## Handling of clusters in transport models

#### Akira Ono

Tohoku University

#### NuSYM13, July 22 - 26, 2013.

- Why clusters are important (for NuSYM)
- Why clusters are difficult, and how to solve
- Effects of clusters



An event of central collision of Xe + Sn at 50 MeV/nucleon (AMD calculation)

• <sup>4</sup>He clusters are symmetric (N = Z = 2). However, after emitting many <sup>4</sup>He clusters, the rest of the system is more neutron rich than the initial system.

$$(N_{\text{tot}}, Z_{\text{tot}}) - n_{\alpha}^{4} \text{He} = (N_{\text{tot}} - 2n_{\alpha}, Z_{\text{tot}} - 2n_{\alpha})$$

In dilute nuclear matter, it is known that clusters play essential roles.

Clusters (e.g. <sup>3</sup>H / <sup>3</sup>He) are measured by experiments to probe NuSYM.

Clusters are a major part of the disintegrating system in heavy-ion collisions, so collision dynamics may be influenced by the existence of clusters.

- Four uncorrelated nucleons at T = 10 MeV:  $\langle E \rangle = \frac{3}{2}T \times 4 = 60 \text{ MeV}$
- An  $\alpha$  cluster at T = 10 MeV:  $\langle E \rangle = \frac{3}{2}T \times 1 28.3$  MeV = -13.3 MeV

### Low-density matter and clusters

Natowitz et al., PRL104 (2010) 202501. Exp.: <sup>64</sup>Zn + <sup>92</sup>Mo, <sup>197</sup>Au at 35 MeV/u Composition of nucleons and clusters

 $\Rightarrow$  Temperature, Density, Symmetry energy



In dilute matter, clusters are important.

EOS with chemical equilibrium

- Shen EOS
- Lattimer-Swesty EOS
- Ishizuka et al.,
- Botvina & Mishustin,
- Horowitz & Schwenk,
- Typel et al.,



Generalized RMF by Typel

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# Clusters measured for NuSYM

#### MSU data for Sn+Sn at 50 MeV/u



SAMURAI-TPC at RIKEN RIBF will measure light charged particles including <sup>3</sup>H and <sup>3</sup>He as well as pions.



Au + Au at 400 MeV/u, central.

Di Toro et al., J. Phys. G 37(2010) 083101.

# Large fraction of clusters in head-on collisions



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#### Various Microscopic Approaches



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Mean field approaches (TDHF or Vlasov/BUU)

$$\phi_{d}(\mathbf{r}_{1} - \mathbf{r}_{2}) \Psi(\frac{\mathbf{r}_{1} + \mathbf{r}_{2}}{2}) \xrightarrow{\text{exact } e^{-iHt}} \phi_{d}(\mathbf{r}_{1} - \mathbf{r}_{2}) \Psi(\frac{\mathbf{r}_{1} + \mathbf{r}_{2}}{2}, t)$$

$$\stackrel{\mathfrak{R}}{\longrightarrow} \psi_{p}(\mathbf{r}_{1}) \psi_{n}(\mathbf{r}_{2}) \xrightarrow{\mathsf{TDHF}} \psi_{p}(\mathbf{r}_{1}, t) \psi_{n}(\mathbf{r}_{2}, t)$$

Deuteron probability disappears due to the spurious coupling to the center-of-mass motion.

Wave-packet molecular dynamics approaches (e.g. AMD)

$$e^{-\nu \mathbf{r}_1^2 + i \mathbf{P} \cdot \mathbf{r}_1} e^{-\nu \mathbf{r}_2^2 + i \mathbf{P} \cdot \mathbf{r}_2} \xrightarrow{\mathsf{MD}} e^{-\nu (\mathbf{r}_1 - \mathbf{v}t)^2 + i \mathbf{P} \cdot \mathbf{r}_1} e^{-\nu (\mathbf{r}_2 - \mathbf{v}t)^2 + i \mathbf{P} \cdot \mathbf{r}_2}$$

No problem once a cluster is formed, but the cluster-forming probability is the problem.

#### Danielewicz et al., NPA 533 (1991) 712.

Coupled equations for  $f_n(\mathbf{r}, \mathbf{p}, t)$ ,  $f_p(\mathbf{r}, \mathbf{p}, t)$ ,  $f_d(\mathbf{r}, \mathbf{p}, t)$ ,  $f_t(\mathbf{r}, \mathbf{p}, t)$ ,  $f_h(\mathbf{r}, \mathbf{p}, t)$  are solved by the test particle method.

$$\begin{aligned} \frac{\partial f_n}{\partial t} + \mathbf{v} \cdot \frac{\partial f_n}{\partial \mathbf{r}} &- \frac{\partial U_n}{\partial \mathbf{r}} \cdot \frac{\partial f_n}{\partial \mathbf{p}} = I_n^{\text{coll}}[f_n, f_p, f_d, f_t, f_h] \\ \frac{\partial f_p}{\partial t} + \mathbf{v} \cdot \frac{\partial f_p}{\partial \mathbf{r}} &- \frac{\partial U_p}{\partial \mathbf{r}} \cdot \frac{\partial f_p}{\partial \mathbf{p}} = I_p^{\text{coll}}[f_n, f_p, f_d, f_t, f_h] \\ \frac{\partial f_d}{\partial t} + \mathbf{v} \cdot \frac{\partial f_d}{\partial \mathbf{r}} &- \frac{\partial U_d}{\partial \mathbf{r}} \cdot \frac{\partial f_d}{\partial \mathbf{p}} = I_d^{\text{coll}}[f_n, f_p, f_d, f_t, f_h] \\ \frac{\partial f_t}{\partial t} + \mathbf{v} \cdot \frac{\partial f_t}{\partial \mathbf{r}} &- \frac{\partial U_t}{\partial \mathbf{r}} \cdot \frac{\partial f_t}{\partial \mathbf{p}} = I_d^{\text{coll}}[f_n, f_p, f_d, f_t, f_h] \\ \frac{\partial f_h}{\partial t} + \mathbf{v} \cdot \frac{\partial f_h}{\partial \mathbf{r}} &- \frac{\partial U_h}{\partial \mathbf{r}} \cdot \frac{\partial f_h}{\partial \mathbf{p}} = I_h^{\text{coll}}[f_n, f_p, f_d, f_t, f_h] \end{aligned}$$

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# Effects of clusters on isospin diffusion (BUU)



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#### AMD wave function

$$|\Phi(Z)\rangle = \frac{\det}{ij} \Big[ \exp\Big\{ -\nu \Big( \mathbf{r}_j - \frac{\mathbf{Z}_i}{\sqrt{\nu}} \Big)^2 \Big\} \chi_{\alpha_i}(j) \Big]$$

$$\begin{split} \mathbf{Z}_{i} &= \sqrt{\nu} \mathbf{D}_{i} + \frac{i}{2\hbar \sqrt{\nu}} \mathbf{K}_{i} \\ \nu &: \text{Width parameter} = (2.5 \text{ fm})^{-2} \\ \chi_{\alpha_{i}} &: \text{Spin-isospin states} = p \uparrow, p \downarrow, n \uparrow, n \downarrow \end{split}$$

Time-dependent variational principle

$$\delta \int_{t_1}^{t_2} \frac{\langle \Phi(Z) | (i\hbar \frac{d}{dt} - H) | \Phi(Z) \rangle}{\langle \Phi(Z) | \Phi(Z) \rangle} dt = 0, \qquad \delta Z(t_1) = \delta Z(t_2) = 0$$

#### Equation of motion for the wave packet centroids Z

$$\frac{d}{dt}\mathbf{Z}_{i} = \{\mathbf{Z}_{i}, \mathcal{H}\}_{\mathsf{PB}} \qquad \text{or} \qquad i\hbar \sum_{j=1}^{A} \sum_{\tau = x, y, z} C_{i\sigma, j\tau} \frac{dZ_{j\tau}}{dt} = \frac{\partial \mathcal{H}}{\partial Z_{i\sigma}}$$

 $\mathcal{H} = \frac{\langle \Phi(Z) | H | \Phi(Z) \rangle}{\langle \Phi(Z) | \Phi(Z) \rangle} + (\text{c.m. correction}), \qquad H: \text{ Effective interaction (e.g. Skyrme force)}$ 

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## AMD with Two-Nucleon Collisions

Stochastic two-nucleon collisions

- Cross section  $\frac{d\sigma_{NN}}{d\Omega}(E,\theta)$  in nuclear medium.
- Pauli blocking for the final state. (Almost automatic in AMD)



$$W_{i \to f} = \frac{2\pi}{\hbar} |\langle \Psi_f | V | \Psi_i \rangle|^2 \delta(E_f - E_i)$$



#### Stochastic equation of motion

$$\frac{d}{dt}\mathbf{Z}_i = \{\mathbf{Z}_i, \mathcal{H}\}_{\mathsf{PB}} + (\mathsf{NN \ collisions})$$

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## Results of AMD with Two-Nucleon Collisions



Xe + Sn central collisions at 50 MeV/u



• AMD with NN collisions

• INDRA data, Hudan et al., PRC 67 (2003)

	AMD	INDRA
<i>M</i> ( <i>p</i> )	40.2	8.4
$M(\alpha)$	2.5	10.1

Two-nucleon collision:

$$\begin{split} W_{i \to f} &= \frac{2\pi}{\hbar} |\langle \Psi_f | V | \Psi_i \rangle|^2 \delta(E_f - E_i) \\ &\sum_f |\Psi_f \rangle \langle \Psi_f| = 1 \end{split}$$

What is a suitable complete basis set for the final states of a two-nucleon scattering?

• A usual choice is to change only the two.  $\sum_{1,k_2} \left| \varphi_{k_1}(1)\varphi_{k_2}(2)\Psi(3,4,\ldots) \right\rangle \left\langle \varphi_{k_1}(1)\varphi_{k_2}(2)\Psi(3,4,\ldots) \right|$ 

 If a deuteron will propagate in medium, a more suitable basis will include

 $\left|\varphi_{k_{1}}(1)\psi_{\mathsf{d}}(2,3)\Psi(4,\ldots)\right\rangle\left\langle\varphi_{k_{1}}(1)\psi_{\mathsf{d}}(2,3)\Psi(4,\ldots)\right|+\cdots$ 

#### Deuteron pole in medium (T = 0)



#### Danielewicz and Bertsch, NPA 533 (1991) 712.

More recent calculation by a quantum statistical approach by G. Röpke, NPA 867 (2011) 66.

### Clusters have to be handled in a special way

Two-nucleon collision:

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# Deuteron pole in medium (T = 0)[MeV/c] 1000 800 deuteron 600 Density of states for p-n system Exact Quantum Mechanics Molecular Dynamics Êrel -BF 0 $\langle K \rangle$

 $\langle V \rangle$ 

#### Similar to Danielewicz et al., NPA533 (1991) 712.

 $N_1 + B_1 + N_2 + B_2 \rightarrow C_1 + C_2$ 

- N<sub>1</sub>, N<sub>2</sub> : Colliding nucleons
- B<sub>1</sub>, B<sub>2</sub>: Spectator nucleons/clusters
- $C_1, C_2 : N, (2N), (3N), (4N)$  (up to  $\alpha$  cluster)

$$\begin{aligned} v_{\rm NN} \, d\sigma({\sf NBNB} \to {\sf CC}) \\ &= |\langle \varphi_1' | \varphi_1^{+{\sf q}} \rangle|^2 \, |\langle \varphi_2' | \varphi_2^{-{\sf q}} \rangle|^2 \, |M|^2 \, \delta(\mathcal{H} - E) \, p_{\rm rel}^2 dp_{\rm rel} d\Omega \\ &\left( \, v_{\rm NN} \, d\sigma_{\rm NN} = |M|^2 \, \delta(\mathcal{H} - E) \, p_{\rm rel}^2 dp_{\rm rel} d\Omega \, \right) \\ &\frac{d\sigma}{d\Omega} = F_{\rm kin} \, |\langle \varphi_1' | \varphi_1^{+{\sf q}} \rangle|^2 \, |\langle \varphi_2' | \varphi_2^{-{\sf q}} \rangle|^2 \left( \frac{d\sigma}{d\Omega} \right)_{\rm NN \to NN} \end{aligned}$$

The cross section is given from the NN cross section.



$$\begin{split} \mathbf{p}_{\text{rel}} &= \frac{1}{2} (\mathbf{p}_1 - \mathbf{p}_2) = p_{\text{rel}} \hat{\boldsymbol{\Omega}} \\ \mathbf{q} &= \mathbf{p}_1 - \mathbf{p}_1^{(0)} = \mathbf{p}_2^{(0)} - \mathbf{p}_2 \\ \varphi_1^{+\mathbf{q}} &= \exp(+i\mathbf{q} \cdot \mathbf{r}_{\mathbf{N}_1})\varphi_1^{(0)} \\ \varphi_2^{-\mathbf{q}} &= \exp(-i\mathbf{q} \cdot \mathbf{r}_{\mathbf{N}_2})\varphi_2^{(0)} \end{split}$$

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# Construction of Final States

Clusters (in the final states) are assumed to have  $(0s)^N$  configuration.



Final states are not orthogonal:  $N_{ij} \equiv \langle \Phi'_i | \Phi'_i \rangle \neq \delta_{ij}$ 

The probability of cluster formation with one of B's:

$$\hat{P} = \sum_{ij} |\Phi'_i\rangle N_{ij}^{-1} \langle \Phi'_j|, \qquad P = \langle \Phi^{\mathbf{q}} | \hat{P} | \Phi^{\mathbf{q}} \rangle \qquad \neq \sum_i |\langle \Phi'_i | \Phi^{\mathbf{q}} \rangle|^2$$

 $\begin{cases} P \implies \text{Choose one of the candidates and make a cluster.} \\ 1 - P \implies \text{Don't make a cluster (with any n)}. \\ \square \models e^{-\frac{1}{2}} \models e^{-\frac{1}{2}} \models e^{-\frac{1}{2}} \end{cases}$ 

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Handling of clusters in transport models

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# Effect of Clusters on the Density Evolution

Without cluster correlations (AMD with NN collisions)



#### With cluster correlations



During the time evolution, clusters are ...

- formed at NN collisions.
- propagated by AMD equation. (nothing special)
- broken by NN collisions. (nothing special)







Very strong tendency of turning into cluster gas.

	w/o C	with C	INDRA
M(p)	40.2	10.9	8.4
$M(\alpha)$	2.5	23.2	10.1
$Z_{\rm gas}/Z_{\rm tot}$	55%	78%	(40-50%)

- Gas =
  - $\sum$  (particles of  $A \le 4$ )
- Liquid = ∑ (heavier fragments)

# **Cluster-Cluster Correlations**

Relative motions between clusters should be treated quantum mechanically. In AMD,

- The binding energy a few clusters is reasonably correct,
- but the phase space of bound configuration is too small.

e.g. <sup>7</sup>Li =  $\alpha + t - 2.5$  MeV

 $|\alpha + t\rangle \rightarrow |^{7}$ Li $\rangle$  with probability  $\approx |\langle^{7}$ Li $|\alpha + t\rangle|^{2}$ 



- if  $C_i$  is the cluster closest to  $C_i$ , (i, j) = (1, 2) or (2, 1),
- and if they are moderately separated,  $|\mathbf{R}_{rel}| < R_{max}$ ,
- and if they are moving slowly away from each other, |P<sub>rel</sub>| < P<sub>max</sub> and P<sub>rel</sub> · R<sub>rel</sub> > 0.

 $P_{\text{max}}^2/2\mu = 8 \text{ MeV}, \qquad R_{\text{max}} = 5 \text{ fm}$  (adjustable)

Energy is conserved by scaling the relative momentum between the  $C_1$ - $C_2$  pair and a third cluster  $C_3$ .







#### Au + Au Central Collisions at Higher Energies



# **Energy Spectra of Clusters**

 $\frac{124}{\text{Sn}}$  Sn +  $\frac{124}{\text{Sn}}$  and  $\frac{112}{\text{Sn}}$  Sn +  $\frac{112}{\text{Sn}}$  central collisions at 50 MeV/nucleon  $\Rightarrow$  Energy spectra of tritons and <sup>3</sup>He emitted to transverse directions



SLy4 (L = 46 MeV)

L = 108 MeV

• Triton/<sup>3</sup>He difference is consistent with the gas part of fractionation.

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# **Energy Spectra of Clusters**

 $\frac{124}{\text{Sn}}$  Sn +  $\frac{124}{\text{Sn}}$  and  $\frac{112}{\text{Sn}}$  +  $\frac{112}{\text{Sn}}$  central collisions at 50 MeV/nucleon  $\Rightarrow$  Energy spectra of tritons and <sup>3</sup>He emitted to transverse directions



- Triton/<sup>3</sup>He difference is consistent with the gas part of fractionation.
- To reproduce data, there should be more low-energy tritons and less high-energy tritons, and low-energy <sup>3</sup>He particles (or protons) should be less.

(known as <sup>3</sup>He puzzle)

Akira Ono (Tohoku University)

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# Compression and Expansion Dynamics of Neutrons and Protons



Compared to the current AMD results (with SLy4), neutrons have to be more slowly expanding in order to explain the data of

- the triton spectrum
- the small yield of proton-rich nuclei
- the large energy of proton-rich nuclei

Momentum dependence of the symmetry potential

 $(m_n^* \text{ v.s. } m_p^*)$  and something more should be studied.

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Data @NSCL/MSU Liu et al., PRC86(2012)024605 Kinetic energies of proton-rich fragments are anomalously large. (Yields of low-energy proton-rich fragments are anomalously small.) (generalized <sup>3</sup>He puzzle)

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#### Summary

- Importance of clusters
  - as probes for nuclear symmetry energy
  - Cluster correlations are strong enough to affect the equation of state and the collision dynamics
- Handling of clusters in transport models
  - Treat clusters as particles (BUU), or specific quantum final states in two-nucleon collisions (AMD: clusters with *A* = 2, 3, 4)
  - Correlations between clusters are also important for fragment formation.
- Clusters (<sup>3</sup>H and <sup>3</sup>He) in central collisions at 50 MeV/u
  - Dependence on symmetry energy, as expected from the behavior of gas part in fractionation
  - Need to understand the <sup>3</sup>He puzzle. Due to the momentum dependence of the symmetry potential, and/or something unknown?



MSU Data: T.X. Liu et al., PRC 014603 (2004).



- The average asymmetry and the width are sensitive to the symmetry energy.
- Compared to data,  $Z \ge N$  fragments are overproduced.

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