}} \frac{dk_4}{E_{k_4}} \sum_{j_1j_2j_3j_4} W(kk_2|k_3k_4)[f_1f_4f_2f_3 - f_1f_3f_2f_4]. \tag{2.21}
\]

This approach is reported to explain the cross section for kaon momentum distribution at SIS energies quite well as measured by the KaoS Collaboration at GSI [43]. Equation (2.21) gives the evolution of single particle distribution \( f_i \equiv f(x, k_i^\nu) \) under the influence...
of a mean field that enters via effective mass $M^*$ and the field tensor $F_{\mu\nu}$. The r.h.s. term is the collision integral in which $f_i \equiv f(x, k_i^*)$ for the particle and $\bar{f}_i \equiv (1 - f(x, k_i^*))$ for the hole distributions with four-momentum $k^\mu = (E_i^*, \mathbf{k})$. In fact, the collision integral includes all inelastic channels such as resonances production and absorption along with meson production. This theory recently explained the $K^+$ mesons energy spectrum in C+C $\oplus$ 2 AGeV collisions which was measured by HypHI Collaboration at GSI [44,45]. This theory is well suited for energetic collisions between light nuclei. Choice of heavier nuclei hinders identification of hyper nuclei via weak decay of hyperons into pions.

2.5 Molecular dynamics approaches

Inherent problems of these models is to extract more complicated 2-body observables. It has always remained a problem of how to deal with composite particles formation. At present, dynamical models based upon molecular dynamics picture are well suited to handle phenomena such as multi-fragment emission. Molecular dynamics approaches ensure retention of multi-particle correlations and are able to address the phenomena like cluster formation. This has led to preference for molecular dynamics model to remove the grey area of mean field models which treat the single particle phase space density $f(\mathbf{r}, \mathbf{p})$ and are most suitable for the calculation of quantities which are expressed as expectation values of one-body observables. Basic character of QMD is similar to classical molecular dynamics model [10] i.e. it solves classical equations of motion for the position and momenta of A-particles:

$$\mathbf{r}_i = \nabla_{\mathbf{p}_i}(H) ; \quad \mathbf{p}_i = -\nabla_{\mathbf{r}_i}(H) ; \quad i = 1, ..., A. \tag{2.22}$$

The QMD model differs from its classical versions in two aspects. One is the inclusion of Fermi character in ground state of nuclei and second is appearance of both a collision and a potential term generated by same bare interaction. Our findings in present work have been compiled in the framework of quantum molecular dynamics (QMD) model which will be discussed in detail in chapter 3.

For the study of heavy-ion collisions at relativistic energies, ultra-relativistic quantum molecular dynamics (UrQMD) model has also been designed [47,48]. This theory is well suited to describe nucleus-nucleus collisions at AGS and SPS energies where quark and gluon degrees of freedom become relevant. This relativistic version contains 55 baryons
and 32 meson states together with their antiparticles and isospin projected states. For masses greater than 2.0 GeV/c², a string picture is used by incorporating color string formation and resonance decay. Nucleons interact via two- and three-body Skyrme potential supplemented with Yukawa and Coulomb potentials as in non-relativistic version of the QMD model. The total nucleon-nucleon cross section $\sigma_{nn}$ depends upon isospin of the colliding nucleons, their flavor and center-of-mass energy. A collision between two hadrons would occur if relative distance $d < \sqrt{\frac{\sigma_{nn}(d)}{\pi}}$, where 'd' and 'σ_{nn}' are the impact parameter and total scattering cross section of two hadrons. The neutron-neutron cross section is assumed to be equal to proton-proton cross section [49]. The total and elastic proton-antiproton cross section at higher incident energies are calculated according to CERN-HERA parameterization:

$$\sigma_{pp}^{el} = A + Bp^n + C\ln^2(p) + D\ln(p),$$

with laboratory momentum 'p' in GeV/c and cross section $\sigma$ in mb. Parameters of this fit are listed in Ref. [48]. Recently nuclear matter stopping was studied over wide range of beam energy from SIS, and AGS upto SPS within UrQMD model. There, medium modification of n-n cross section and stiffness of equation of state are found to strongly affect the nuclear stopping at SIS energies [50]. With increase in energy from AGS to SPS, the so-called gaussian shape rapidity distribution gets changed to two-bump structure. This reflected dominance of transparency behavior in the high SPS energy region.

### 2.6 Molecular dynamics for fermions (FMD/AMD)

Recently, molecular dynamics approach has been advanced to describe the fermionic nature of nuclear matter using antisymmetrized wave packets. The fermionic molecular dynamics (FMD) model was proposed by Feldmeier et al [37, 51, 52]. In this approach, the total wave function of the system is represented by a Slater determinant of gaussian wave packets. The width of gaussian wave packet is treated as a variable in time which is an important non-classical degree of freedom [52, 53]. This helps to allow for evaporation of nucleons. This model is well suited for the study of low-energy fusion fission events and nuclear structure [54, 55]. The FMD approach has been recently employed to study the ground state band in $^{12}$C nucleus [56]. The FMD calculations are found to give good description of negative parity states [55], whereas $\alpha$-cluster model predicted too
small excitation energy for the $2^+$ state. On the similar lines, antisymmetrized molecular
dynamics (AMD) model has been extended in which A-nucleon system is represented by
a Slater determinant of single particle gaussian wave packets [34, 35, 57, 58]. The AMD
model assumes width of gaussian wave packet as a constant parameter unlike FMD model.
This simplification nevertheless reduces computational time and ensures that there is no
spurious coupling of internal motion and c.m. motion of a cluster or a nucleus. The set
of single particle wave function is given as:

$$\phi_i(t) = \{Z_i(t), \chi_i, \xi_i\}$$

where the centroid of wave function $Z_i(t)$ is a complex variable defined as:

$$Z_i = \sqrt{L} \mathbf{r}_i + \frac{i}{2\hbar \sqrt{L}} \mathbf{p}_i,$$

with $L$ as width parameter taken to be equal to 0.16 fm$^{-2}$ and is time independent. The
variables $(\chi_i, \xi_i)$ represent the spin-isospin states of a nucleon in $p^\uparrow, p_\downarrow, n^\uparrow,$ and $n_\downarrow$
states. $(\mathbf{r}_i, \mathbf{p}_i)$ corresponds to position and momentum coordinates of each nucleon. The
time evolution of centroids $Z_i$ in Eq.(2.25) is treated in a classical manner. The important
point on which these approaches differ from the QMD model is that physical momentum in
AMD model is taken to be centroid of the gaussian wave packet in momentum distribution.
In QMD model, usually, it represents the definite momentum of a nucleon. The AMD
simulations of Ca+Ca reactions have recently shown that rms radii, fragment kinetic
energies, and yield of light charged particles ($Z=1$, and 2) were larger than those of
equilibrium ensemble prepared by confining the many body system in a container at all
reaction times [59]. These calculations depict the significance of flow effects and transverse
kinetic energy of fragments.

### 2.7 Summary

In this chapter, we have recaptured the basic details of transport models used in low
and intermediate energy heavy-ion reactions. The mean field approaches like TDHF are
suitable candidates for low energy heavy-ion reactions. At intermediate energies, phenomena
such as multi-fragment emission, particle production and collective flow require more
advanced transport models that can handle mean field and nucleon-nucleon collisions at
the same level. We address the importance of one-body approach namely Boltzmann-
Uehling-Uehlenbeck (BUU) equation and many-body approaches such as QMD, FMD
and AMD models. The quantum molecular dynamics (QMD) approach is an important tool to describe the multi-fragment emission and related phenomena such as transverse expansion, entropy production, system size effects etc. For the present thesis work we shall use the QMD model that is described in detail in the next chapter. The QMD calculations are suitably compared with experimental observables, wherever it is needed. An attempt shall also be made to probe nuclear incompressibility via spectator matter fragmentation at ultra-low excitation energies.
Bibliography


