Chapter 2
Methodology

2.1 Introduction

As discussed in Chap. 1, the dynamical study of heavy-ion collisions at intermediate energy needs correct information about the real and imaginary parts of the potential. In addition, one has to also deal with the initial non-equilibrated situation that changes with the course of the reaction. Any dynamical model, designed for the intermediate energy heavy-ion collisions, should be able to handle these different situations emerging at different stages of the reaction. The conventional theories like the Hartree-Fock and Schrödinger equation are good for a system propagating under the influence of mean field alone, which is valid at low incident energies only. However, the problems at intermediate energies can be dealt with the help of transport models that are capable of following the dynamics from the start (where matter is non-equilibrated) to the final state (where matter is cold and fragmented). These transport models are supposed to include the essential collision physics. In the following, we shall first present some of the earlier attempts and then shall discuss in detail the quantum molecular dynamics (QMD) model used in the present study.

2.2 The time dependent Hartree-Fock (TDHF) theory

The low energy heavy-ion collisions can be described by the time dependent Hartree-Fock theory which is a quantum mechanical theory [1]. The TDHF assumes independent particle behaviour for nearly equilibrated states to non-equilibrated situations if the ex-
citation energy is less than 10 MeV/nucleon. The TDHF describes the many body wave function by a single Slater determinant. The wave function for a system at a time \( t \) is given by [2]

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

where \( H \) is a many body Hamiltonian given by

\[
H = T + V = \sum_{i,j} T_{ij} c_i^+ c_j + \frac{1}{2} \sum_{i,j,k,l} U_{ijkl} c_i^+ c_j^+ c_k c_l,
\]

with \( T \) as the single particle kinetic energy operator and \( U \) as the two-body interactions. The one-body density matrix is then given by

\[
\rho_{ij} = \langle \psi | c_i^+ c_j | \psi \rangle.
\]

It has been shown by many authors that this time dependent density equation will not reduce to a pure one-body equation. The equation of motion shows that the one-body density matrix is related to the two-body density matrix. Similarly, the equation of motion for two-body density matrix is related to three-body density matrix, and so on. This series of the equations, which are called Bogoliubov-Bonn-Green-Kirkwood-Yvon hierarchy (BBGKY) [3], is equivalent to the full solution of the time dependent Schrödinger equation. In order to reduce this equation to one-body equation, we have to introduce some approximations. The TDHF assumes

\[
\rho^{(2)}_{ijkl} = \rho_{ik} \rho_{jl} - \rho_{ij} \rho_{kl}.
\]

This terminate the BBGKY hierarchy and yields the TDHF equation:

\[
i\hbar \frac{d\rho}{dt} = [h, \rho],
\]

where \( h \) is the Hartree-Fock Hamiltonian:

\[
h = \sum_{ij} T_{ij} + \sum_{kl} (V_{ijkl} - V_{iklj}) \rho_{kl}.
\]
The particle number as well as the energy of the system and Slater determinant are always conserved in TDHF theory [3]. The TDHF theory has been applied at low incident energies to study different physical processes such as compound nucleus formation, dissipation, shock wave propagation etc. [4]. Some attempts are also made in the literature to extend the above equation to include the residual nucleon-nucleon interactions which are responsible for two-body collisions. This attempt is called as Extended Time Dependent Hartree-Fock (ETDHF) equation [5]. Unfortunately, ETDHF is too complicated to be used for large scale investigations in heavy-ion collisions at low and intermediate energies where frequent nucleon-nucleon collisions are in dominant mode [5].

2.3 The intranuclear cascade (INC) model

In contrast to the TDHF theory, the intranuclear cascade model is capable of describing the very high energy heavy-ion collisions [6]. In this model, the mean field is completely neglected and the nucleon-nucleon collisions are taken without Pauli-blocking. Note that this was the first microscopic dynamical model used to understand the experimental data of heavy-ion collisions [6]. The INC model simulates the heavy-ion collisions as a superposition of independent two-body nucleon-nucleon collisions. In the absence of mean field, all nucleons move on straight line trajectories until they collide.

In this model, each nucleus is considered as a collection of point particles distributed within a sphere of radius $R$ without any Fermi momentum. When two nuclei approach each other, the position of each nucleon is assigned by Monte-Carlo sampling. The time evolution is followed by dividing the whole reaction time into the small intervals $\Delta t$. Two nucleons are supposed to collide if they pass the point of closest approach within a given time interval. The distance of closest approach $d_{\text{max}}$ is $\sqrt{\sigma_{\text{tot}}(\sqrt{s})}/\pi$, where $\sigma_{\text{tot}}(\sqrt{s})$ is the total nucleon-nucleon cross section in their center-of-mass system and $\sqrt{s}$ is the center-of-mass energy. The colliding nucleons can also scatter elastically or inelastically. The main processes include:

$$
\text{elastic} : \begin{cases}
N + N \rightarrow N + N & (a), \\
N + \Delta \rightarrow N + \Delta & (b), \\
\Delta + \Delta \rightarrow \Delta + \Delta & (c).
\end{cases}
$$

(2.8)
The cross sections for channels (a) and (d) are taken from experiments. The cross sections for channels (b) and (c) are taken to be same as (a). The cross section for channel (e) is obtained by detailed balance method.

At the end of the reaction, all $\Delta$'s decay isotropically into nucleons and pions by conserving the charge and isospin quantum numbers. In other words, the number of $\Delta$'s at the end of the reaction gives the number of pions. The INC model gave excellent opportunity to extract the information about several experimental observables [6]. As the mean field of the nucleons as well as the crucial quantum features are neglected in this approach, its applicability is limited to high energy heavy-ion collisions only.

We shall now discuss some other transport models that treat the mean field as well as nucleon-nucleon collisions at the same level. In this series, the microscopic Nuclear Fluid Dynamics (NFD) model [7] was the first to exhibit the relation between the equation of state, collective flow, and pion production. The main disadvantage of the NFD model is, however, that much of the microscopic dynamics is lost. In particular, the initial non-equilibrium state of the collision is not possible within this theory [7]. The Boltzmann-Uehling-Uhlenbeck (BUU) model [2,8] is among the first microscopic models developed for heavy-ion collision at intermediate energies. In the following, we shall discuss in brief the BUU model.

2.4 The Boltzmann-Uehling-Uhlenbeck (BUU) model

The BUU model follows the time evolution of one body function $f$ [2,8]:

$$
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f - \nabla_r U \cdot \nabla_p f = -\frac{1}{(2\pi)^6} \int d^3p_2d^3p_1 \frac{d\sigma}{d\Omega} \delta_{12} \times \left\{ \left[ ff_2(1-f_1)(1-f_2)-f_1f_2(1-f)(1-f_2) \right] \right\} \times \left(2\pi\right)^3 \delta^3(\mathbf{p} + \mathbf{p}_2 - \mathbf{p}_1 - \mathbf{p}_2).$$

(2.10)
Here $f$ is the one-body distribution function and $f_1$ is defined as $\frac{n_1}{n-1}$ where $n_1$ is the number of test particles in the phase-space volume excluding the test particle at $(r_i, p_i)$. Similarly $f_2$ is $\frac{n_2}{n-1}$. The collision integral (which also includes the Pauli-blocking) is shown on the right hand side of Eq. (2.10). The above equation [Eq. (2.10)] is solved by test particle method. Here phase-space of each nucleon is represented by a large number of pseudo-particles (called test particles). In its numerical implementation, the above equation reduces to a set of $6 \times (A_T + A_P) \times N$ coupled first order differential equations in time. Here $N$ represents the number of test particles per nucleon and $A_T$ and $A_P$ are, respectively, the target and projectile. The test particle method replaces the expectation value of a single particle observable:

$$\langle O(t) \rangle = \int f(r, p, t)O(r, p)d^3rd^3p, \quad (2.11)$$

by a Monte-Carlo integration

$$\langle O(t) \rangle = \frac{1}{n(A_T + A_P)} \sum_{i=1}^{n(A_T + A_P)} O(r_i(t), p_i(t)), \quad (2.12)$$

with $r_i(t)$ and $p_i(t)$ being the points in phase-space which are distributed according to $f(r, p, t)$:

$$f(r, p, t) = \lim_{n \to \infty} \frac{1}{n(A_T + A_P)} \sum_{i=1}^{n(A_T + A_P)} \delta(r - r_i(t))\delta(p - p_i(t)). \quad (2.13)$$

Obviously, large number of test particles will be needed to avoid the numerical noise. In earlier attempts, test particles were represented by classical point particles. The recent calculations, however, use Gaussian wave packets for test particles [2]. The time evolution of these test particles is governed by the classical Hamilton’s equations of motion

$$\dot{p}_i = -\frac{\delta(H)}{\delta r_i}, \quad (2.14)$$

$$\dot{r}_i = \frac{\delta(H)}{\delta p_i}. \quad (2.15)$$

It is worth mentioning that the forces acting on the test particles are calculated from the entire distribution which includes the test particles of all events. In other words, the $n$ parallel events are inter-connected and therefore, event by event correlations cannot be analyzed. In the limit $n \to \infty$, the distribution of these test particles should represent a
true one-body distribution function.

Another method to solve the collision integral of Eq. (2.10) was developed by Bonasera et al. [9]. In this method, concept of mean free path was used to solve the collision integral where mean free path was defined as

\[ \lambda = \frac{1}{\sigma_{NN} \rho_{\text{test}} / N} \]  

(2.16)

where \( \sigma_{NN} \) is the free nucleon-nucleon cross section. \( N \) is the number of test particles per nucleon. \( \rho_{\text{test}} \) is the test particle density. One can have

(a) Parallel ensembles approximation in which \( N = 1 \) and \( \rho_{\text{test}} = \rho_0 \) (normal nuclear matter density). Since one ensemble is not enough to avoid numerical noise, one needs to perform \( n \) parallel events.

(b) Full phase-space evaluation of the collision integral which is similar to the method described above in BUU model. In this case \( N \gg 1 \) and \( \rho_{\text{test}} = N \rho_0 \). Only one ensemble is necessary to calculate the average physical quantities. Note that in both the cases, mean free path remains the same, i.e., if one increase the test particle density, one accordingly reduce the nucleon-nucleon cross section.

Any one-body observable can be calculated by averaging the values weighted with the distribution function. In brief, the BUU model is able to explain the one-body observables like the collective flow, stopping as well as particle spectra [2, 8]. Recent developments in BUU model incorporates the inclusion of momentum dependent potential [10] and isospin dependent potential as well as isospin dependent nucleon-nucleon scattering cross section [11]. In the following, we describe in detail the quantum molecular dynamics (QMD) model [7, 12–17] which is an \( N \)-body model.

### 2.5 The quantum molecular dynamics (QMD) model

The correlations among nucleons can be described within the classical molecular dynamics (MD) or “equation of motion” approaches which, in principle, are capable of treating both the compression and fragment formation, albeit on a completely classical level: the Hamilton’s equations of motion are integrated for \( N \)-classical point particles,
with finite range nucleon-nucleon potential. Based on MD approach, Aichelin and Stöcker [7] designed a novel method that incorporates N-body correlations, an equation of state and most important quantum correlations, namely the Pauli-principle, stochastic scattering as well as particle production. It is based on an event by event analysis. Here each event is simulated independent of other events. In contrast to the BUU model, no averaging is done over various events and hence, the correlations among nucleons can be preserved. Note that every transport model (like the QMD model [12–17]) has three fold dynamics: First, one has to generate the projectile/target. This procedure is called as initialization. The nucleons of projectile/target, then, propagate under the influence of surrounding mean field. This step is termed as propagation. The nucleons are bound to scatter (elastically or inelastically) if they come too close to each other. This part is dubbed as nucleon-nucleon collision. In the following, we shall discuss each of these parts in detail.

2.5.1 Initialization

The close agreement between the results of the TDHF theory and classical Vlasov equation led to conclusion that the form of the wave function has insignificant influence on the time evolution of a system, if it fulfills the minimal requirements like the approximate constant density over the proper region in coordinate space, binding energy etc. [12]. In QMD model [12–17], nucleons (represented by Gaussian wave packets) interact via mutual two and three-body interactions. Here each nucleon is represented by a coherent state of the form

$$\psi_i(r, p_i(t), r_i(t)) = \frac{1}{(2\pi L)^{3/4}} \exp \left[ \frac{i}{\hbar} p_i(t) \cdot r - \frac{\{r - r_i(t)\}^2}{4L} \right].$$

(2.17)

For the detailed discussion on the parameter \(L\) (which is related to the extension of the wave packet in phase-space), see Chap. 6 of Ref. [18]. The total \(N\)-body function is assumed to be a direct product of the coherent states [Eq. (2.17)]

$$\Phi = \prod_i \psi_i(r_i, p_i, t).$$

(2.18)

By doing this, one neglects the antisymmetrization. First successful attempts to simulate the heavy-ion reactions with antisymmetrized states have been reported in Refs. [19, 20]. The Wigner transformations of the coherent states are the Gaussians in coordinate and
momentum space. The Wigner density reads as

\[
f_i(r, p, r_i(t), p_i(t)) = \frac{1}{(2\pi \hbar)^3} \int e^{-i\frac{p}{\hbar} r_i(t) - \frac{p_i(t)}{2}} \psi_i^*(r - \frac{r_i(t)}{2}, t) d^3r d^3p,
\]

Here \( r_i(t) \) and \( p_i(t) \) define the classical orbit or the center of Gaussian wave packet in phase-space. The density of the \( i \)th particle is

\[
\rho_i(r) = \int f_i(r, p, r_i(t), p_i(t)) d^3p,
\]

\[
= \frac{1}{(2\pi \hbar)^3} e^{-\frac{(r - r_i(t))^2}{2L^2} - \frac{(p - p_i(t))^2}{2\hbar^2}}. \tag{2.20}
\]

To build a nucleus, we have to first assign the coordinates and momenta to all the nucleons. In three dimensional space (inside a sphere of radius \( R = 1.14A^{1/3} \), where \( A \) stands for either nucleus), the centroid of Gaussian wave packet is uniformly distributed in polar coordinate by:

\[
r = Rx_1^{1/3}, \quad \cos \theta = 1 - 2x_2, \quad \phi = 2\pi x_3, \tag{2.21}
\]

where \( x_1, x_2, \) and \( x_3 \) are the random numbers. The coordinates of nucleons are rejected if their distance is less than 1.5 fm. The local Fermi momentum is determined by the relation

\[
P_F(r_i) = \sqrt{-2mU(r_i)}, \tag{2.22}
\]

where \( U(r_i) \) is the local potential. The center of each Gaussian wave packet in momentum space is uniformly distributed in polar coordinate by:

\[
p_i = P_F(r_i)x_4^{1/3}, \quad \cos \theta = 1 - 2x_5, \quad \phi = 2\pi x_6 \tag{2.23}
\]

where \( x_4, x_5, \) and \( x_6 \) are again random numbers. We reject those distributions where two nucleons are closer than minimum distance \( d_{\text{min}} \). In other words, we demand

\[
(r_i - r_j)^2(p_i - p_j)^2 \geq d_{\text{min}}^2. \tag{2.24}
\]
Typically 1 out of 50,000 initializations is accepted under present criteria. As noted in Ref. [21], the above initial phase-space distribution agrees with the experiments as well as with theoretical calculations of PPW+RPA approach. Extensive tests were conducted by the Heidelberg-Nantes-Frankfurt-Tübingen groups to study the properties of different single (cold) nuclei. This includes the stability of a nucleus, its root mean square radius (in coordinate and momentum space) as well as its binding energy. It is worth mentioning that semi-classical theory may generate nuclei which start emitting nucleons after the lapse of couple of hundred fm/c.

2.5.2 Numerical tests for the stability of nuclei

As stated above, the nuclei prepared within transport model may start emitting nucleons after the lapse of couple of hundred fm/c. Therefore, it is very important to make sure that our initialization does not destabilize the cold nuclei. A large number of tests were conducted by Aichelin and coworkers to check the stability of nuclei [7,12]. The nucleons (inside a nucleus) move under the influence of the mean field of their neighbors. During the propagation, whenever a nucleon comes close to the surface of a nucleus, it is pulled back by other nucleons [12,22]. Due to the local density approximation used here, the light nuclei are little more unstable compared to heavier ones. We have also carried out various checks by calculating the binding energy of different nuclei and also the propagation of heaviest fragment. Most of the nuclei were found to be stable for couple of hundred fm/c which is long enough for our present purpose.

The problem of the stability of nuclei was also looked carefully by the Frankfurt group [23]. They showed that the inclusion of Pauli-potential in the mean field keeps the nuclei stable for several thousand fm/c [24]. In their approach, they included the Gaussian Pauli-potential of Dorso et al. [25]. The total energy of a free Fermi gas is given by

\[ E_{FG} = E_{\text{kin}} + E_{\text{Pauli}} = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} V_p^\sigma \left( \frac{\hbar}{q_0 p_0} \right)^3 \exp\left( -\frac{r_{ij}^2}{2(q_0)^2} - \frac{p_{ij}^2}{2(p_0)^2} \right), \]

with \( V_p^\sigma = 29 \text{ MeV}, q_0 = 3 \text{ fm} \) and \( p_0 = 120 \text{ MeV/c} \). The nuclei like Au, Ru, Ne were found to be close to their ground state.
Once the target and projectile are generated, we boost them with proper center-of-
mass velocity. The propagation and scattering of nucleons, in principle, is represented by
the real and imaginary parts of the G matrix. However, due to practical problems, one
often uses parameterized forms both for the real (representing the mean field) and imagi-
nary parts (taking care of the nucleon-nucleon scattering). In the following, we shall first
discuss the propagation and then shall discuss the nucleon-nucleon scattering/collision.

2.5.3 Propagation

The equations of motion for many-body system are, then, calculated by means of a
generalized variational principle: we start from the action

\[ S = \int_{t_1}^{t_2} \mathcal{L} \left[ \Phi, \Phi^* \right] dt, \]  

with the Lagrange functional

\[ \mathcal{L} = \langle \Phi | i \hbar \frac{d}{dt} - H | \Phi \rangle. \]

The time evolution is obtained by the requirement that the action is stationary under the
allowed variation of the wave function, i.e.,

\[ \delta S = \delta \int_{t_1}^{t_2} \mathcal{L} \left[ \Phi, \Phi^* \right] dt = 0. \]

The Hamiltonian \( H \) contains a kinetic term and mutual interactions \( V_{ij} \), which can be
interpreted as the real part of the Brückner G matrix supplemented by the Coulomb
interaction. The time evolution of the parameters is obtained by the requirement that
the action is stationary under allowed variation of the wave function. This yields an
Euler-Lagrange equation for each parameter. We obtain for each parameter \( \lambda \), an Euler-
Lagrange equation:

\[ \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\lambda}} - \frac{\partial \mathcal{L}}{\partial \lambda} = 0. \]

If the true solution of the Schrödinger equation is contained in the restricted set of wave
functions \( \psi_i(\mathbf{r}, \mathbf{r}_i(t), \mathbf{p}_i(t)) \), this variation of the action will give the exact solution of
the Schrödinger equation. If the parameter space is too restricted, we obtain that wave
function in the restricted parameter space which comes closest to the solution of the
Schrödinger equation. Note that the set of wave functions which can be covered with
special parameterizations is not necessarily a subspace of Hilbert-space, thus the super­
position principle does not hold.

For the coherent states and Hamiltonian of the form \( H = \sum_i T_i + \frac{1}{2} \sum_{ij} V_{ij} \) (\( T_i \) =
kinetic energy and \( V_{ij} \) = potential energy), the Lagrangian and the variation can easily 
be calculated and we obtain:

\[
\mathcal{L} = \sum_i \left[ -\dot{r}_i \dot{p}_i - T_i - \frac{1}{2} \sum_{j \neq i} \langle V_{ij} \rangle - \frac{3}{2} Lm \right],
\]

\[
\dot{r}_i = \frac{p_i}{m} + \nabla_{p_i} \sum_j \langle V_{ij} \rangle = \nabla_{p_i} < H > ,
\]

\[
\dot{p}_i = -\nabla_{r_i} \sum_{j \neq i} \langle V_{ij} \rangle = -\nabla_{r_i} < H > ,
\]

with \( r_i = r_i + \frac{p_i}{m} t \) and \( \langle V_{ij} \rangle = \int d^3r_1 d^3p_1 \langle \psi_i \psi_j | V(r_1, r_2) | \psi_i \psi_j \rangle \). These equations represent the time evolution and can be solved numerically. Therefore, the variational principle reduces the time evolution of n-body Schrödinger equation to the time evolution 6 \times (A_p + A_T) equations. The equations of motion now have a similar structure like the classical Hamiltonian equations

\[
\dot{p}_i = -\frac{\partial \langle H \rangle}{\partial r_i} ; \dot{r}_i = \frac{\partial \langle H \rangle}{\partial p_i} .
\]

The numerical solution can be achieved in the spirit of classical molecular dynamics [26–
28]. The expectation value of the total Hamiltonian reads

\[
\langle H \rangle = \langle T \rangle + \langle V \rangle = \sum_i \frac{p_i^2}{2m_i} + V_{Skyrme} + V_{Yuk} + V_{Coul} + V_{MDI}.
\]

Here \( V_{Skyrme} \), \( V_{Yuk} \), \( V_{Coul} \) and \( V_{MDI} \) are, respectively, the local (two and three-body) 
Skyrme, Yukawa, Coulomb, and momentum dependent potentials. The momentum de­
pendent interactions will be discussed in Chap 4. The local Skyrme interaction is written as

\[
V_{Skyrme} = \frac{1}{2!} \sum_{j \neq i} V_{ij}^{(2)} + \frac{1}{3!} \sum_{j,k \neq i \neq jk} V_{ijk}^{(3)} .
\]

Here \( V_{ij}^{(2)} \) and \( V_{ijk}^{(3)} \) represent, respectively, the two and three-body interactions. The two­
body interactions \( V_{ij}^{(2)} \) are obtained by folding the two-body potential with the densities
of both the nucleons.

\[ \sum_{j \neq j'} V_{ij}^{(2)} = \sum_{j \neq j'} \int f_1(r_i, p_i, t) f_j(r_j, p_j, t) V(r_i, r_j) \times d^3 r_i d^3 r_j d^3 p_i d^3 p_j, \]  
(2.36)

\[ = \sum_{j \neq j'} \int f_1(r_i, p_i, t) f_j(r_j, p_j, t) t_1 \times \delta(r_i - r_j) d^3 r_i d^3 r_j d^3 p_i d^3 p_j, \]

\[ = t_1 \sum_{j \neq j'} f_1(r_i, p_i, t) f_j(r_j, p_j, t) \times d^3 r_i d^3 p_i d^3 p_j, \]

\[ = \sum_{j \neq j'} \int \frac{1}{(\pi \hbar)^3} e^{-\frac{(r_i - r_j)^2}{2L}} e^{-\frac{(p_i - p_j)^2}{2L}} e^{-\frac{(p_i - p_j)^2}{2L}} d^3 r_i d^3 p_i d^3 p_j, \]

\[ = \sum_{j} t_1 \int \frac{1}{(4\pi L)^{3/2}} e^{-\frac{(r_i - r_j)^2}{4L}} \rho_{ij}, \]

\[ \rho_{ij} = \int d^3 r \rho_i(r) \rho_j(r) = \frac{1}{(4\pi L)^{3/2}} e^{-\frac{(r_i - r_j)^2}{4L}}. \]
(2.37)

The three-body interactions can be calculated as follows:

\[ \sum_{j,k,\neq \neq j,k} V_{ijk}^{(3)} = \sum_{j,k,\neq \neq j,k} \int f_1(r_i, p_i, t) f_j(r_j, p_j, t) f_k(r_k, p_k, t) V(r_i, r_j, r_k) \times d^3 r_i d^3 r_j d^3 r_k d^3 p_i d^3 p_j d^3 p_k, \]

\[ = \sum_{j,k,\neq \neq j,k} \int f_1(r_i, p_i, t) f_j(r_j, p_j, t) f_k(r_k, p_k, t) t_2 \times \delta(r_i - r_j) \delta(r_i - r_k) \delta(r_i - r_k) d^3 r_i d^3 r_j d^3 r_k d^3 p_i d^3 p_j d^3 p_k, \]

\[ = \frac{t_2}{(2\pi L)^{3/2}} \sum_{j,k,\neq \neq j,k} e^{\left[-\frac{(r_i - r_j)^2 + (r_i - r_k)^2}{4L}\right] / 2}, \]

\[ = \frac{t_2}{(2\pi L)^{3/2}} \sum_{j,k,\neq \neq j,k} e^{\left[-\frac{(r_i - r_j)^2 + (r_i - r_k)^2}{4L}\right] / 2}, \]

\[ = \frac{t_2}{(2\pi L)^{3/2}} \left[ \sum_{j \neq i} \frac{1}{(4\pi L)^{3/2}} e^{-\frac{(r_i - r_j)^2}{4L}} \right]^2, \]

\[ = \frac{t_2^2}{3^{3/2}} \left[ \sum_{j \neq i} \rho_{ij} \right]^2. \]
(2.39)
From Eq. (2.39), it is clear that the three-body term reduces to two-body term. The finite range Yukawa \((V_{\text{Yuk}})\) and effective Coulomb potential \((V_{\text{Coul}})\) read as:

\[
V_{\text{Yuk}} = \sum_{j:i \neq j} t_3 \frac{\exp(-|r_i - r_j|/\lambda)}{|r_i - r_j|/\lambda},
\]

\[
V_{\text{Coul}} = \sum_{j:i \neq j} \frac{Z_i Z_j e^2}{|r_i - r_j|}
\]

The Yukawa term (with \(t_3 = -6.66 \text{ MeV}\) and \(\mu = 1.5 \text{ fm}\)) has been added to improve the surface properties of the interaction which plays an important role in multifragmentation. In nuclear matter where the density is constant, the interaction density coincides with the single particle density, and the two-body Skyrme as well as Yukawa interactions are directly proportional to \((-\rho \rho_0)\). The three-body part of the Skyrme interaction is proportional to \((-\rho \rho_0)^2\). In nuclear matter, the local potential energy has the form

\[
V_{\text{Skyrme}} = \frac{\alpha}{2}(\frac{\rho}{\rho_0}) + \frac{\beta}{\gamma + 1}(\frac{\rho}{\rho_0})^2.
\]

The above potential has two free \((\alpha \text{ and } \beta)\) parameters, which can be fixed by the requirement that at normal nuclear matter density, the average binding energy should be \(-15.75 \text{ MeV}\) and total energy should have a minimum at \(\rho_0\). In order to investigate the influence of different compressibilities \(K\), the above potential energy [Eq. (2.42)] can be generalized to

\[
V_{\text{Skyrme}} = \frac{\alpha}{2}(\frac{\rho}{\rho_0}) + \frac{\beta}{\gamma + 1}(\frac{\rho}{\rho_0})\gamma.
\]

This equation leads to the nuclear matter equation of state which connects the pressure and energy [12, 29]. It has been shown in Ref. [12] that the energy of equation of state can be divided into compressional and thermal parts. By varying the parameter \(\gamma\), one can study different equations of state. Naturally, larger value of \(\gamma\) leads to hard equation of state whereas smaller value of \(\gamma\) results in soft equation of state. These parameters along with other equations of state are given in Chap. 4. It is worth reminding that the above equation of state represents a cold matter. However, we know that the matter formed in a collision is not only compressed, but is also hot. This aspect was taken care by Faessler et al. [30] in their recent study where they included the temperature dependent mean field.
2.5.4 The nucleon-nucleon collisions

During the course of time if nucleons come too close they can scatter elastically or inelastically. The effect of N-body collisions is found to be rather small and therefore, one talks of two-body collisions only [31]. Two nucleons undergo a scattering if they are closer than a distance $\sqrt{\frac{\sigma_{\text{tot}}(\sqrt{s})}{\pi}}$. This scattering is further subjected to the fulfillment of Pauli-principle. Any scattering that violates the Pauli-principle is neglected. Here $\sigma_{\text{tot}}(\sqrt{s})$ represents the total nucleon-nucleon cross section and $\sqrt{s}$ is the center-of-mass energy. The various nucleon-nucleon cross sections shall be discussed in Chap. 3.

2.5.5 Pauli-blocking

The Pauli-principle is a very important quantum feature. Whenever a collision occurs, the phase-space around the scattering partners is checked. For simplicity, we assume that each nucleon occupies a sphere in coordinate and momentum space [12]. This trick yields the same Pauli blocking ratio as an exact calculation of the overlap of the Gaussians will yield. We calculate the fractions $P_1$ and $P_2$ of final phase-space for each of the two scattering partners that is already occupied by other nucleons. The collision is blocked with a probability

$$P_{\text{block}} = 1 - [1 - \min(P_1, 1)][1 - \min(P_2, 1)],$$

and, correspondingly, is allowed with probability $1 - P_{\text{block}}$. For a nucleus in its ground state, we obtain an averaged blocking probability $<P_{\text{block}}> = 0.96$ which also shows the limit of our theory. Note that this sharp occupancy is valid for cold nuclear matter only. Recently, Faessler and co-workers [30] included the temperature by smearing the Fermi spheres for Pauli-operator using realistic G matrix. The impact of in-medium corrections is drastic at low incident energies which washes away at higher incident energies. On the other hand, the relativistic effects become very important at higher incident energies. Recently, the QMD/BUU models have been extended to relativistic energies. These extensions are known as relativistic quantum molecular dynamics (RQMD)/relativistic Boltzmann-Uehling-Uhlenbeck (RBUU) models [22, 32–35]. Frankfurt group reported a new version ultra relativistic quantum molecular dynamics (UrQMD) [36–38] which is designed specifically for ultra-relativistic energy collisions which was improved by Ref. [39].
by incorporating momentum dependent Pauli potential, in-medium $NN \rightarrow N\Delta$ angular distribution and clusterization procedure. As our present interest is to look for the various phenomena at intermediate energies, the intensity of relativistic effects is assumed to be small [40].

We shall here also mention briefly the relativistic version of the QMD model.

2.6 The relativistic quantum molecular dynamics (RQMD) model

With increasing velocity of the nucleons, need of a fully covariant formalism is always justified. The relativistic version of QMD model, namely, the RQMD model [22,32-34], describes the propagation of all kinds of baryons and mesons in a Lorentz-invariant fashion. A covariant Hamiltonian for $N$-particle system is expressed in terms of $8N$ variables: $4N$ position coordinates $q_{\mu i}$ and $4N$ momentum coordinates $p_{\mu i}$. This implies that here each particle carries its own energy and time. Since the physical events are described as world lines in a 6$N$-dimensional phase-space, extra $2N-1$ degrees of freedom have to be eliminated and a global evolution parameter $\tau$ has to be defined. This can be achieved with the help of $2N$ constraints. In our approach, the first $N$ constraints are chosen as Poincaré invariant mass-on shell constraints [22,32].

$$\xi_i = p^\mu_i p_{\mu i} - m_i^2 - \tilde{V}_i = 0 \quad ; \quad i = 1, \ldots, N.$$  (2.45)

This choice of Poincaré invariant constraints requires that the potential part $\tilde{V}_i$ should be a Lorentz scalar and therefore, function of the Lorentz scalars only. Since, in the RQMD model, a system with mutual two and three-body interactions (like in the QMD model) has to be defined, $\tilde{V}_i$ should be given by the sum of these two-body interactions. Further, as we want to look for the relativistic effects in the dynamics, we have to generalize the non-relativistic Skyrme force in such a way that the force is covariant and reduces also to the usual Skyrme force in non-relativistic limit. This can be achieved as [22]

$$\tilde{V}_i = \sum_{j \neq i} \tilde{V}_{ij}(q^2_{ij}).$$  (2.46)

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This shows that the two-body interactions depend only on the Lorentz invariant squared transverse distance
\[ q_{ij}^2 = q_{ij}^2 - \frac{(q_{ij}^\mu p_{ij}^\mu)^2}{p_{ij}^2}, \tag{2.47} \]
with \( q_{ij}^\mu = q_i^\mu - q_j^\mu \) being the simple four dimensional distance and \( p_{ij}^\mu = p_i^\mu + p_j^\mu \) the sum of the momenta of the two interacting particles \( i \) and \( j \).

The next set of the constraints (which fix the relative times of all particles) should be chosen in such a way that these constraints must respect the principle of causality and \( N - 1 \) of these constraints should be Poincaré invariant so that the world line invariance can also be fulfilled. Another feature which these constraints has to fulfill is the cluster separability. This means that the system can be divided into single particles or clusters as soon as their Minkowski distances are space-like. Furthermore, a global evolution parameter should also be defined. These features can be fulfilled by choosing the following set of time constraints:
\[
\chi_i = \sum_{j \neq i} \frac{1}{q_{ij}^2 / L_C} \exp(q_{ij}^\mu / L_C) p_{ij}^\mu q_{ij\mu} = 0 ; \quad i = 1, \ldots, N - 1, \tag{2.48}
\]
\[
\chi_{2N} = \bar{P}^\mu Q_\mu - \tau = 0. \tag{2.49}
\]
with \( \bar{P}^\mu = P^\mu / \sqrt{P^2}, P^\mu = \sum_i p_i^\mu, Q_\mu = \frac{1}{N} \sum_i q_i^\mu \).

These time fixations take care that the time coordinates of the interacting particles should not be much dispersed in the center-of-mass system of two particles. The Hamiltonian is a linear combination of the Poincaré invariant constraints:
\[
H = \sum_{i=1}^{2N-1} \lambda_i \Psi_i, \tag{2.50}
\]
with
\[
\Psi_i = \begin{cases} 
\xi_i & \text{if } i \leq N \\
\chi_{i-N} & \text{if } N < i \leq 2N - 1.
\end{cases} \tag{2.51}
\]
This Hamiltonian then generates the equations of motion
\[
\frac{dq_i^\mu}{d\tau} = [H, q_i^\mu], \tag{2.52}
\]
\[
\frac{dp_i^\mu}{d\tau} = [H, p_i^\mu]. \tag{2.53}
\]
Here square brackets represent the Poisson brackets. The unknown Lagrange multipliers $\lambda_i$ in Eq. (2.50) are determined by the condition that all constraints must be fulfilled for all times during the simulations. These equations of motion are then used to propagate the baryons during the reaction.

The propagation and the “soft interactions” between baryons are combined with the quantum effects like the stochastic scattering, Pauli blocking etc. In RQMD model, the collision part is treated in a covariant fashion. Hence, all quantities which determine the collision must be Lorentz invariant. In RQMD model, two baryons are allowed to collide if their distance $\sqrt{-q^2_{ij}} \leq \sqrt{\sigma_{tot}(\sqrt{s})/\pi}$ where $q^2_{ij}$ is the Lorentz-invariant squared transversal distance [Eq. (2.47)] and $\sigma_{tot}(\sqrt{s})$ is the cross section depending on the available invariant mass $\sqrt{s}$.

In recent years, several refinements and improvements were made over the original QMD model. The new versions were named as Isospin QMD (IQMD) [41], $G$ matrix QMD (GQMD) [42], Glauber plus QMD (DQMD) [43] etc. The crucial quantum features like the antisymmetrization were implemented in approaches like fermionic molecular dynamics (FMD) [44] and antisymmetrized molecular dynamics (AMD) [19]. Later on, a novel model (AMD-V) was constructed by the stochastic incorporation of the diffusion and the deformation of wave packets which is calculated by the Vlasov equation without any restriction on the one-body distribution [45]. In order to study light unstable nuclei systematically, a new method was proposed in Ref. [46]. Recently, the improved version of AMD, antisymmetrized molecular dynamics superposition of selected snapshots (AMD triple-S), was used to show the cluster-shell competition of these nuclei [47]. However, the serious numerical problems have restricted the use of FMD and AMD approaches to lighter nuclei only. To describe the fermionic nature of the $N$-body system, new microscopic model, dubbed as constrained molecular dynamics (CoMD) was proposed in Ref. [48]. It constrains the phase space to fulfill, at each time step, the Pauli principle. This approach has been applied to the formation and decay of heavy systems above fission barrier [49], $\gamma$-ray emission [50], non-relativistic [48] and relativistic heavy-ion collisions [51] and plasma physics [52] as well. To study the hadron and quark dynamics, new formalism quark molecular dynamics (qMD) was put forward by Hofmann et al. [53].
In summary, we discussed the details of various models in this chapter. In the following chapters, we shall present the detailed studies of various problems encountered in collective transverse in-plane flow as well as in its disappearance, thermalization, density, temperature, participant-spectator matter etc. Our results are also compared with experimental data, whenever needed.
Bibliography


