Improvement of the nucleon emission process and the statistical property in molecular dynamics

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Abstract

We propose to introduce a new stochastic process in molecular dynamics in order to improve the description of the nucleon emission process from a hot nucleus. We give momentum fluctuations originating from the momentum width of the nucleon wave packet to the nucleon stochastically when it is being emitted from the nucleus. We show by calculating the liquid gas phase equilibrium in the case of antisymmetrized molecular dynamics, that with this improvement, we can recover the quantum mechanical statistical property of the nucleus for the particle emission process.

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In multifragmentation reactions in intermediate energy heavy ion collisions, many intermediate mass fragments are produced. Data of the mass distribution and other exclusive quantities have been reproduced rather well by the statistical models [1,2] which assume the decay of the thermal source into fragments according to the statistical weights of the possible final states. It is therefore reasonably considered that the multifragmentation process is largely governed by the statistical property. On the other hand, molecular dynamics simulations try to describe the fragmentation based on the microscopic dynamical evolution of the system [3–5]. With molecular dynamics simulations we can study the dynamical and statistical aspects in a unified framework without assuming any thermal equilibrium. However, for the reliable description of the fragmentation, we should check the validity of the statistical aspect of molecular dynamics and, if necessary, modify the dynamics of molecular dynamics so as to get the appropriate statistical aspect.

In our previous studies [6,7] of heavy ion collisions with antisymmetrized molecular dynamics (AMD) in the incident energy region between 30 MeV/nucleon and 100 MeV/nucleon, we observed that light nuclei such as ^{12}C break up into fragments easily in the dynamical stage of the reaction but intermediate mass fragments are seldom produced in the collision of heavier nuclei such as ^{40}Ar. We are also aware that the decay of excited nuclei produced in the reaction is too slow when the AMD calculation is continued for a long time, compared to the prediction by the statistical decay model. These points strongly suggested that we should improve particle emission processes in AMD. In this letter, we propose a method how to improve AMD in the nucleon emission process from the excited nucleus and show by calculating the liquid gas phase equilibrium that the improved AMD describes the quantum mechanical statistical property of hot nuclei for the particle emission process while the original AMD describes only the classical statistical property for that process. Our method of improvement is of general nature and can be applied to other molecular dynamics simulations.

Before the discussion of the statistical aspect and the improvement of AMD, we will explain the usual AMD [6] very briefly for the convenience of the readers. AMD describes

the nuclear many body system by a Slater determinant of Gaussian wave packets as

$$\Phi(Z) = \det\left[\exp\left\{-\nu(\mathbf{r}_j - \mathbf{Z}_i/\sqrt{\nu})^2\right\}\chi_{\alpha_i}(j)\right], \tag{1}$$

where the complex variables $Z \equiv \{\mathbf{Z}_i\}$ are the centers of the wave packets. We took the width parameter $\nu = 0.16\,\mathrm{fm}^{-2}$ and the spin isospin states $\chi_{\alpha_i} = \mathrm{p}\uparrow,\ \mathrm{p}\downarrow,\ \mathrm{n}\uparrow,$ or $\mathrm{n}\downarrow$. The time evolution of Z is determined by the time-dependent variational principle and the two-nucleon collision process. The equation of motion for Z derived from the time-dependent variational principle is

$$i\hbar \sum_{j\tau} C_{i\sigma,j\tau}\frac{dZ_{j\tau}}{dt} = \frac{\partial\mathcal{H}}{\partial Z_{i\sigma}^*}. \tag{2}$$

$C_{i\sigma,j\tau}$ with $\sigma,\tau = x,y,z$ is a hermitian matrix, and $\mathcal{H}$ is the expectation value of the Hamiltonian after the subtraction of the spurious kinetic energy of the zero-point oscillation of the center-of-masses of fragments,

$$\mathcal{H} = \langle H \rangle - \frac{3\hbar^2\nu}{2M}A + T_0(A - N_\mathrm{F}), \tag{3}$$

where N_F is the fragment number and T_0 is $3\hbar\nu/2M$ in principle, but treated as a free parameter for the adjustment of the binding energies. In two-nucleon collisions, physical coordinates $\mathbf{W}_i$ are introduced as

$$\mathbf{W}_i = \sum_{j=1}^{A}\left(\sqrt{Q}\right)_{ij}\mathbf{Z}_j, \quad Q_{ij} = \frac{\partial\log\langle\Phi(Z)|\Phi(Z)\rangle}{\partial(\mathbf{Z}_i^* \cdot \mathbf{Z}_j)}. \tag{4}$$

Except for the two-nucleon collision process, the AMD equation of motion (2) constitutes a kind of Hamilton system, and therefore one may think that the statistical property of AMD is not quantum mechanical [8]. It is not true because AMD can give the exact time evolution of the wave function for the harmonic oscillator mean field. Namely although the motion of the wave packet centers is classical, the AMD wave function containing the spatial and momentum spread of wave packets can have quantum mechanical statistical property. However, for the process of particle emission, the statistical property of AMD may be of classical nature, because the AMD description of the particle emission does not duely take

into account the momentum spread of wave packets. In order to get physical picture and to enable further development, we calculate the statistical property of the excited nucleus for the particle emission process in a new method explained in the following. We added to the Hamiltonian (3) the potential wall with a large radius of the form

$$\frac{k}{2}\sum_i f(|\mathbf{D}_i - \mathbf{D}_{\mathrm{CM}}|) \tag{5}$$

with

$$f(x) = (x - a)^2 \theta(x - a),$$
$$\sqrt{\nu}\mathbf{D}_i = \mathrm{Re}\,\mathbf{Z}_i, \quad \mathbf{D}_{\mathrm{CM}} = \frac{1}{A_{\mathrm{tot}}}\Sigma_j\mathbf{D}_j,$$
$$a = 12\,\mathrm{fm}, \quad k = 5\,\mathrm{MeV/fm}^2,$$

and put A_{tot} nucleons into the potential wall and give the total energy E_{tot}. The time evolution is calculated for a long time ($\sim 10^5$ fm/c). As shown in Fig. 1 there are usually a nucleus and nucleons in the potential wall. Nucleons are sometimes emitted and absorbed by the nucleus. This situation can be interpreted as the phase equilibrium of liquid (nucleus) and gas (nucleons). Typical values of the mass number of the largest fragment A_{liq} and its internal energy E_{liq} depend on the choice of A_{tot} and E_{tot}. We select the moments at which A_{liq} takes a given value in order to get the statistical property of the nucleus of the given mass number, and the long time average value of E_{liq} and the temperature are calculated. The temperature T, which should be common to both phases, is calculated as the long time average value of τ, where $(3/2)\tau$ is the kinetic energy (plus the potential energy from the wall) per nucleon in gas phase. Since the gas phase is dilute, the effect of the Pauli principle is neglected. When there are small fragments in the gas phase, they are excluded in the calculation of the temperature. The calculated relation between E_{liq} and T is shown in the left part of Fig. 2 by squares, which lie just on the line $\langle E_{\mathrm{liq}}\rangle/A_{\mathrm{liq}} = 3T - \mathrm{B.E.}$ of the classical statistics. Each calculated point corresponds to a specific choice of A_{tot} and E_{tot}. In the calculation of the temperature T, i.e., the kinetic energy of gas nucleons, we only used the central value of the wave packet $\mathrm{Im}\,\mathbf{Z}_i$ in momentum space. The neglect of the momentum

4

width is consistent with the subtraction of the spurious zero-point kinetic energy from the Hamiltonian (3). If we consider the momentum width, the temperature will shift by $(2/3)T_0$ (~ 6 MeV) and there will not be any states with temperature less than $(2/3)T_0$.

Microscopic processes which are important for the liquid gas phase equilibrium is the emission and the absorption of nucleons by the nucleus. The above result indicates that AMD has a problem in the description of the nucleon emission from the excited nucleus, since nucleon absorption is naturally described by AMD. Each nucleon in the nucleus has a momentum width of the wave packet which is an important part of its Fermi motion in the nucleus. When such a nucleon is emitted from the nucleus in AMD, it will have the momentum corresponding to the central value of its momentum distribution in the nucleus. Especially if the central value is not sufficiently large, the nucleon will never be able to go out, even if there should be some probability of going out due to the tail of the momentum distribution. In order to cure this problem, we regard the emitted nucleon as a classical particle without momentum distribution or a plane wave, though it is a wave packet in a nucleus. And we add a new stochastic process of giving the momentum fluctuation of the wave packet to a nucleon when it is being emitted from a nucleus. The total momentum and energy is conserved by adjusting the state of the nucleus. This new version of AMD is called AMD-MF and the details will be described in following paragraphs. By this incorporation of the momentum fluctuation into AMD, the situation of the liquid-gas phase equilibrium changes as shown in Fig. 3. Even when the excitation energy of the nucleus is smaller than in the case of usual AMD (Fig. 1), the number and the averaged energy of the gas nucleons are much larger. The AMD-MF is not a Hamilton system any more, and the statistical property of the excited nucleus for the particle emission process has changed drastically into quantum mechanical one, as shown in Fig. 2 by diamonds, which is similar to the empirical Fermi gas formula $\langle E_{\mathrm{liq}} \rangle / A_{\mathrm{liq}} = T^2/(12 \, \mathrm{MeV}) - \mathrm{B.E.}$.

It should be noted that our statistical ensemble for an excited nucleus is between the canonical ensemble and the microcanonical ensemble. Although both of E_{liq} and τ are fluctuating in time, they are correlated due to the energy conservation relation

FIG. 1. The density snapshots of the many-nucleon system contained in a potential wall (shown by circles) calculated with the usual AMD. These figures are for the total number of the nucleons $A_{\mathrm{tot}} = 15$ and the total energy $E_{\mathrm{tot}} = -50$ MeV, and the calculated temperature and the energy of the nucleus are $T = 1.48$ MeV and $\langle E_{\mathrm{liq}} \rangle / A_{\mathrm{liq}} = -3.65$ MeV for the mass number of the nucleus $A_{\mathrm{liq}} = 14$. The Volkov force is used for this calculation.

FIG. 2. The statistical property of the excited nucleus calculated with the usual AMD and the AMD-MF. The adopted effective interaction is the Volkov force in the left part, and the Gogny force in the right part. Lines of $(E/A)_{\mathrm{liq}} = 3T + \mathrm{const.}$, $T^2/(12\,\mathrm{MeV}) + \mathrm{const.}$, and $T^2/(8\,\mathrm{MeV}) + \mathrm{const.}$ are drawn for the comparison.

FIG. 3. Similar to Fig. 1 but calculated with the AMD-MF. $A_{\text{tot}} = 28$ and $E_{\text{tot}} = 60$ MeV for these figures, and calculated temperature and the energy of the nucleus are $T = 6.12$ MeV and $\langle E_{\text{liq}} \rangle / A_{\text{liq}} = -5.52$ MeV for the mass number of the nucleus $A_{\text{liq}} = 14$.

8

$$\Delta E_{\text{liq}} + \frac{3}{2} A_{\text{gas}} \Delta \tau = 0 \tag{6}$$

with $A_{\text{gas}} = A_{\text{tot}} - A_{\text{liq}}$, as long as one can neglect the probability of the existence of light fragments in gas phases and the small interaction energy between both phases and among the gas nucleons. By choosing a large potential wall so that A_{gas} is very large, it is possible to get the canonical ensemble with small $\Delta \tau$. On the other hand, if one take small volume for gas phase, microcanonical ensemble with small ΔE_{liq} can be obtained. With our choice of parameters for the case of Fig. 3, for example, the energy fluctuation is found to be $\sqrt{\langle \Delta E_{\text{liq}}^2 \rangle}/A_{\text{liq}} = 1.2$ MeV, which corresponds to the fluctuation of temperature $\sqrt{\langle \Delta \tau^2 \rangle} = 0.8$ MeV.

In AMD-MF, the momentum fluctuation is given to a nucleon when it is being emitted from a nucleus. At each time step, it is judged whether each nucleon is in a nucleus or it is isolated in free space. For each nucleon i, a representative point $\mathbf{r}_i$ is randomly generated around $\text{Re}\,\mathbf{W}_i/\sqrt{\nu}$ according to the Gaussian distribution, where $\mathbf{W}_i$ is the physical coordinate (4). The density at $\mathbf{r}_i$ without self-contribution is calculated in an approximate way as

$$\rho_i \sim \left(\frac{2\nu}{\pi}\right)^{3/2} \sum_{j(\neq i)} \exp\left[-2(\sqrt{\nu}\mathbf{r}_i - \text{Re}\,\mathbf{W}_j)^2\right]. \tag{7}$$

If $\rho_i < 0.1\rho_0$ with $\rho_0 = 0.17$ fm^{-3}, the nucleon is considered to be isolated in free space; else it is in a nucleus. In the same way, it is checked whether at the previous time step the representative point $\mathbf{r}_i - \text{Re}(\mathbf{W}_i(t) - \mathbf{W}_i(t - \Delta t))$ was in a nucleus or isolated. Momentum fluctuation is given to the nucleon i if it was in a nucleus at the previous time step and it is now isolated in free space.

When it is decided that the nucleon i should be given the momentum fluctuation now, the following procedures are made. First of all, the nucleus from which the nucleon i is being emitted is defined as the cluster judged by the chain clustering method. The mass number of the nucleus is denoted by A_{nuc}, which do not include the nucleon i. Then the relative momentum between the nucleon i and the nucleus is decided stochastically, by taking

9

account of the fact that the momentum distribution of the nucleon and the distribution of the momentum per nucleon of the center-of-mass of the nucleus are approximately represented by Gaussian distributions

$$\exp\left[-(\mathbf{p} - \mathbf{P}_i)^2/2\hbar^2\nu\right] \quad \text{and} \quad \exp\left[-A_{\mathrm{nuc}}(\mathbf{p} - \mathbf{P}_{\mathrm{nuc}})^2/2\hbar^2\nu\right], \tag{8}$$

respectively, where

$$\mathbf{P}_i = 2\hbar\sqrt{\nu}\,\mathrm{Im}\,\mathbf{W}_i \quad \text{and} \quad \mathbf{P}_{\mathrm{nuc}} = \frac{2\hbar\sqrt{\nu}}{A_{\mathrm{nuc}}}\sum_{j\in\mathrm{nuc}}\mathrm{Im}\,\mathbf{W}_j. \tag{9}$$

In order to keep consistency with the method of subtraction of spurious center-of-mass motion of fragments (3), the energy T_0 is subtracted from the relative kinetic energy by reducing the relative momentum. If the relative momentum is too small for this procedure, this momentum fluctuation is canceled.

The first candidate of the final state of the momentum fluctuation process is determined by changing only the relative physical momentum between the nucleon i and the nucleus to the value decided in the previous paragraph. However, since the energy is not conserved with this state, the energy is adjusted to the initial energy with the least modification of the state by applying the frictional cooling/heating method with $\lambda + i\mu = \mp i$, for the limited coordinates $\mathbf{Z}_j$ with j in the nucleus. And after each step of the friction, the physical coordinate of the nucleon i and the physical center-of-mass and the total momentum of the nucleus are restored to the values of the first candidate.

There are several possibilities for the above procedure to fail. The friction leads to a converged energy but still may not reach the initial energy. Or the transformation from $\mathbf{W}$ variables to $\mathbf{Z}$ variables may not exist due to the Pauli-blocking. In these cases, the momentum fluctuation is tried again by generating a different sample of relative momentum.

In summary, a new stochastic process has been added to AMD in order to improve the description of the nucleon emission process from a hot nucleus. The momentum fluctuation originating from the momentum width of the nucleon wave packet in the nucleus is given to the nucleon stochastically when it is being emitted from the nucleus (AMD-MF). With this

improvement, the quantum mechanical statistical property of the excited nucleus for the particle emission process has been obtained, which are calculated in the phase equilibrium of the liquid phase and the gas phase of nucleons. It should be noted that we need not totally modify the dynamics of the AMD equation of motion. As we mentioned before, we can believe that the AMD wave function gives fairly good time-evolution of the hot nucleus, because AMD can give the exact time evolution of the wave function for the harmonic oscillator mean field. What we have incorporated in this work is a minor branching process which is brought about by the tail of the nucleon wave packet. It may be necessary to generalize the modification so as to improve the cluster emission process in addition to the nucleon emission. For the application to heavy ion collisions, other processes caused by the wave packet tail should be considered such as the nucleon transfer between the projectile and the target. The wave packet width in spatial coordinate space may also play some role. Such extensions have been formulated and calculations of nuclear collisions have shown that fragmentation processes are largely influenced by the introduction of the new stochastic process described here and its extensions. We will discuss these in other papers.

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