Progress of Quantum Molecular Dynamics model and its applications in Heavy Ion Collisions

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arxiv: 2005.12877

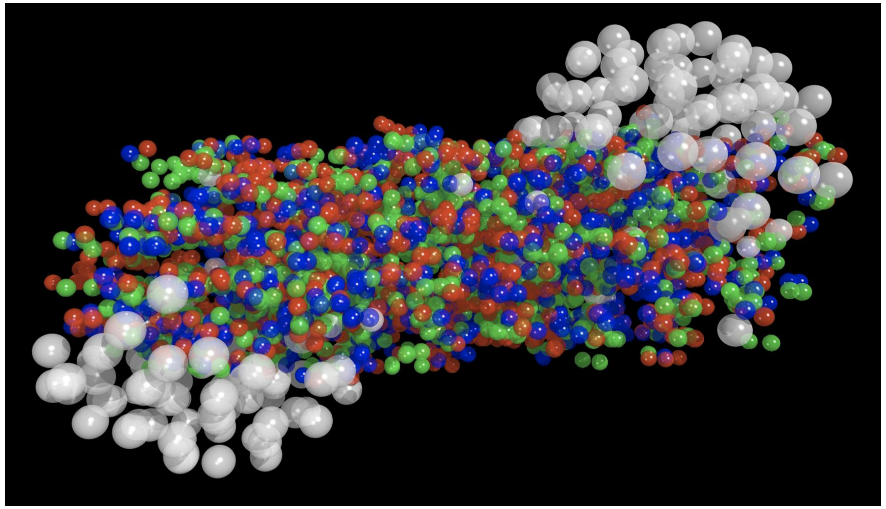
Transport Theory:

① Transport theory for N-body system

② Quantum Molecular Dynamics (QMD)

③ Improved QMD (ImQMD)

Transport Theory



Heavy-Ion Collisions (HICs)

(for low energy fusion cross sections,
diffusion model, di-nuclear model.

for intermediate model, statistical
multifragmentation model (SMM).)

describe evolution → microscopic transport models →

Boltzmann-Uehling-Uhlenbeck (BUU) model

evolution of the one-body phase
space occupation probability

quantum molecular dynamics (QMD) model

evolution of the N-body phase
space density distribution

Transport Theory: Transport theory for N-body system

$\psi(\mathbf{r}_1, ..., \mathbf{r}_N)$ **is given** $\Longrightarrow$ **N-body phase space distribution** $f_N(\mathbf{r}_1, ...\mathbf{r}_N; ...\mathbf{p}_1, ..., \mathbf{p}_N)$

$\Downarrow$ **density matrix**

$$(\frac{1}{2\pi\hbar})^N \int_{-\infty}^{\infty} ... \int d\mathbf{y}_1 ... d\mathbf{y}_N \psi^*(\mathbf{r}_1 - \mathbf{y}_1, ..., \mathbf{r}_N - \mathbf{y}_N)$$
$$\psi(\mathbf{r}_1 + \mathbf{y}_1, ..., \mathbf{r}_N + \mathbf{y}_N) e^{-2i(\mathbf{p}_1 \cdot \mathbf{y}_1 + ... + \mathbf{p}_N \cdot \mathbf{y}_N)/\hbar},$$

$\Downarrow$ **by Aichline**

$$(\frac{\partial}{\partial t} + \sum_i \frac{\mathbf{p}_i}{m} \cdot \nabla_{\mathbf{r}_i}) f_N(\mathbf{r}_1, \ldots \mathbf{r}_N, \mathbf{p}_1, \ldots \mathbf{p}_N, t)$$
$$= \int \Pi_i d^3 p_i d^3 Q_i d^3 q_i e^{i\mathbf{r}_i \cdot \mathbf{p}_i}$$
$$f_0^{(n)}(Q_1, \ldots, Q_N, q_1, \ldots, q_N, t)$$
$$(I_1(T) + I_2(T) + I_3(T)),$$

It's difficult to be solved!

(Aichline, "Quantum" molecular dynamics—a dynamical microscopic n-body approach to investigate fragment formation and the nuclear equation of state in heavy ion collisions , Phys. Rep. 202, 233 (1991).)

Transport Theory: Quantum Molecular Dynamics (QMD)

In QMD approach, each nucleon is represented by a Gaussian wave packet:

$$\psi_i(\mathbf{r}_i) = \frac{1}{(2\pi\sigma_r^2)^{3/4}} e^{-\frac{(\mathbf{r}_i - \mathbf{r}_{i0})^2}{2\sigma_r^2} + i(\mathbf{r_i} - \mathbf{r}_{i0})\cdot\mathbf{p}_{i0}/\hbar}$$

σ_r $\mathbf{r}_{i0}$ **are width and centroid**

$$\Big\Downarrow \text{ Wigner density}$$

$$\begin{aligned} f_i(\mathbf{r}, \mathbf{p}, t) &= \frac{1}{(2\pi\sigma_r^2)^{3/2}} e^{-(\mathbf{r}-\mathbf{r}_{i0})^2/2\sigma_r^2} \\ &\quad \frac{1}{(2\pi\sigma_p^2)^{3/2}} e^{-(\mathbf{p}-\mathbf{p}_{i0})^2/2\sigma_p^2} \\ &= \frac{1}{(\pi\hbar)^3} \exp[-\frac{(\mathbf{r}_i - \mathbf{r}_{i0})^2}{2\sigma_r^2} - \frac{(\mathbf{p}_i - \mathbf{p}_{i0})^2}{2\sigma_p^2}] \end{aligned}$$

$$\sigma_r\sigma_p = \hbar/2$$

Transport Theory: Quantum Molecular Dynamics (QMD)

For N-body system: $\psi(\mathbf{r}_1, ..., \mathbf{r}_N) = \phi_{k_1}(\mathbf{r}_1)\phi_{k_2}(\mathbf{r}_2)...\phi_{k_n}(\mathbf{r}_N)$

a direct product of N coherent state

$\phi_{k_i}(\mathbf{r}_i)$ **is the ith particle at state** k_i $(p_i = \hbar k_i \text{ form})$

N-body Wigner function

$$f_N(\mathbf{r}_1, ..., \mathbf{r}_N; \mathbf{p}_1, ..., \mathbf{p}_N) = \prod_{i=1}^{N} f(\mathbf{r}_i, \mathbf{p}_i)$$

$$= \prod_{i=1}^{N} \frac{1}{(\pi\hbar)^3} \exp[-\frac{(\mathbf{r}_i - \mathbf{r}_{i0})^2}{2\sigma_r^2} - \frac{(\mathbf{p}_i - \mathbf{p}_{i0})^2}{2\sigma_p^2}]$$

$$\mathbf{r}_{i0} = \langle \mathbf{r}_i \rangle$$
$$\mathbf{p}_{i0} = \langle \mathbf{p}_i \rangle$$

width is fixed

Time evolution of the centroids in the coordinate and momentum spaces, which are driven by the mean field potential and nucleon-nucleon collisions.

Transport Theory: Quantum Molecular Dynamics (QMD)

$$(\frac{\partial}{\partial t} + \sum_i \frac{\mathbf{p}_i}{m} \cdot \nabla_{\mathbf{r}_i}) f_N(\mathbf{r}_1, \ldots \mathbf{r}_N, \mathbf{p}_1, \ldots \mathbf{p}_N, t)$$
$$= \int \Pi_i d^3p_i d^3Q_i d^3q_i e^{i\mathbf{r}_i \cdot \mathbf{p}_i}$$
$$f_0^{(n)}(Q_1, \ldots, Q_N, q_1, \ldots, q_N, t)$$
$$(I_1(T) + I_2(T) + I_3(T)),$$

only the mean field $\Longrightarrow$ **w/o collision part**

$$\frac{\partial < \mathbf{p_i} >}{\partial t} \approx -\frac{\partial U(\mathbf{r}_{10}, ..., \mathbf{r}_{N0})}{\partial \mathbf{r}_{i0}},$$
$$\frac{\partial < \mathbf{r_i} >}{\partial t} = \frac{\mathbf{p}_{i0}}{m}.$$

The potential energy *U* can be caculated from the potential operator $\hat{V} = v_{ij} + v_{ijk} + \ldots$ **as followed:**

$$\begin{aligned}
U &= \sum_{i<j} \int d\Gamma_i d\Gamma_j v_{ij} f_i(\mathbf{r}_i, \mathbf{p}_i) f_j(\mathbf{r}_j, \mathbf{p}_j) \\
&+ \sum_{i<j<k} \int d\Gamma_i d\Gamma_j d\Gamma_k v_{ijk} \\
&\quad f_i(\mathbf{r}_i, \mathbf{p}_i) f_j(\mathbf{r}_j, \mathbf{p}_j) f_k(\mathbf{r}_k, \mathbf{p}_k) + \ldots \\
&\equiv \sum_{i<j} < r_i, r_j | v_{ij} | r_i, r_j > \\
&\quad + \sum_{i<j<k} < r_i, r_j, r_k | v_{ijk} | r_i, r_j, r_k > + ..., \\
&= \sum_{i<j} U_{ij} + \sum_{i<j<k} U_{ijk} + ...,
\end{aligned}$$

$$d\Gamma_i = d^3r_i d^3p_i$$

v_{ij}, v_{ijk} **are two-body interaction, three-body interaction**

Transport Theory: Quantum Molecular Dynamics (QMD)

The interactions may consist of local interaction, Yukawa and Coulomb interactions:

local interaction: $v_{ij} = t_1\delta(\mathbf{r}_1 - \mathbf{r}_2), v_{ijk} = t_2\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3)$ $\Longrightarrow$

$$U_{ij} = t_1\tilde{\rho}(\mathbf{r}_{i0}, \mathbf{r}_{j0}) = \frac{t_1}{(4\pi\sigma_r^2)^{3/2}} e^{-(\mathbf{r}_{i0}-\mathbf{r}_{j0})^2/4\sigma_r^2},$$

$$\begin{aligned} U_{ijk} &= \frac{t_2}{(2\pi\sigma_r^2)^3 \cdot 3^{3/2}} \\ &\quad e^{-((\mathbf{r}_{i0}-\mathbf{r}_{j0})^2+(\mathbf{r}_{i0}-\mathbf{r}_{k0})^2+(\mathbf{r}_{k0}-\mathbf{r}_{j0})^2)/6\sigma_r^2} \\ &\approx \frac{t_2}{(2\pi\sigma_r^2)^3 \cdot 3^{3/2}} e^{-((\mathbf{r}_{i0}-\mathbf{r}_{j0})^2+(\mathbf{r}_{i0}-\mathbf{r}_{k0})^2)/4\sigma_r^2} \end{aligned}$$

(t1, t2 are paramaters determined by fitting nuclear matter potential)

Yukawa interaction: $V^{Yuk} = t_3 \frac{e^{-|\mathbf{r}_1-\mathbf{r}_2|/\mu}}{|\mathbf{r}_1 - \mathbf{r}_2|/\mu}$

Here mu=1.5 fm, t3=-6.66 MeV

Momentum dependent interaction: $U_{md} = \sum_{k=1,2} \frac{C_{ex}^{(k)}}{\rho_0} \int d\mathbf{r}d\mathbf{p}d\mathbf{p}' \frac{f(\mathbf{r},\mathbf{p})f(\mathbf{r},\mathbf{p}')}{1 + [(\mathbf{p} - \mathbf{p}')/\mu_k]^2}$

Transport Theory: Improved QMD (ImQMD)

1. Nucleonic mean field

In the ImQMD, improving the mean-filed part by using a reasonable energy density functional, in Hamiltonian equation:

$$\dot{\mathbf{r}}_i = \frac{\partial H}{\partial \mathbf{p}_i} + \frac{\partial H^{Pau}}{\partial \mathbf{p}_i},$$
$$\dot{\mathbf{p}}_i = -\frac{\partial H}{\partial \mathbf{r}_i} - \frac{\partial H^{Pau}}{\partial \mathbf{r}_i}.$$

potential energy U from its energy density functional: $U = \int u[\rho] d^3 r$ $\quad \rho(\mathbf{r}) = \sum \rho_i = \frac{1}{(2\pi\sigma_r^2)^{3/2}} e^{-(\mathbf{r}-\mathbf{r}_{i0})/2\sigma_r^2}$

Transport Theory: Improved QMD (ImQMD)

1. Nucleonic mean field

In ImQMD, three kinds of **Skyrme-type energy density functional** are used according to the energy region:

(1) low beam energy (ImQMD-v2):

a reasonable energy density functional (EDF) derived from the Skyrme EDF and the Fermi constraints are used:

$$
\begin{aligned}
u_\rho = \quad & \frac{\alpha}{2}\frac{\rho^2}{\rho_0} + \frac{\beta}{\gamma+1}\frac{\rho^{\gamma+1}}{\rho_0^\gamma} + \frac{g_{sur}}{2\rho_0}(\nabla\rho)^2 \\
& + \frac{C_s}{2\rho_0}[\rho^2 - \kappa_s(\nabla\rho)^2]\delta^2 + g_{\rho\tau}\frac{\rho^{\eta+1}}{\rho_0^\eta}
\end{aligned}
$$

$\delta = (\rho_n - \rho_p)/(\rho_n + \rho_p)$ g_{sur} is coefficient related to the density gradient C_s is the symmetry potential coefficient

κ_s is related to isospin dependent density gradient term $g_{\rho\tau}$ is obtained from the contribution of $\rho\tau$ term in Skyrme energy density functional,

Transport Theory: Improved QMD (ImQMD)

1. Nucleonic mean field

(2) beam energies are high enough to trigger the multifragmentation (ImQMD05): (from 20 MeV/nucleon to 300 MeV/nucleon)

nucleonic potential energy density functional has two parts: $u = u_\rho + u_{md}$

$$u_\rho = \frac{\alpha}{2}\frac{\rho^2}{\rho_0} + \frac{\beta}{\gamma+1}\frac{\rho^{\gamma+1}}{\rho_0^\gamma} + \frac{g_{sur}}{2\rho_0}(\nabla\rho)^2 + \frac{g_{sur,iso}}{\rho_0}(\nabla(\rho_n-\rho_p))^2 + g_{\rho\tau}\frac{\rho^{8/3}}{\rho_0^{5/3}} + u_\rho^{sym}.$$

$$u_\rho^{sym} = [A_{sym}\frac{\rho}{\rho_0} + B_{sym}(\frac{\rho}{\rho_0})^\gamma + C_{sym}(\frac{\rho}{\rho_0})^{5/3}]\delta^2\rho$$

the symmetry potential energy density functional

$$u_{md} = \frac{1}{2\rho_0}\sum_{N_1,N_2}\frac{1}{16\pi^6}\int d^3p_1 d^3p_2 f_{N_1}(\mathbf{p}_1) f_{N_2}(\mathbf{p}_2)\, 1.57[\ln(1+5\times10^{-4}(\Delta p)^2)]^2\ ,$$

Transport Theory: Improved QMD (ImQMD)

1. Nucleonic mean field

(3) standard parametrization of the Skyrme potential energy density functional with only the spin-orbit interaction neglected (ImQMD-SKY):

(from 20 MeV/nucleon to 300 MeV/nucleon)

The nucleonic potential energy density functional is

$$
\begin{aligned}
u &= \frac{\alpha}{2}\frac{\rho^2}{\rho_0} + \frac{\beta}{\gamma+1}\frac{\rho^{\gamma+1}}{\rho_0^{\gamma}} + \frac{g_{sur}}{2\rho_0}(\nabla\rho)^2 \\
&+ \frac{g_{sur,iso}}{\rho_0}(\nabla(\rho_n - \rho_p))^2 \\
&+ A_{sym}(\frac{\rho}{\rho_0})\delta^2\rho + B_{sym}(\frac{\rho}{\rho_0})^{\gamma}\delta^2\rho \\
&+ u_{md}^{sky}.
\end{aligned}
$$

$$
\begin{aligned}
u_{md}^{sky} &= u_{md}(\rho\tau) + u_{md}(\rho_n\tau_n) + u_{md}(\rho_p\tau_p) \\
&= C_0 \int d^3p d^3p' f(\mathbf{r},\mathbf{p}) f(\mathbf{r},\mathbf{p}')(\mathbf{p}-\mathbf{p}')^2 + \\
&\quad D_0 \int d^3p d^3p' [f_n(\mathbf{r},\mathbf{p}) f_n(\mathbf{r},\mathbf{p}')(\mathbf{p}-\mathbf{p}')^2 \\
&\quad + f_p(\mathbf{r},\mathbf{p}) f_p(\mathbf{r},\mathbf{p}')(\mathbf{p}-\mathbf{p}')^2].
\end{aligned}
$$

Transport Theory: Improved QMD (ImQMD)

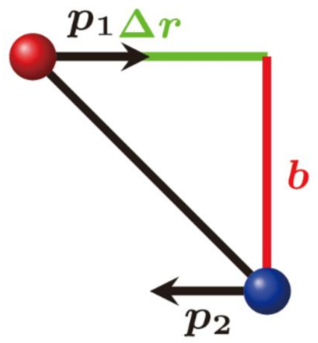
2. Collision part

(1) transform from system center of mass reference to the two-particle center of mass reference frame

(2) make judgements from geometry:

几何条件判断

- $b \leq b_{\max} = \sqrt{\sigma_{NN}^{tot}/\pi}$
- $\left(\frac{p_1}{\sqrt{p_1^2+m_1^2}} + \frac{p_2}{\sqrt{p_2^2+m_2^2}}\right)\frac{\delta t}{2} \geq \Delta r$



(3) make judgements from cross section:

Monte-Carlo反应截面判断

- $\xi < \sigma_{el}/\sigma_{NN}^{tot}$ 弹性散射，根据微分截面由Monte-Carlo给出散射后动量
- $\xi > \sigma_{el}/\sigma_{NN}^{tot}$ 非弹性散射，散射后动量空间均匀分布

(4) transfrom back to system center of mass reference

Transport Theory: Improved QMD (ImQMD)

3. Pauli blocking

The occupation probability is:

$$\begin{aligned} f_i' &= f_\tau(\vec{R}_i, \vec{P}_i') \\ &= \frac{1}{2/(2\pi\hbar)^3} \frac{1}{(\pi\hbar)^3} \sum_{k\in\tau(k\neq i)} \mathrm{e}^{-(\vec{R}_i-\vec{R}_k)^2/2\sigma_r^2} \\ &\quad \times \mathrm{e}^{-2(\sigma_r/\hbar)^2(\vec{P}_i'-\vec{P}_k)^2}, \end{aligned}$$

$\tau = n$ or p

Transport Theory: Improved QMD (ImQMD)

4. Initialization

坐标球：$R = r_0 A^{1/3}$

动量球：$p_i^F = \hbar k^F = \hbar\left(3\pi^2\rho/2\right)^{1/3}$

约束条件$\Delta r \geq 1.5\text{fm} \quad \Delta r \Delta p \geq h/4$

稳定性：结合能、方均根半径……

THANK YOU!