Fragment Formation Studied with Antisymmetrized Version of Molecular Dynamics with Two-Nucleon Collisions

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A new microscopic simulation method of heavy-ion collisions is formulated by incorporating the two-nucleon collision process into the antisymmetrized version of molecular dynamics. This method can describe quantum-mechanical features such as shell effects. The fragment mass distribution of the $^{12}C+^{12}C$ reaction at 28.7 MeV/nucleon is shown to be reproduced very well by this new method combined with the treatment of statistical cascade decays of excited fragments, which verifies the usefulness of the new method.

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The study of fragment formation is indispensable for the understanding of heavy-ion reaction mechanisms. "Quantum" molecular dynamics (QMD) [1] and the Landau-Vlasov method combined with the percolation analysis [2] are representative practical methods of microscopic simulation for the description of fragment formation. These two methods are, however, largely of classical nature and, for example, they can describe shell effects neither of the colliding individual nuclei nor in the reaction process. The antisymmetrized version of molecular dynamics [3–5], which Feldmeier called fermionic molecular dynamics, treats explicitly the wave function of the total system and hence is able to describe quantum-mechanical effects such as shell effects. However, until now the two-nucleon collision process has not been incorporated into the framework, which has made this framework insufficient for the description of fragment formation.

The present authors have succeeded in incorporating two-nucleon collisions into the antisymmetrized version of molecular dynamics. This means the construction of a new microscopic simulation framework of the heavy-ion reaction. Hereafter we call this new simulation framework simply AMD. The aims of this paper are first to explain this new framework of AMD and second to show an example of applications of AMD to fragment formation which verifies the usefulness of AMD.

In AMD, the wave function of the A-nucleon system $|\Phi\rangle$ is described by a Slater determinant $|\Phi(\mathbf{Z})\rangle$:

$$|\Phi(\mathbf{Z})\rangle=\frac{1}{\sqrt{A!}}\det[\varphi_i(j)],\quad \varphi_i=\phi_{\mathbf{Z}_i}\chi_{\alpha_i}, \tag{1}$$

where α_i represents the spin-isospin label of the ith single-particle state, $\alpha_i=p\uparrow$, $p\downarrow$, $n\uparrow$, or $n\downarrow$, and χ is the spin-isospin wave function. $\phi_{\mathbf{Z}_i}$ is the spatial wave function of the ith single-particle state which is a Gaussian wave packet:

$$\langle\mathbf{r}|\phi_{\mathbf{Z}_i}\rangle=(2\nu/\pi)^{3/4}\exp[-\nu(\mathbf{r}-\mathbf{Z}_i/\sqrt{\nu})^2+\tfrac{1}{2}\mathbf{Z}_i^2], \tag{2}$$

where the width parameter ν is treated as time independent in the model presented in this paper. If we define $\mathbf{D}$ and $\mathbf{K}$ as $\mathbf{Z}=\sqrt{\nu}\mathbf{D}+(i/2\hbar\sqrt{\nu})\mathbf{K}$, then $\langle\phi_{\mathbf{Z}}|\mathbf{r}|\phi_{\mathbf{Z}}\rangle/\langle\phi_{\mathbf{Z}}|\phi_{\mathbf{Z}}\rangle=\mathbf{D}$, and $\langle\phi_{\mathbf{Z}}|\mathbf{p}|\phi_{\mathbf{Z}}\rangle/\langle\phi_{\mathbf{Z}}|\phi_{\mathbf{Z}}\rangle=\mathbf{K}$. The time developments of the centers of Gaussians, $\{\mathbf{Z}\}=\{\mathbf{Z}_i\ (i=1,2,\ldots,A)\}$, are determined by the time-dependent variational principle [6], and the resultant equation of motion for $\{\mathbf{Z}\}$ is similar to Hamilton's equation with its Hamiltonian being given by the expectation value $\langle H\rangle$ of the nucleonic Hamiltonian operator H by the A-body wave function $|\Phi(\mathbf{Z})\rangle$.

When the fragmentation of a nucleus into N_F fragments is described by wave-packet theories like AMD and QMD, the center-of-mass zero-point kinetic energy $T_0=3\hbar^2\nu/2M$ of each fragment causes serious trouble because the effective value of the fragmentation threshold energy is higher than its real value by the amount $(N_F-1)T_0$. In order to avoid this spurious energy effect, we modify the definition of the total system energy, namely, the Hamiltonian $\mathcal{H}$, by adding a correction term to $\langle H\rangle$: $\mathcal{H}=\langle H\rangle-T_0A+T_0'(A-N_F)$. In order to get a better reproduction of binding energies of nuclei, we regard T_0' as an adjustable parameter whose value is close to T_0 but is not necessarily equal to T_0. The fragment number N_F for a given set of $\{\mathbf{D}_i\ (i=1,2,\ldots,A)\}$ can be calculated in principle by using relative distances $\{d_{ij}=|\mathbf{D}_i-\mathbf{D}_j|\}$. We have used the following formula for the calculation of N_F:

$$N_F=\sum_{i=1}^{A}\frac{1}{n_i}\frac{1}{m_i},\quad n_i=\sum_{j=1}^{A}\hat{f}_{ij},\quad m_i=\sum_{j=1}^{A}\frac{1}{n_j}f_{ij}, \tag{3}$$

where $f_{ij}=F(d_{ij},\nu,0.5\text{ fm})$, $\hat{f}_{ij}=F(d_{ij},2\nu,0.25\text{ fm})$, and

$$F(d,\mu,b)=\begin{cases}\exp[-\mu(d-b)^2] & \text{if } d>b,\\ 1 & \text{if } d\le b.\end{cases} \tag{4}$$

This formula is a refined version of a simpler sum formula $N_F=\sum_{j=1}^{A}(1/n_j)$ which is easy to understand since n_j denotes the mass number of the fragment to which the nucleon j belongs.

We use the frictional cooling method [4] for the construction of the ground states of nuclei, namely, the determination of $\{\mathbf{Z}\}$ which minimize $\mathcal{H}$. The Volkov

No. 1 force [7] with $m=0.576$ is adopted as the effective two-nucleon force and the Coulomb force is also included. The width parameter $\nu=0.16$ fm^{-2} is chosen. The parameter $T_0'=7.7$ MeV is taken in order to reproduce the binding energies of α and ^{12}C. We show in Fig. 1 the calculated binding energies of light nuclei which reproduce the observed values very well. The ground state of ^{12}C constructed in this way, which is used for our later study of the ^{12}C+^{12}C reaction, has proved to be identical to the shell-model state $(0s)^4(0p)^8$ and hence it is completely stationary. The rms radius of this ^{12}C is calculated to be 2.49 fm, while its observed value is 2.48 fm.

In order to incorporate two-nucleon collisions into AMD, we have constructed physical nucleon coordinates $\{\mathbf{W}\}=\{\mathbf{W}_i\ (i=1,2,\ldots,A)\}$ from $\{\mathbf{Z}\}$ because $\{\mathbf{Z}\}$ do not always have the same meaning as the positions and momenta of nucleons due to the antisymmetrization effect. The definition of $\{\mathbf{W}\}$ is given by

$$\mathbf{W}_i=\sum_{j=1}^{A}(\sqrt{Q})_{ij}\mathbf{Z}_j,\quad Q_{ij}=\frac{\partial}{\partial(\mathbf{Z}_i^*\cdot\mathbf{Z}_j)}\ln\langle\Phi(\mathbf{Z})|\Phi(\mathbf{Z})\rangle. \tag{5}$$

The position $\mathbf{R}_j$ and momentum $\mathbf{P}_j$ of $\mathbf{W}_j=\sqrt{\nu}\mathbf{R}_j+(i/2\hbar\sqrt{\nu})\mathbf{P}_j$ have properties very similar to those of the position and momentum coordinates of QMD. For example, we can show that the total number of oscillator quanta $\langle N_{\rm tot}\rangle$ and the total angular momentum $\langle\mathbf{L}\rangle$ can be expressed by $\{\mathbf{R}_j\}$ and $\{\mathbf{P}_j\}$ as if they were QMD coordinates, namely,

$$\langle N_{\rm tot}\rangle=\sum_{j=1}^{A}\mathbf{W}_j^*\cdot\mathbf{W}_j,\quad \langle\mathbf{L}\rangle=\frac{\hbar}{i}\sum_{j=1}^{A}\mathbf{W}_j^*\times\mathbf{W}_j. \tag{6}$$

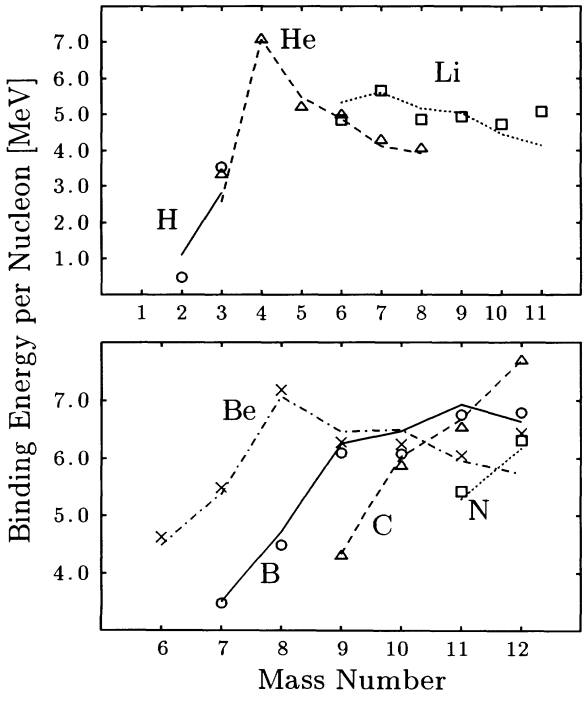

FIG. 1. Good reproduction of the binding energies by theory. Calculated values are shown by ○, △, ×, and □, while data are given by various lines. Energies are in MeV/nucleon.

In the case of a two-nucleon system ($A=2$) of the same spin and isospin, we see easily that $\{\mathbf{W}\}$ coincide with the canonical coordinates of Saraceno, Kramer, and Fernandez [8,9] and in fact the introduction of $\{\mathbf{W}\}$ has been made by extending the idea of Ref. [8]. For $A=2$, we can prove that $|\mathbf{W}_i-\mathbf{W}_j|\geq\sqrt{2}$ always holds; namely, the region of $|\mathbf{W}_i-\mathbf{W}_j|<\sqrt{2}$ is the Pauli-forbidden region in the phase space. For general A, we define $\{\mathbf{W}\}$ to be Pauli forbidden when there exists no $\{\mathbf{Z}\}$ which satisfies Eq. (5). We can easily show that the square root of the average value of $|\mathbf{W}_i-\mathbf{W}_j|^2$ over all pairs (i,j) is larger than $\sqrt{2}$. We have performed many numerical experiments for general A, and have found that $|\mathbf{W}_i-\mathbf{W}_j|$ cannot be too small for any pair (i,j) if $\{\mathbf{W}\}$ is Pauli allowed, though the minimum value is not exactly $\sqrt{2}$.

Based on the above-mentioned properties of $\{\mathbf{W}\}$, we treat two-nucleon collisions as follows: Two nucleons i and j are made to scatter with the probability $P(b)=(\nu\sigma_{NN}/\pi)\exp(-\nu b^2)$, where b is the impact parameter between i and j, and the in-medium two-nucleon cross section is given by $\sigma_{NN}=(100\ \text{mb})/[1+E_{NN}/(200\ \text{MeV})]$. By the collision the positions $\mathbf{R}_i$ and $\mathbf{R}_j$ are not changed but the momenta $\mathbf{P}_i$ and $\mathbf{P}_j$ are changed so as to make isotropic scattering. The length of the final relative momentum $|\mathbf{P}_i'-\mathbf{P}_j'|$ is changed from the initial one $|\mathbf{P}_i-\mathbf{P}_j|$ so that the total energy $\mathcal{H}$ is conserved. If the resultant $\{\mathbf{W}'\}$ is Pauli forbidden, namely, no corresponding $\{\mathbf{Z}'\}$ is obtained by solving Eq. (5), this two-nucleon collision is judged to be Pauli blocked. In order to facilitate the judgment of the Pauli blocking, we regard that $\{\mathbf{W}'\}$ is Pauli forbidden if another nucleon exists in any of two spheres with radius a centered at $\mathbf{W}_i'$ and $\mathbf{W}_j'$ in phase space, where we have taken $a=1.348$.

We have applied AMD to the study of the fragment mass distribution of the ^{12}C+^{12}C reaction at 28.7 MeV/nucleon. In Fig. 2 we compare the calculated results with the data of Czudek *et al.* [10]. The mass distribution is calculated at $t=200$ fm/c after the first contact of two ^{12}C nuclei. We have checked that the mass distribution is almost stationary between $t=155$ and 200 fm/c. We have taken account of only those fragments that have emission angles $4^\circ<\theta_F<36^\circ$ and momenta per nucleon $p_F/A_F>100$ MeV/c in the laboratory system, because this angle selection exactly corresponds to the experimental situation and the momentum selection approximately corresponds to it. In Fig. 2, ^{12}C is not displayed since it is difficult to distinguish between scattered and unscattered ^{12}C. We see large calculated yields of α and ^{8}Be fragments, which shows the ability of AMD to describe the shell effect or α-clustering effect. We can say that the qualitative feature of the data is reproduced

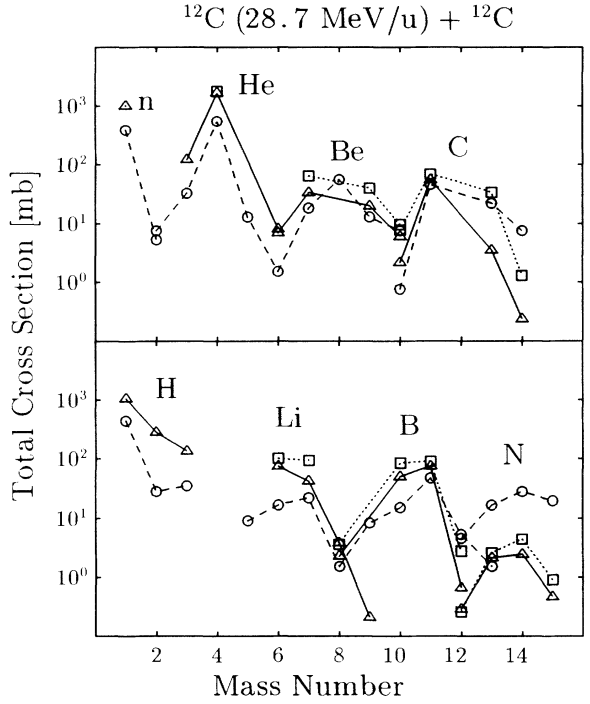

FIG. 2. Comparison of calculated fragment production cross sections with data (□). Calculations at $t = 200$ fm/c are shown by ○, and those after the treatment of statistical decays are shown by △.

by this calculation at $t = 200$ fm/c, if we take into account the subsequent decay of ^{8}Be fragments. The role of two-nucleon collisions is essential to this fragment mass distribution. When two-nucleon collisions are switched off, two ^{12}C nuclei pass through each other with little excitations in most events.

We have calculated excitation energies and spin values of fragments produced by the AMD simulation, which are usually well separated from one another in the configuration space. Since most fragments are highly excited, we have made a calculation of statistical cascade decays of these fragments. Our calculation code written by one of the authors (T.M.) is a modified version of the code CASCADE [11]. The mass distribution after the treatment of cascade decays is compared with data in Fig. 2. We see a good reproduction of the data by the theory, which verifies the usefulness of our new microscopic simulation framework AMD.

The total angular momentum conservation is violated by our method of two-nucleon collisions and therefore the calculated values of spins of the AMD fragments may not be so reliable. However, we can believe that this violation does not cause serious effects on the mass distribution after statistical cascade decays, because we have checked that it remains almost unchanged even when we artificially increase the spins of the AMD fragments by $2\hbar$.

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