The role of the Heisenberg principle in the Constrained Molecular Dynamics model

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We implement the Heisenberg principle into the Constrained Molecular Dynamics model with a similar approach to the Pauli principle using the one-body occupation probability $\bar{f}_i$. Some results of the modified and original model and comparison to the data are given. The binding energies and radii of light particles reproduced by the modified model are more consistent with the experimental data than the original model. Some simulations for superheavy nuclei are discussed.

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I. INTRODUCTION

In recent decades, heavy-ion reactions have been an important approach to study the properties of nuclear structure and dynamics, such as the properties of exotic nuclei, the equation of state, and superheavy nuclei among other features. Besides experiments, theoretical models become more and more useful in these researches. Among them, molecular dynamics models achieved great success since they dealt better with the N-body problem[1]. The Fermionic Molecular Dynamics model(FMD)[2, 3] and the Antisymmetrized Molecular Dynamics model(AMD)[4, 5] has successfully preserved the fermionic nature of the many body system by expressing the wave function of the system as a single Slater determinant of N wave packets. As a result, the numerical effort of these two models grows with N^4. It takes very large CPU time for calculations of large mass systems (≥80 nucleons) so that approximations are needed[6]. The Quantum Molecular Dynamics model (QMD)[7, 8] takes much less time since it need only double-fold loops to calculate two-body interactions, making its numerical effort grow with N^2[1]. It has made great achievements in heavy-ion reactions from intermediate to high energies[9–12]. However, the fermionic feature is lacking in the QMD model, especially in the ground states or in low-energy reaction phenomena[1]. Several modified quantum molecular dynamics models have been proposed to solve this problem, like the extended Quantum Molecular Dynamics(EQMD) model[13], and the constrained Molecular Dynamics(CoMD) model[1, 14].

The EQMD model tried to mimic the fermionic features by introducing the Pauli potential, which forbids nucleons of the same spin and isospin from coming close to each other in phase space[13]. The model shows some good features such as stable ground states and saturation properties of nuclear matter, but it also has some problem like the spurious repulsion in the collisions[1, 15, 16].

By constraining the phase space to fulfil the Pauli principle at each time step, the CoMD model has successfully introduced the effect of the fermionic nature to the nuclear many-body system. It is able to reproduce with the same set of parameters not only the average binding energy and radii of nuclei in a wide mass region (A = 30-208) but also the experimental fragment charge distribution in many collisions such as ^{40}Ca+^{40}Ca, ^{197}Au+^{197}Au, ^{112,123}Sn+^{58,64}Ni systems at 35 MeV/nucleon, and ^{40}Ca+^{48}Ca system at 25 MeV/nucleon[1, 17]. However, the binding energies and theoretical prediction of light particles particularly the Z=2 yield are not consistent with experimental results[1]. In this paper, we try to modify these features by introducing the Heisenberg principle into the CoMD model.

II. MODEL AND FORMALISM

The nucleon wave functions and mean field used in this work are the same with the original model to maintain the equation of state. Details about the effective interaction were described in Ref. [1].

In the original CoMD model, the algorithm constraints for Pauli principle at each time step are achieved via the following quantities:

$$\bar{f}_i \leq 1, \tag{1}$$

$$\bar{f}_i \equiv \sum_j \delta_{\tau_i,\tau_j}\delta_{s_i,s_j}\int_{h^3} f_j(r,p)d^3rd^3p, \tag{2}$$

in which the coordinate s_i represents the nucleon spin projection quantum number[1].

At each time step and for each particle i, an ensemble K_i of nearest identical particles (including the particle i) is determined within the distances $\sqrt{\pi\hbar\sigma_r/2\sigma_p}$ and $\sqrt{\pi\hbar\sigma_p/2\sigma_r}$ from particle i in r and p spaces, respectively[1]. Then we calculate the phase space occupation $\bar{f}_i$ for the identical particles. If $\bar{f}_i$ has a value greater than 93.0/128.0, which we modified from the original value 1 in Ref. [1] to get better average binding energy, we change randomly the momenta of the particles

belonging to the ensemble K_i. The mechanism we use is a many-body elastic scattering so that the total momentum and the total kinetic energy of the newly generated sample is conserved. The new sample is accepted only if the phase-space occupation $\bar{f}_i$ is smaller than before.

We decided to use a similar approach to introduce the Heisenberg principle into the modified model. After the check for Pauli principle for identical particles (same spin and isosipin) as mentioned before, for each of those particles that do not violate Pauli principle, we search the ensemble L_i of nearest non-identical particles (including the particle i) within the distances $\sqrt{\pi\hbar\sigma_r/2\sigma_p}$ and $\sqrt{\pi\hbar\sigma_p/2\sigma_r}$ from particle i in r and p spaces, respectively[1]. Then we calculate the average $\bar{f}_i$ for the non-identical particles in the ensemble L_i. If the average of $\bar{f}_i$ has a value greater than 25.0/128.0 (a value ~~we got~~ by calculating the $\bar{f}_i$ of two nucleons with their $\Delta r\Delta p$ equals to $\hbar/2$[18]), we change the momenta of the particles belonging to the ensemble L_i as we did for K_i before. Notably, those particles which have been scattered because of the Pauli principle will not be included in the check for Heisenberg principle. This ensures that one particle will not be scattered twice.

Similarly to the Pauli blocking, we introduced the "Heisenberg blocking" in the collision term. For each NN collision, we calculate the occupation probability as we did before and check for both Pauli principle and Heisenberg principle. Only if they are both satisfied with the requirements ~~can~~ the collision ~~be~~ accepted, ~~and~~ rejected otherwise. In this way, the Heisenberg principle is important for light nuclei ($Z \leq 4$) and Pauli principle becomes dominant for heavy nuclei.

III. RESULTS AND DISCUSSION

In order to examine the CoMD model with Heisenberg principle (CoMD-H), we compare some calculated results to the original model and also to experimental data.

For the initialization step, we modified the cooling procedure. We use the constraint to solve the equations of motion with friction terms. The nucleons are first distributed in spheres of radius $1.2\times A^{1/3}$ fm and P_F^{nm} (Fermi momentum for infinite nuclear matter) in coordinate and momentum space, respectively. Then at each time step, we first calculate the value of $\bar{f}_i$ to fulfil the Pauli principle. If $\bar{f}_i$ is greater than 93.0/128.0, the momenta of the particles belonging to the ensemble K_i are scaled by a factor of 1.005. If $\bar{f}_i$ is less than 93.0/128.0, we calculate the value of $\bar{f}_i$ to fulfill the Heisenberg principle. If the average $\bar{f}_i$ for Heisenberg principle is greater than 25.0/128.0, we set the scale factor to 1.0005. If this $\bar{f}_i$ is also less than the critical value, the scale factor is set to 0.99. Then roughly in 1000 fm/c, we get stationary values of the total binding energy and radius. After this cooling procedure, the friction term is switched off and we check the time dependence of the nuclear radius R. The initial condition will be accepted only if R is stable for at least 1000 fm/c.

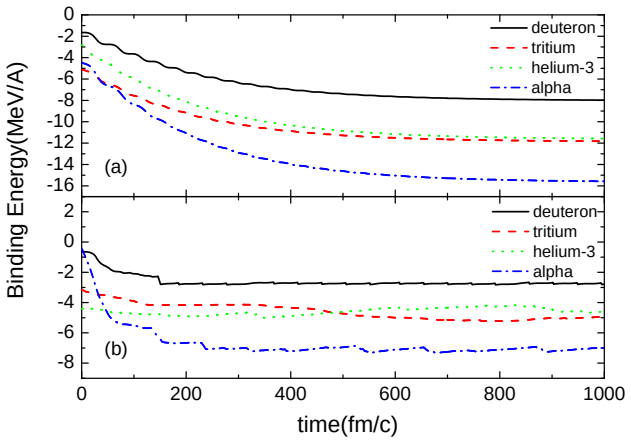

FIG. 1: (Color online) Time evolution of binding energies during the cooling step for the original model without Heisenberg principle (a) and the modified model with Heisenberg principle (b).

In the original model, the binding energies of light particles are not ~~satisfying~~. Figure 1 shows comparisons of the binding energies calculated by the original and the modified model. From the results of the original model, we see that the binding energies keep going down to a very low value. This is due to the fact that these light particles, i.e., deuteron, tritium, helium-3, and alpha particles do not violate Pauli principle thus friction moves the gaussian wave packets on top of each other. We stress that this feature is common to all molecular dynamics models but other authors choose to include the gaussian finite width as the kinetic energy part. Thus the ground states are solids[6, 14]. When adding the Heisenberg principle, we see that the binding energies oscillate around some average values. These are the real ground state of the model depending only on the interaction parameters and especially the surface term for light nuclei. The binding energies are closer to the experimental data, as shown in Fig. 2. The experimental data are taken from National Nuclear Data Center. We calculate nuclei with masses ranging from 2(deuteron) to 238(^{238}U). The modified model seems to work better throughout the whole nuclei chart than the original one. We stress also that in order to fulfill the Heisenberg principle, we enforce its effect in the collision term as well for non-identical particles.

To test the ability of the modified model to work with exotic nuclei, we calculated the binding energies of whole calcium isotopes as shown in Fig. 3. It seems that the results of the modified model are more consistent with the data than those of the original one. Figure 4 shows the binding energies of the nuclei with mass $A = 40$. Both models reproduce the binding energies in a similar fashion within the error bars, thus suggesting that with larger nuclei the Heisenberg principle is less and less important

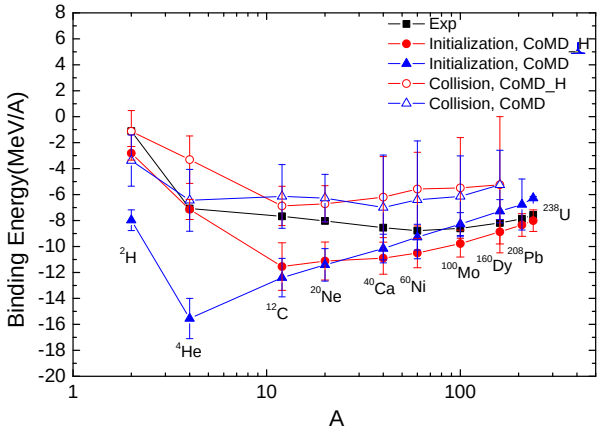

FIG. 2: (Color online) Binding energies of nuclei with mass ranging from 2 to 238 in initializations and collisions. The black squares represent the experimental data. The red solid circles and blue solid triangles represent the binding energies of nuclei during the initialization step calculated by the modified model with the Heisenberg principle (CoMD_H) and by the original model without that (CoMD), respectively, while the red open circles and blue open triangles represent the binding energies of the fragments obtained in the nucleus-nucleus fragmentation collisions. The latter fragments might be stable but not in their ground state because they would normally deexcite say by γ rays at very long times, a mechanism not included in the model.

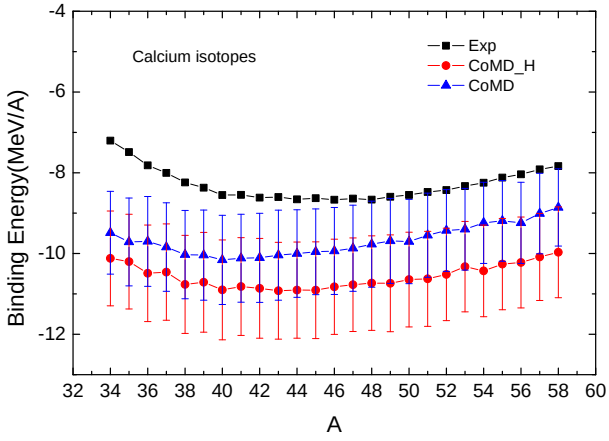

FIG. 3: (Color online) Binding energies of the calcium isotopes.

than the Pauli one as expected. Clearly the reproduction of the data is not perfect and we did not try to adjust parameters since we believe that important effects, such as spin-spin forces are missing and we plan to include those effects in future works.

As for the reactions, we also performed some simulations. Figure 5 shows the charge distribution of ^{197}Au + ^{197}Au at 35 MeV/A with impact parameters ranging

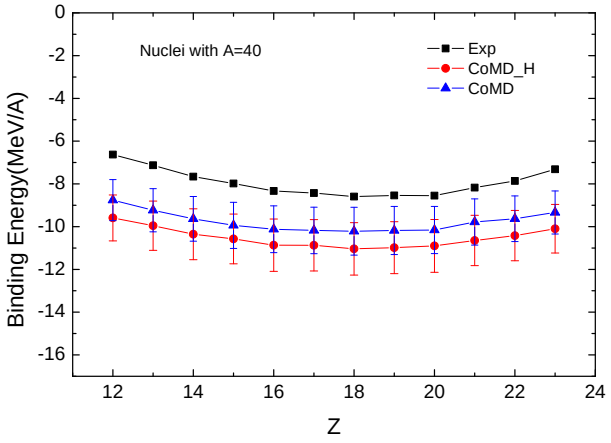

FIG. 4: (Color online) Binding energies of nuclei with mass $A = 40$.

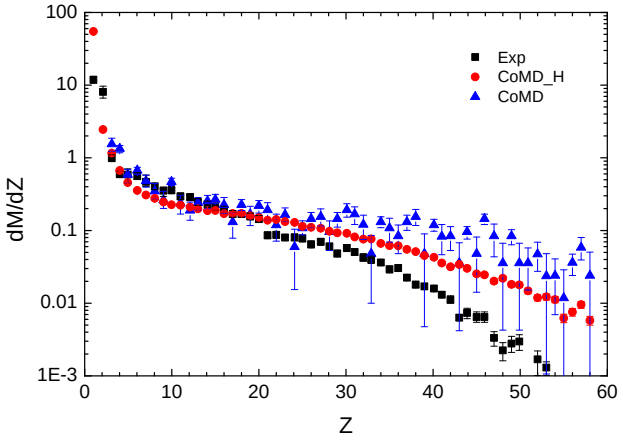

FIG. 5: (Color online) Comparison between the experimental isotope distribution and the calculated results of the modified model and the original model for ^{197}Au + ^{197}Au at 35 MeV/A with impact parameters ranging from 0 to 3.5 fm up to 1500 fm/c[1].

from 0 to 3.5 fm up to 1500 fm/c. The modified model seems better than the original one, especially in the light nuclei region, noticing that the original model gives too many protons and alpha particles(not displayed in the figure - out of scale)[1]. At Z =20, the data show a jump due to the detectors used. We will get a better agreement of the data with the calculations if we slightly shift the data yield up for Z >20[1].

Figure 6 shows the the isotope distribution of the ^{238}U + ^{238}U at 15 MeV/A with impact parameter of 0 fm up to 4000 fm/c. For some isotopes coming out from the reaction region, their binding energies are shown in Fig. 2. We see that all the binding energies of the nuclei from the collisions are smaller than those in the initialization step, since they are still excited after 4000 fm/c evolu-

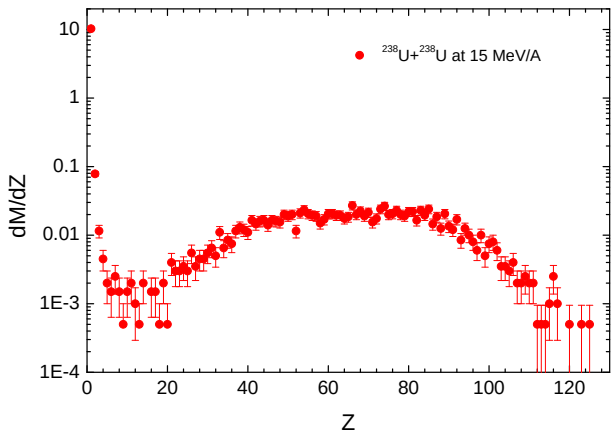

FIG. 6: (Color online) Isotope distribution of ^{238}U + ^{238}U at 15 MeV/A with impact parameter of 0 fm up to 4000 fm/c by CoMD_H.

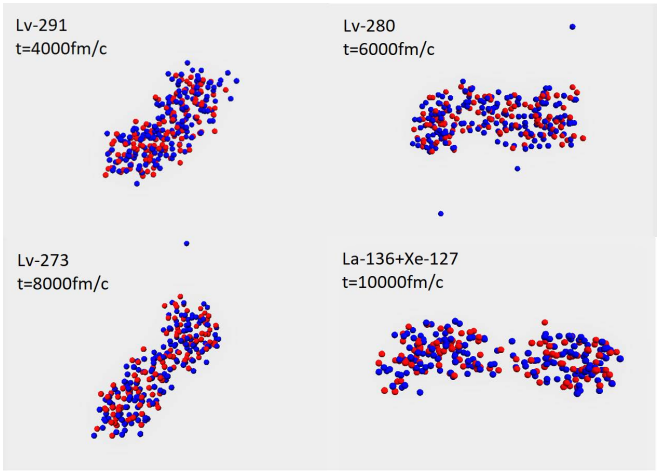

FIG. 7: (Color online) Time evolution of Livermorium-291 by CoMD_~~H~~. The red spheres represent protons, while the blue ones represent neutrons. Only the largest clusters are ~~marked out~~.

tion (they cannot emit say gamma rays to decay to their ground states). The binding energies of deuterons and alpha particles of the modified model are smaller than those of the original one, while for heavy nuclei, they are more or less the same, consistent with the initialization step. In the superheavy region, a peak around Z = 116 was found. We selected one nucleus with Z = 116 and A = 291, and let it evolve with time. One out of 500000 events survived for a total time of another 6000 fm/c with only several neutrons emitted as shown in Fig. 7, then finally it underwent fission and broke into ^{136}La+^{127}Xe, one alpha particle with the kinetic energy of 15.78 MeV (close to the value predicted by the nuclear density functional theory, which is around 14 MeV[19, 20]), and several protons and neutrons. This might be a different path to study super-heavy production[21] and we will discuss more in detail in future works since a large calculation effort is required.

IV. SUMMARY

In this paper, we have succeeded in modifying the CoMD model by introducing the Heisenberg principle. The binding energies of the light particles are more comparable to the experimental data in both initializations and collisions. The modified model seems to work better with exotic nuclei than the original one. We have also performed some superheavy nuclear reactions with the new model. Though we got some events, more efforts, both numerically and theoretically needs to be done and we decided to postpone it until further refinements in the model are included such as the (iso)spin-(iso)spin forces.

Acknowledgments

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