Extension of Quantum Molecular Dynamics and its Application to Heavy-Ion Collisions

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Abstract

In order to treat low-energy heavy-ion reactions, we make an extension of quantum molecular dynamics method. A phenomenological Pauli potential is introduced into effective interactions to approximate the nature of the Fermion many-body system. We treat the widths of nucleon wave-packets as time-dependent dynamical variables. With these modifications, our model can well describe the ground-state properties in wide mass range. Improvements due to the extension are also obtained in the nucleus-nucleus collision calculations.

I. INTRODUCTION

With the progress of computers, microscopic simulation methods have become popular in the heavy-ion reaction studies. The benefit of microscopic simulation method is that one can investigate nuclear reactions without making any specific assumption on the reaction mechanism. There are many kinds of microscopic simulations such as the time-dependent Hartree Fock (TDHF) which is a mean-field theory, Vlasov equation which is the semiclassical approximation of TDHF, Vlasov-Uehling-Uhlenbeck (VUU) equation or Boltzmann-Uehling-Uhlenbeck (BUU) equation in the other name, which consist of Vlasov and the two-body collision term, the Cascade model which includes only two-body collision term, and so on. Especially, VUU/BUU equation, which includes both of mean-field and two-body collision term, has become a standard framework for the heavy-ion reaction study from the low or intermediate energy to the high energy region. However, VUU/BUU equation, which is basically one-body theory, has a difficulty in dealing with the phenomena of fluctuation such as the fragment formation.

Molecular dynamics approaches like quantum molecular dynamics (QMD) have been developed in order to calculate the fragmentation process. In QMD, we assume a single-particle distribution function of a nucleon as a Gaussian wave packet, and calculate the time evolution of the system according to the classical Newtonian equation of motion plus the two-body collision term. It contains both aspects of the mean-field and the two-body collisions, and is applicable to the wide energy-region. Furthermore, QMD can deal with the
Due to its applicability and its ability to describe fragment formation, QMD is widely used recently for heavy-ion reactions from intermediate to high energies. For low-energy reactions such as fusion, fission and deep inelastic collision process, however, microscopic simulations by using the molecular dynamics have not been studied except for a few works. One example is the analysis of the fusion reaction using QMD [8]. It was reported, however, that several extra nucleons are emitted during the collision process in the calculation. This is due to the insufficient stability of initial ground state nuclei. We have to settle this problem to study low-energy collisions of heavy-ions using the molecular dynamics.

For the simulation of low-energy nuclear reactions, frameworks with anti-symmetrization of the total wave function like FMD [6] and AMD [7] are suitable for describing ground state properties and reaction processes. However, they are not applicable for very heavy systems since they need much CPU time which is approximately proportional to the fourth power of the particle number. For calculations of heavy systems, application of the QMD framework (without anti-symmetrization) is still necessary.

In this paper we propose an extended version of QMD method in view of the simulation of low-energy phenomena. Its applicability to treat ground state properties and nuclear reaction is investigated. Several improvements over standard QMD are found in this study. In Sec. 2 we describe the formalism of the extended QMD method, and the ground state properties by our model is discussed in Sec. 3. Its application to the nuclear reaction is reported in Sec. 4. Finally, summary and the discussion is given in section 5.

II. EXTENSION OF QMD

The insufficient stability of the standard QMD ground state is mainly due to the fact that they are not at their energy-minimum states. In the standard QMD, the kinetic energy term arising from the momentum variance of wave-packets is spurious and we do not take into account this term. Thus the constituent nucleons have finite momenta and are moving around in the ground state with appropriate binding energies. If we take the energy-minimum states, all the nucleons stop their motion and get into the over-bound states where the Pauli principle is broken. To solve this difficulty we make an extension of QMD in two points so as to take energy-minimum state as an initial ground nucleus: First, we include the so-called Pauli potential into effective interactions [9] in order to approximate the nature of Fermion many-body system. Second, we take into account the kinetic-energy term of the momentum variance of wave-packets to the Hamiltonian. In accordance with this we treat the width of each wave packet as a dynamical variable [10]. We call here this extension of QMD as “EQMD”.

A. Equation of motion of the system

The equation of motion is obtained by the time-dependent variational principle. We assume the total wave function of the system as a direct product of Gaussian wave packets of nucleons
\[ \Psi = \prod_i \phi_i(\mathbf{r}_i), \]  
\[ \phi_i(\mathbf{r}_i) = \left( \frac{\nu_i + \nu_i^*}{2\pi} \right)^{3/4} \exp \left[ -\frac{\nu_i}{2}(\mathbf{r}_i - \mathbf{R}_i)^2 + i\frac{\mathbf{P}_i \cdot \mathbf{r}_i}{\hbar} \right]. \]

Here \( \mathbf{R}_i \) and \( \mathbf{P}_i \) are the centers of position and momentum of the \( i \)-th wave packet. We introduce the complex Gaussian width \( \nu_i \) as
\[ \nu_i \equiv 1 + i\delta_i, \]
where \( \lambda_i \) and \( \delta_i \) are its real and imaginary parts, respectively. The Hamiltonian is written as
\[ H = \langle \Psi | \sum_i -\frac{\hbar^2}{2m} \nabla^2_i - \hat{T}_{CM} + \hat{H}_{\text{int}} | \Psi \rangle \]
\[ = \sum_i \left[ \frac{\mathbf{P}_i^2}{2m} + 3\hbar^2 \frac{(1 + \lambda_i^2 \delta_i^2)}{4m\lambda_i} \right] - T_{CM} + H_{\text{int}}, \]
where \( T_{CM} \) and \( H_{\text{int}} \) denote the spurious zero-point center-of-mass kinetic energy and the potential energy term, respectively. Here, one should note that the Hamiltonian includes terms originating from momentum variances of wave packets which were neglected as spurious constant terms in the standard QMD. Subtraction of the spurious zero-point CM kinetic energy is necessary since we include the kinetic energy from the momentum variance of wave-packets.

The equations of motion of these variables are determined by the time-dependent variational principle
\[ \delta \int_{t_1}^{t_2} \mathcal{L} dt = 0, \]
\[ \mathcal{L}(\{\mathbf{R}_i, \mathbf{P}_i, \lambda_i, \delta_i, \dot{\mathbf{R}}_i, \dot{\mathbf{P}}_i, \dot{\lambda}_i, \dot{\delta}_i\}) \equiv \langle \Psi | i\hbar \frac{d}{dt} - \hat{H} | \Psi \rangle. \]

Then we get 8\( A \) dimensional classical equations of motion, i.e. equations of motion of 4\( A \) parameters (\( A \) means the number of constituent particles)
\[ \dot{\mathbf{R}}_i = \frac{\partial H}{\partial \mathbf{P}_i}, \quad \dot{\mathbf{P}}_i = -\frac{\partial H}{\partial \mathbf{R}_i}, \]
\[ \frac{3\hbar}{4} \dot{\lambda}_i = -\frac{\partial H}{\partial \delta_i}, \quad \frac{3\hbar}{4} \dot{\delta}_i = \frac{\partial H}{\partial \lambda_i}. \]

**B. Subtraction of zero-point CM kinetic energy**

We subtract the zero-point center-of-mass kinetic energy of the system \( T_{CM} \) following the basic idea of Ref. [7]. In our case, however, all the wave-packets have different contributions to zero-point kinetic energy. Therefore we take \( T_{CM} \) as
\[ T_{\text{CM}} = \sum_i t_{i,\text{CM}}^{\text{CM}} / M_i , \]  
\[ (9) \]

where \( t_{i,\text{CM}}^{\text{CM}} \) is the zero-point kinetic energy of the wave-packet \( i \) written as

\[ t_{i,\text{CM}}^{\text{CM}} = \frac{\langle \phi_i | \nabla | \phi_i \rangle^2}{2m} - \frac{\langle \phi_i | \nabla^2 | \phi_i \rangle}{2m} . \]  
\[ (10) \]

and \( M_i \) is the “mass number” of the fragment to which the wave-packet \( i \) belongs. The “mass number” is calculated as the sum of the “friendships” of other nucleons

\[ M_i = \sum_j F_{ij} \]  
\[ (11) \]

\[ F_{ij} \equiv \begin{cases} 1 & (|R_i - R_j| < a) \\ e^{-((R_i - R_j)^2 / b)} & (|R_i - R_j| \geq a) \end{cases} \]  
\[ (12) \]

where we use the parameters \( a = 1.7 \text{ fm} \) and \( b = 4 \text{ fm}^2 \).

C. Effective interaction

For the effective interaction, we use Skyrme, Coulomb, Symmetry and the Pauli potential

\[ H_{\text{int}} = H_{\text{Skyrme}} + H_{\text{Coulomb}} + H_{\text{Symmetry}} + H_{\text{Pauli}} . \]  
\[ (13) \]

For the form of Skyrme interaction, we use the most simple one

\[ H_{\text{Skyrme}} = \frac{\alpha}{2\rho_0} \int \rho^2(r) d^3 r + \frac{\beta}{(\gamma + 1)\rho_0^\gamma} \int \rho^{\gamma+1}(r) d^3 r \]  
\[ (14) \]

\[ \rho(r) = \sum_i^A \rho_i(r) , \]  
\[ (15) \]

\[ \rho_i(r) = \frac{1}{(\pi\lambda_i)^{3/2}} \exp[-(r - R_i)^2 / \lambda_i] . \]  
\[ (16) \]

In the treatment of real system, however, we exclude the self interaction

\[ H_{\text{Skyrme}} = \frac{\alpha}{2\rho_0} \sum_{i,j \neq i} \int \delta(r_i - r_j) \rho_i(r_i)\rho_j(r_j) d^3 r_i d^3 r_j \]
\[ + \frac{\beta}{(\gamma + 1)\rho_0^\gamma} \sum_{i,j \neq i} \int \delta(r_i - r_j) \rho(r_i)^{\gamma-1} \rho_i(r_i)\rho_j(r_j) d^3 r_i d^3 r_j , \]  
\[ (17) \]

\[ \equiv H_2 + H_{\gamma+1} . \]  
\[ (18) \]

For the numerical calculation of the density-dependent term \( H_{\gamma+1} \), we perform a three-fold loop computation since we use the density-dependent term with \( \gamma = 2 \) which is identical to the three-body interaction. Although the approximate treatment of density-dependent term with the two-fold loop computation much reduces the CPU time, it causes much ambiguity.

We also employ the symmetry potential as
\[ H_{\text{Symmetry}} = \frac{c_s}{2\rho_0} \sum_{i,j \neq i} \int [2\delta(T_i, T_j) - 1] \rho_i(r)\rho_j(r) d^3r, \tag{19} \]

where \( T_i \) is the isospin index of nucleon \( i \). In the nuclear matter limit, this term goes to

\[ \int \frac{c_s}{2} \left( \frac{\rho_p - \rho_n}{\rho_0} \right)^2 d^3r, \tag{20} \]

where \( \rho_p \) and \( \rho_n \) denote proton and neutron densities, respectively.

### D. Pauli potential

We introduce a phenomenological repulsive potential which inhibits nucleons of the same spin \( S \) and isospin \( T \) to come close to each other in the phase space. We assume a very simple form for this potential,

\[ H_{\text{Pauli}} = \frac{c_p}{2} \sum_i (f_i - f_0) \theta(f_i - f_0), \tag{21} \]

\[ f_i \equiv \sum_j \delta(S_i, S_j)\delta(T_i, T_j) |\langle \phi_i | \phi_j \rangle|^2, \tag{22} \]

where \( f_i \) is the overlap of a nucleon \( i \) with the same kind of nucleons (including itself), and we take the threshold parameter \( f_0 \approx 1 \). \( c_p \) is the strength of the potential.

In order to see the statistical behavior of infinite system with our Pauli potential, we show in Fig. 1 the energy per nucleon of free nucleon gas with the density- and temperature-dependence. In the limit of infinite system, we assume all the wave packets approach to plane waves with uniform coordinate-space distribution. Then we perform the Metropolis simulation in the momentum space as in Refs. \[11,12\]. As for the parameters of Pauli potential in the figure, we take \( c_p = 15 \text{ MeV}, f_0 = 1.05 \) and \( \mu = 2.0 \). No nuclear potential and Coulomb potential is included. In the low-temperature region our gas is closer to the Fermi gas rather than the Boltzmann gas. In the high-temperature region, however, it approaches to the classical limit of the Boltzmann gas rapidly. Although this is a general tendency with any set of parameters, the behavior of our gas is apparently different from that of the simple classical gas and we can describe, to a certain extent, the property of Fermi gas. For the ground state nuclei and for low- and medium energy reactions treated in this paper, the inclusion of Pauli potential greatly improves the standard QMD as seen in this paper.

There are two possible ways to fix the interaction parameters. One is to keep the saturation condition of nuclear matter with nuclear and Pauli potentials. In this case we have to adjust the Skyrme interaction parameters as well as the Pauli potential. We calculate the energy of the infinite system at zero-temperature as a function of its density. Then the Skyrme interaction parameter is adjusted to give 16 MeV binding energy at the saturating point. Keeping the saturation property of nuclear matter, we search good parameters of Pauli potential for finite nuclear systems. We call the parameters fixed in this way as “parameter set 1”. Another way is to fix the Skyrme parameters in their original values neglecting the contribution of Pauli potential to the saturation property of matter. In this
FIG. 1. Energies per nucleon of infinite system without nuclear and Coulomb potentials. Open circles and crosses denote the total and the kinetic energy of the gas with Pauli potential with $c_p = 15$ MeV, $f_0 = 1.05$ and $\mu = 2.0$. Dashed and dot-dashed lines denote Fermi gas and the classic Boltzmann gas.
TABLE I. Parameter values used in the Skyrme, Symmetry and Pauli potentials.

|                | $\alpha$ | $\beta$  | $\gamma$ | $c_S$  | $c_P$  | $f_0$ | $\mu$ |
|----------------|----------|----------|----------|--------|--------|-------|-------|
| parameter set 1| $-116.6$ MeV | $70.8$ MeV | $2$       | $25$ MeV | $15$ MeV | $1.05$ | $2.0$  |
| parameter set 2| $-124.3$ MeV | $70.5$ MeV | $2$       | $25$ MeV | $15$ MeV | $1.0$  | $1.3$  |

case we adopt standard parameters of the Skyrme interaction. The parameters of Pauli potential is searched to give a good agreement to the systematic trend of binding energies of finite systems. We call these parameters “parameter set 2”. The values of the parameter of both sets are listed in Table I.

E. Two-body collision term

For the treatment of two-body collisions, we follow the prescription of the standard QMD. If a pair of two nucleons fulfill these conditions, i.e., i) their relative distance takes its minimum value within the time-step, and ii) the minimum distance being smaller than a certain value $d_{coll}$, then a stochastic two-body collision is set to occur iii) with the probability $P_{coll}$ decided as

$$P_{coll} = \frac{\sigma_{NN}}{\pi d_{coll}^2}. \quad (23)$$

Here we take $2.0$ fm for the value of $d_{coll}$ and $\sigma_{NN}$ is the energy-dependent nucleon-nucleon collision cross section parameterized \(^4\) given as

$$\sigma_{NN} = \frac{100}{1 + \epsilon/200 \text{ MeV}} \text{ mb}, \quad (24)$$

$$\epsilon \equiv p_{coll}^2/2m. \quad (25)$$

In this paper the angular distribution of the final state of collision is assumed to be isotropic. The final relative momentum of colliding nucleons is searched so as to conserve the total energy of the system, since the total energy conservation is not guaranteed due to the momentum dependence of Pauli potential. The Pauli principal is also checked and the collisions with unsatisfactory final states are canceled.

III. THE GROUND STATE PROPERTIES

One has to prepare energy-minimum states as initial ground nuclei. They are obtained by starting from a random configuration and by solving the damped equations of motion as

$$\dot{R}_i = \frac{\partial H}{\partial P_i} + \mu_n \frac{\partial H}{\partial R_i}, \quad \dot{P}_i = -\frac{\partial H}{\partial R_i} + \mu_p \frac{\partial H}{\partial P_i},$$

$$\frac{3h}{4} \dot{\lambda}_i = -\frac{\partial H}{\partial \delta_i} + \mu_s \frac{\partial H}{\partial \lambda_i}, \quad \frac{3h}{4} \dot{\delta}_i = \frac{\partial H}{\partial \lambda_i} + \mu_s \frac{\partial H}{\partial \delta_i}. \quad (26)$$
Here $\mu_R$, $\mu_P$, $\mu_\lambda$, and $\mu_\delta$ are damping coefficients. With negative values of these coefficients the system goes to its (local) minimum point,

$$\frac{dH}{dt} = \sum_i \left[ \frac{\partial H}{\partial \mathbf{R}_i} \dot{\mathbf{R}}_i + \frac{\partial H}{\partial \mathbf{P}_i} \dot{\mathbf{P}}_i + \frac{\partial H}{\partial \lambda_i} \dot{\lambda}_i + \frac{\partial H}{\partial \delta_i} \dot{\delta}_i \right]$$

$$= \sum_i \left[ \mu_R \left( \frac{\partial H}{\partial \mathbf{R}_i} \right)^2 + \mu_P \left( \frac{\partial H}{\partial \mathbf{P}_i} \right)^2 + \frac{4\mu_\lambda}{3\hbar} \left( \frac{\partial H}{\partial \lambda_i} \right)^2 + \frac{4\mu_\delta}{3\hbar} \left( \frac{\partial H}{\partial \delta_i} \right)^2 \right] .$$

$$\leq 0$$

(27)

(28)

(29)

All the nucleon wave-packets obeying Eq. 26 stop their motions at the energy-minimum state,

$$\dot{\mathbf{R}}_i = 0 , \quad \dot{\mathbf{P}}_i = 0 ,$$

$$\dot{\lambda}_i = 0 , \quad \dot{\delta}_i = 0 ,$$

(30)

while in the standard QMD model nucleons are moving around in the ground-states. Fermi motions are shared by the momentum variance of wave-packets and the non-zero values of momenta $\mathbf{P}_i$ which come from the momentum-dependence of Pauli potential.

**A. Mass number dependence of the binding energy**

The binding energy of a nucleus in the present framework is obtained from the minimum-energy condition for the ground state, while in the standard QMD framework it is only an input to fit the empirical value. Our interest is therefore how well the calculated values reproduce the experimental data. Figure 2 shows the comparison of binding energy per nucleon $E_{\text{bind}}$ of our calculation and the experimental value.

With interaction parameter set 1 which guarantees the infinite matter properties, we can reasonably reproduce the binding energies of finite systems shown with circles in Fig. 2. With parameter set 2 (shown with triangles in Fig. 2) which uses the standard value of Skyrme interaction without considering the matter properties, we can reproduce the binding energy of nucleus almost perfectly.

**B. Some typical features of individual nuclei**

The shapes and density distributions of ground states are also well reproduced. In the case of light nuclei, e.g., $^{12}$C, we can reproduce the alpha-clustering structures as displayed in Fig. 3. On the left are shown the radial density distribution (upper) and distribution of the real parts of nucleon wave-packet widths (lower) and on the right is shown the contour plot of density. This $^{12}$C nucleus is calculated with parameter set 2 and has the binding energy of 92.7 MeV and the rms radius of 2.31 fm which agree to the experimental values (92.2 MeV and 2.46 fm). By using interaction parameter set 1, we can also make a very similar ground state of $^{12}$C except for the binding energy. This three-alpha structure
FIG. 2. Binding energies per nucleon of ground state nuclei. Circles and triangles denote our model with parameter set 1 and 2, crosses denote corresponding experimental values. Of $^{12}\text{C}$ is almost the same as those obtained in AMD [7] and FMD [8]. This gives a support of introducing the Pauli potential as a phenomenological substitute of anti-symmetrization.

For heavy nuclei, the density profiles is shown in the upper parts of Fig. 4. We see that the general feature of the density and the surface thickness are well reproduced in our calculations. The value of density, however, is somewhat higher than normal matter density. This is one of the problems of our model which makes the size of nuclei and therefore the reaction cross section slightly smaller than the data. We guess one reason is the Pauli principle is not perfectly realized in the ground nuclei since the Pauli potential we are using is rather moderate. One can see this fact in the Fig. 1 at low temperature where our system is slightly deviating from the Fermi gas.

The lower parts of Fig. 4 shows the distribution of the real parts of nucleon wave-packet widths. The absicssas represent the distance of the wave packet from the center. Wave packets near the center are spatially more spread than those near the surface. Note that this fact does not mean the kinetic-energy density is higher at the surface since the density and the imaginary part of the width also contribute to the kinetic-energy density. In fact we obtain the kinetic-energy density distribution higher at the center and lower at the surface of a nucleus. A narrow width for a surface nucleon is required because otherwise the surface diffuseness becomes unrealistically large. A wide width for a central nucleon is also expected because our model predicts naturally a kind of matter limit (large width limit) for the nucleon sitting in the central part of the nucleus of large mass limit.
FIG. 3. Radial distribution (upper-left), the contour plot (upper-right) of density and the real part of the Gaussian widths (lower part) of the ground states of $^{12}$C. Interaction parameter set 2 is used.

FIG. 4. Density distribution (upper parts) and Gaussian widths (lower parts) of the ground states of $^{93}$Nb and $^{197}$Au. Abscissas for both denote the distance from the center. Interaction parameter set 2 is used.
IV. NUCLEUS-NUCLEUS COLLISIONS

We apply our model to nucleus-nucleus collisions in this section. In the calculation of nuclear reactions we boost two initial nuclei according to the incident energy and then solve the EQMD equation of motion together with the two-body collision term as in the standard QMD. For all the fragments produced, their statistical decay processes to the final products are calculated. Typically, within a time-scale of about 100 fm/c the dynamical part of nuclear reaction is completed, and is followed by the statistical decay process for a time-scale of several-order longer. Since it is not practical nor reliable to treat this statistical process in a framework of simulation, we adopt the standard statistical model for the latter process. With this hybrid model of QMD plus statistical decay calculation, we can calculate observables such as the mass distribution and the energy spectra of fragments.

A. Fragment mass distribution in the medium energy collisions

Figure 5 shows our calculation of fragment production cross sections in the $^{12}\text{C} + ^{12}\text{C}$ (29 MeV/nucleon) reaction compared with the standard QMD (QMDstd) and AMD. The AMD results reproduce the experimental data well especially for light fragments. Solid lines show the final fragment distribution after the statistical decay calculation while dashed lines show fragments produced in the dynamical process before the statistical decay.

Though the final results of three models are quite similar, there are some differences between them before the statistical decay. Especially, AMD and QMDstd apparently differ with each other: In the AMD result, enhancement of $A_f = 4$ and 8 ($N$ alpha fragments) is seen while there is no peak at $4N$ in the QMDstd result. This is mainly because AMD can describe three-alpha structure of $^{12}\text{C}$ while QMDstd can not. There exist peaks at $A_f = 4$ in the present results of EQMD with parameter sets 1 and 2. Dynamical emissions of alpha clusters are enhanced due to the improvement of ground states in our model.

To see the effect of dynamical treatment of wave-packet width, we compare in Fig. 6 the full EQMD calculation with that of fixed-width constraint for the same quantity as Fig. 5. In the fixed width calculation we solve the equation of motion only for $R_i$ and $P_i$ keeping the widths $\nu_i \equiv \lambda_i^{-1} + i\delta_i$ as constants (6A-dimensional calculation) using exactly the same interactions and the initial conditions as in the full EQMD. Thus this calculation also differs from the QMDstd. With fixed wave-packet widths, the distribution of dynamically produced fragments has strong peaks at $A_f = 4N$ and productions of other fragments and nucleons are rather hindered. Underestimation of nucleon yield is seen even after the statistical decay. For the description of nucleon emission process, the dynamical treatment of wave-packet widths is essential in the QMD calculation.

B. Fusion cross section of $^{16}\text{O} + ^{16}\text{O}$ reaction

We examine our model in the case of the $^{16}\text{O} + ^{16}\text{O}$ fusion reaction. The same reaction has been calculated by the standard QMD model in Ref. [8]. It was found there that if one admits events of up to three nucleons escape into the fusion events, fusion cross section is nicely reproduced by the standard QMD model. If one demands no nucleon emission,
FIG. 5. Fragment mass distribution in $^{12}\text{C} + ^{12}\text{C}$ (29 MeV/nucleon) reaction calculated with standard QMD, AMD and EQMD with parameter sets 1 and 2. Dashed lines denote fragments produced in dynamical process before statistical decay calculation, while solid lines denote final fragments after statistical decay.

FIG. 6. Fragment mass distribution in $^{12}\text{C} + ^{12}\text{C}$ (29 MeV/nucleon) reaction. Dashed lines denote fragments produced in dynamical process before statistical decay calculation, while solid lines denote final fragments after statistical decay.
FIG. 7. Fusion cross section for $^{16}\text{O} + ^{16}\text{O}$ reaction. Crosses denote experimental data from Refs. [17,18]. The full circles and full triangles denote our results of full EQMD calculation with parameter set 1 and 2, respectively. Open circles and open triangles denote the results of EQMD calculation with constraint of fixed wave-packet widths.

However, the calculated fusion cross section is almost zero. In the present calculation, we demand that in the fusion event there is no nucleon/fragment emission within a certain time (in this paper we have chosen 450 fm/c after the contact of two nuclei). Classification of nucleons into fragments is done by the condition that nucleons within the distance of 3.0 fm belong to the same fragment. Since we judge the fusion events at finite time, we don’t calculate the statistical decay process in this case. This calculation corresponds to a complete fusion reaction, and such exclusive calculation is possible in EQMD owing to the fact that EQMD ground state is stable enough so that no spurious particle emission happens.

The fusion cross section is obtained by calculating the fusion probabilities for impact parameters of 0.0, 3.0, 4.0, 5.0, 5.5 and 6.0 fm by simulating 40 events for each impact parameter. In Fig. 7 we show the incident-energy dependence of the fusion cross section. Crosses denote experimental data from Refs. [17,18] and full circles and triangles denote our calculation with parameter sets 1 and 2. There is no significant difference between the results with two parameter sets. They reproduce about 85 % of experimental data but somewhat underestimate them. The ground state of $^{16}\text{O}$ we have used has the binding energy of 130.8 MeV and the rms radius of 2.5 fm which is about 92 % of the experimental value 2.73 fm [14]. We guess the small size of $^{16}\text{O}$ causes this underestimation of fusion cross section. Though we can not, at present, reproduce perfectly the fusion cross section, one should remember that we get almost zero fusion cross section with the standard QMD by using the same criterion of fusion event.

We discuss again the effect of dynamical treatment of wave-packet width by comparing the full calculation with that of fixed width constraint as in the previous section. In the
fixed width calculation, the initial condition and interaction is exactly the same as in the full EQMD calculation. As shown with open circles and triangles in Fig. 7, the fusion cross sections with fixed width calculation are close to the full calculation in low-energy region and are much smaller for higher incident energies. At very low energies, two nuclei can easily fuse if they overcome the fusion barrier. At higher energies, however, the dissipation of the incident energy into the internal excitation is necessary. The dynamical change of wave-packet widths offers larger degree of freedom for the dissipation than the case of fixed width. Thus the dynamical treatment of wave-packet width plays much important roles rather at higher energies where dissipation of the incident energy is important for the fusion process.

V. SUMMARY

In this paper we have discussed how to treat low-energy reactions in the framework of quantum molecular dynamics (QMD). We have introduced a phenomenological Pauli potential into effective interactions and have made the width of each wave packet as a dynamical variable. With this extended QMD (EQMD) method, we can well describe the ground state properties such as binding energies, density profiles or alpha-clustering structure in light nuclei.

In the calculation, we have introduced two sets of interaction parameters. Set 1 is obtained by adjusting the nuclear potential by keeping the matter saturation properties which depends both on Pauli potential and on the nuclear potential. Set 2 is obtained by the standard parameterization of nuclear potential and the Pauli potential is searched to give a good agreement to the systematic trend of binding energies of finite systems. With the latter parameter set, we can reproduce the binding energies of nuclei almost completely from very light to very heavy systems. As for the nucleus-nucleus collisions, however, we did not see any significant difference between different interaction parameter sets.

The width of Gaussian wave-packets, which are taken as a constant of arbitrary value in standard QMD, were determined from the minimum energy condition for the ground state. We showed that for $^{12}$C, the real parts of the widths become identical for whole 12 nucleons and a clear alpha structure appears where 3 alphas are located at the vertices of equilateral triangle. For medium and heavy nuclei the real parts of the width show a systematic distribution; wider widths in the central region and narrower ones near the surface, which was first obtained with this work. Remaining problems to be solved are somewhat higher matter density near the center and somewhat smaller root mean square radius.

In the calculation of nucleus-nucleus collisions, we showed that EQMD is able to enhance the dynamical alpha emission process. This enhancement was seen in AMD calculation but not in the standard QMD.

The effect of the dynamical change of the widths of wave-packets were clearly seen in two points: One is nucleon emission or disintegration of clusters in medium energy collisions. With the dynamical change of Gaussian widths, nucleons can escape easily from the cluster. If we freeze the widths, dynamical emission of nucleons is much hindered. The other is the fusion reaction where dissipation of the incident energy become essential. We showed that the change of widths for fusion of $^{16}$O + $^{16}$O causes a big enhancement of the cross section at
higher incident energies. Without this freedom, the EQMD model gives unphysically small fusion cross section.

The study of EQMD in this paper showed that this is a promising direction to generalize the QMD simulations. The systematic calculation of EQMD, however, is now in a beginning stage. We need further calculations to clarify the basic features of this model. One of the most interesting item to study with EQMD calculation is the low energy reactions between heavy nuclei, because no other many-body model has been successfully applied to it. The study in this direction is in progress.

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