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Role of wave packet width in quantum molecular dynamics in fusion reactions near barrier

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Abstract. The dynamical fusion process of \textsuperscript{48}Ca + \textsuperscript{144}Sm with different impact parameters near barrier is studied by an extended quantum molecular dynamics (EQMD) model, where width of wavepacket is dynamically treated based on variational principle. The time evolution of different energy components such as potential energy, kinetic energy, Coulomb energy and Pauli potential are analyzed when dynamical or fixed width is assumed in calculation. It is found that the dynamical wavepacket width can enhance the dissipation of incident energy and the fluctuations, which are important to form compound nuclei. Moreover, we compare the fusion barrier dependence on the incident energy when it is determined by both dynamical and fixed wavepacket width.

1. Introduction

The use of dynamical process is important in order to understand the formation of complete fusion in a heavy ion reaction. In experiment, it is hard to correctly determine the compound nucleus cross section in massive nucleus reactions since it is difficult to unambiguously identify the complete fusion products from quasifission fragments [1–5]. The determination of superheavy nuclei (SHN) cross section is overestimated if the fusion-fission products from compound nuclei strongly overlap with the one of quasifission process. Therefore it is highly needed to study the quasifission and fusion-fission dynamics and how the nuclear system evolves from the capture forming the dinuclear system to statistically equilibrated compound nucleus (CN).

In the last decades, in some almost mass symmetric reaction (namely “cold fusion reaction”) were used to synthesize some superheavy elements (SHEs) with atomic numbers from 107 to 112, by using double magic target nuclei such as \textsuperscript{208}Pb, \textsuperscript{209}Bi, and projectile nuclei heavier than \textsuperscript{40}Ar [6]. For heavier SHEs, mass asymmetric reactions (namely “hot fusion reaction”) were used to synthesize elements with Z up to 118, by using \textsuperscript{48}Ca as beam and actinide nuclei as targets [7].
However, to go beyond \( Z = 118 \), there are not results for \( Z = 119 \) and \( Z = 120 \) elements by using reactions such as like \(^{50}\)Ti, \(^{54}\)Cr, \(^{58}\)Fe and \(^{64}\)Ni (as beams) + Actinides (as targets) \([8]\). Furthermore, all synthesized transfermium nuclei are neutron-deficient, lying above the \( \beta \) stability line. Therefore, new reaction mechanisms and methods are mandatory for exploring neutron rich superheavy nuclei in north-east direction. Alternative reaction mechanisms –such as fusion with radioactive neutron-rich projectile, transfer reactions in damped collisions with very heavy projectile and target nuclei– are very promising to access neutron-rich side and superheavy nuclei beyond \( Z = 118 \).

The macroscopic liquid and dinuclear models are widely used in fusion reactions near barrier. However, for damped collisions with massive nuclei, a large number of degrees of freedom related to the excitation and deformed projectile and target nuclei, the neck formation, nucleon transfer, different types of re-separation of the composite system and nucleon emission, will simultaneously play relevant roles. Therefore, it is difficult to have a realistic description of the dynamical process.

The microscopic dynamic approaches, such as time-dependent Hartree-Fock (TDHF) \([9]\) and quantum molecular dynamics (QMD) \([10,11]\) have been used to consider the full dynamical degrees of freedom highly needed to determine the fusion reaction with massive nuclei. For TDHF and QMD, the calculations are fully microscopic, without assuming any reaction mechanism and cluster formation in advance. It is found that the dynamical conditions produce apparent effects on a series of processes such as barrier distribution, pre-equilibrium collective motion, nucleons transfer, dynamical deformation and equilibration of the shape etc..

TDHF is essentially one-body theory, where the fluctuation and correlation are not treated sufficiently and explicitly. QMD is based on many-body theory and it can link the simulation to experimental observables. In comparison with TDHF, the QMD model can also be used at higher energies besides around barrier. The recent Langevin dynamics + quantum molecular dynamics calculations show that the non-Gaussian random forces play a very important role in the dissipation dynamics of the relative motion between target and projectile nuclei \([12]\). However, the wavepacket width is treated as fixed and uniform for every nucleon in QMD-like models \([13–15]\) except that the extended quantum molecular dynamics (EQMD) \([16,17]\), fermionic molecular dynamics (FMD) \([18]\) and one generalization of Gaussian trial wave functions in quantum molecular dynamics \([20]\). The dynamical width provides the nonclassical degree of freedom and it is expected to compensate some important quantum effects, which is insufficiently considered in the traditional QMD model. In this paper, the fusion process of \(^{48}\)Ca + \(^{144}\)Sm near barrier is studied by the EQMD model. The role of how dynamical width of wavepacket affects the energy dissipation of incident energy is carefully checked by comparing with the case of fixed and uniform wavepacket.
2. Model and approach

In the present paper, we use a microscopic transport dynamics model, EQMD, to simulate the time evolution of nuclear phase-space. This model was presented by Maruyama [16], and also used in [17]. In addition to advantage of dynamical wavepacket width, this model has a much better conversion of energy and enough long stability for initialized ground nucleus. It can also well describe the ground properties of nuclei through the periodic table. Therefore, it is very suitable to study low energy fusion reactions. A brief introduction of EQMD model is shown as following.

In the EQMD model, the total wave function of the nuclear system was assumed as a product of Gaussian wave packets of all nucleons

\[ \Psi = \prod_i \phi_i(\mathbf{r}_i), \]

where

\[ \phi_i(\mathbf{r}_i) = \left( \frac{\nu_i + \nu_i^*}{2\pi} \right)^{3/4} \exp \left[ -\frac{\nu_i}{2} (\mathbf{r}_i - \mathbf{R}_i)^2 + \frac{i}{\hbar} \mathbf{P}_i \cdot \mathbf{r}_i \right]. \]

Here \( \mathbf{R}_i \) and \( \mathbf{P}_i \) are the centers of position and momentum of the \( i \)th wavepacket. \( \nu_i \) is the Gaussian width written as

\[ \nu_i \equiv \frac{1}{\lambda_i} + i\delta_i, \]

where \( \lambda_i \) and \( \delta_i \) are its real and imaginary parts, respectively. The Hamiltonian is written as

\[ H = \left\langle \Psi \left| \sum_i -\frac{\hbar^2}{2m} \nabla_i^2 - \hat{T}_{c.m.} + \hat{H}_{int} \right| \Psi \right\rangle \]

\[ = \sum_i \left[ \frac{\mathbf{P}_i^2}{2m} + \frac{3\hbar^2}{2m} (1 + \lambda_i^2\delta_i^2) \right] - \hat{T}_{c.m.} + H_{int}, \]

where \( \hat{T}_{c.m.} \) and \( H_{int} \) denote the spurious zero-point center-of-mass (CM) kinetic energy and the potential energy term, respectively. For the effective interaction, this model uses Skyrme, Coulomb, symmetry, and the Pauli potential

\[ H_{int} = H_{Skyrme} + H_{Coulomb} + H_{symmetry} + H_{Pauli}. \]

Specifically, the Pauli potential is written as

\[ H_{Pauli} = \frac{c_P}{2} \sum_i (f_i - f_0)^2 \theta(f_i - f_0), \]

\[ f_i \equiv \sum_j \delta(S_i, S_j)\delta(T_i, T_j) |< \phi_i | \phi_j > |^2, \]

where \( f_i \) is the overlap of a nucleon \( i \) with the same kind of nucleons (including itself), \( c_P \) is the strength of the potential and \( f_0 \) is the threshold parameter \( \sim 1 \). \( S \) and \( T \) denote spin and isospin of a nucleon, respectively.
The phase-space is obtained firstly from a random configuration. To get the energy-minimum states as initial ground state, one can solve the damped equations of motion as

\[
\dot{R}_i = \frac{\partial H}{\partial P_i} + \mu_R \frac{\partial H}{\partial R_i}, \quad \dot{P}_i = \frac{\partial H}{\partial R_i} + \mu_P \frac{\partial H}{\partial P_i},
\]

(9)

\[
3\hbar^2 \dot{\lambda}_i = -\frac{\partial H}{\partial \delta_i} + \mu_\lambda \frac{\partial H}{\partial \lambda_i}, \quad 3\hbar^2 \dot{\delta}_i = \frac{\partial H}{\partial \lambda_i} + \mu_\delta \frac{\partial H}{\partial \delta_i}.
\]

Here \(\mu_R, \mu_P, \mu_\lambda,\) and \(\mu_\delta\) are damping coefficients. After this cooling process, the system goes to its energy minimum point. For free evolution of coordinate, momentum and corresponding widths in reaction, \(\mu_R, \mu_P, \mu_\lambda,\) and \(\mu_\delta\) are set to zero.

The proper initialization of target and projectile nuclei are necessary to describe reasonably the reactions. Especially for fusion near barrier, one of the necessary conditions, which must be satisfied, is that the stability of initialized nuclei has to be taken for enough time and at meantime no spurious nucleon and cluster emission occur, in comparison with the time scale of fusion dynamical process. The stability checks: binding energy and root mean square (RMS) radius vs evolution time are shown in Fig. 1 (a) and (b), respectively. The binding energy of initialized \(^{48}\text{Ca}\) and \(^{144}\text{Sm}\) is 8.305 MeV and 7.659 MeV, respectively, which are near the experimental binding energy: 8.667 MeV and 8.304 MeV [19], respectively, for \(^{48}\text{Ca}\) and \(^{144}\text{Sm}\). These good initialized samples are stored for fusion simulations. The fluctuation of binding energy and RMS radius are more than one order smaller compared with many other version QMD models, where fluctuation of binding energy and RMS radius can be as large as 0.15 MeV/u and 0.3 fm, respectively, for the best initialized nucleus such as \(^{144}\text{Sm}\). The small enough and negligible energy fluctuation is very important for fusion with massive nuclei at very low energy since a fraction fluctuation of binding energy per nucleon will bring a big enough total energy fluctuation into the fusion system, compared with the incident energy.

![Figure 1](image1.png)

**Figure 1.** (Color online). (a) The examination of the average binding energy for initialized \(^{48}\text{Ca}\) and \(^{144}\text{Sm}\) versus the evolution time; (b) The examination of the root mean square radius for initialized \(^{48}\text{Ca}\) and \(^{144}\text{Sm}\) vs the evolution time.
3. Results and discussion

One of the distinct features in our fusion calculations is the dynamical evolution of the wavepacket width. The dynamical evolution of one wavepacket width in $^{48}$Ca + $^{144}$Sm with CM frame energy 180 MeV is shown in Figure 2. Large fluctuations can be seen clearly, which has not been considered in fusion reaction before. The average width increases till 1400 fm/$c$ and then saturates even if large fluctuations are present. The rise of average width corresponds to the early stage of projectile-target touching. In later stage, the larger width is due to the compound system formation, and to the nucleon diffusion between the projectile and target contact region. The momentum width largely fluctuates. However, it is perfectly anti correlated with the coordinate width. The product of them well satisfies the uncertainty principle shown by the green dotted line in Figure 2. The lines in Figure 2 show that the width evolutions are reasonable and reliable in our calculations.

In Figure 3, the functions of dynamical width of wavepacket can be clearly seen through the time evolution of the dynamical nucleus-nucleus interaction potential in comparison with fixed wavepacket calculations. The nucleus-nucleus interaction potential is defined as

$$V(R) = E_{tot} - E_{tar}(R) - E_{proj}(R),$$

where $R$ is relative distance between centers of mass of target and projectile, and $E_{tot}$, $E_{tar}(R)$, and $E_{proj}(R)$ represent the total energy of the system, target, and projectile, respectively; they can be calculated from the energy density function. Each of them includes kinetic energy as well as all potential energy components as reported in equation (6). From panel (a) we can see that the dynamical width leads to a more faster fusion process and a more deeper binding between target and projectile, in comparison with the fixed width. However, there is no much difference for these two cases when the distance
between target and projectile is larger than 10 fm, as shown in panel (b) of Figure 3. After the touching point, a large difference emerges between the two approaches. The nucleus-nucleus potential becomes more soft due to the fact that the dynamical width plays an important role of additional degree of freedom. Therefore, it should be easier and quicker to reach equilibrium for energy, shape, isospin, etc. when the dynamical width is considered.

![Figure 3](image-url)

**Figure 3.** (Color online). (a) Potential between target and projectile for fixed and dynamical wavepacket width in the process of approaching as a function of the evolution time in the $^{48}\text{Ca} + ^{144}\text{Sm}$ head-on fusion with 180 MeV CM energy; (b) The same as (a) but for dependence of distance between target and projectile.

In order to clarify the energy dissipation process before equilibrium, the total potential energy, total kinetic energy, Coulomb energy of projectile and Pauli potential of target and projectile as functions of the distance between target and projectile, are shown in panels (a), (b), (c), (d), and (e) of Figure 4, respectively. The anti correlation between potential energy and kinetic energy is described well since EQMD keeps energy conservation with a very good accuracy. Projectile with dynamical width has larger Coulomb energy than the one with fixed width at short distance, since the former has more compact shape when the target and projectile merge together. At the path of approaching, the Coulomb energy does not have apparent difference. However, for Pauli potential, the case is different. Pauli potential from target anti correlates strongly with projectile for dynamical width, which is based on the fact that the Pauli potential is calculated from overlap between wave packets shown by equation (7) and (8). From Liouville theorem, we know that the total size of phase space of system is constant. Therefore, more larger overlap between nucleons in target, more smaller overlap in projectile, and vice versa. The Coulomb and Pauli potential play dominant roles on the dynamical nucleus-nucleus potential at large distance. They both push the target and projectile to adjust their density distributions in the approaching process.

The dependence of the potential evolution on different impact parameter is calculated, as shown in Figure 5. From panel (a) we can see that the speed of energy dissipation in head-on collisions is not the fastest compared with all other cases. Fusion with impact parameter around 2 fm evolves fastest towards equilibrium.
Figure 4. (Color online). Total potential energy, total kinetic energy in CM frame, Coulomb energy of projectile, Pauli potential of target and projectile in $^{48}$Ca + $^{144}$Sm fusion with 180MeV CM energy head-on collision as functions of distance between target and projectile are shown by (a), (b), (c), (d) and (e), respectively, where the calculations with fixed and dynamical wavepacket width are compared in each figures.

For impact parameters larger than 4 fm, obviously a longer time is needed to reach equilibrium. Panel (b) shows that the evolution path with larger impact parameters is more complicated with walking back.

Figure 5. (Color online). Potential between target and projectile with dynamical width in $^{48}$Ca + $^{144}$Sm fusion with 180MeV CM energy as a function of evolution time and distance between target and projectile are shown by (a) and (b), respectively, where the calculations with different impact parameters are compared in each figures.
The energy dependence of the fusion barrier is extracted from head-on collisions for both dynamic and fixed wavepacket width shown in Figure 6. The barrier decreases with the decrease of incident energy in the two different calculations. However, the dynamical wavepacket width reduces the barrier height a lot, which is based on the fact that dynamical wavepacket width, acting as another additional degree of freedom, allows the approaching target and projectile to adjust their densities quickly. This should be very different from the nucleus-nucleus barrier extracted from frozen approximation.

![Figure 6.](image)

**Figure 6.** (Color online). Fusion barrier from $^{48}$Ca + $^{144}$Sm head-on fusion as a function of incident energy in CM frame, where the fixed wavepacket width is calculated with two incident energies.

4. Summary

The role of the dynamical width of wavepacket is studied in the $^{48}$Ca + $^{144}$Sm fusion reaction near barrier energy by the EQMD model. In comparison with the fixed width (widely used before), the dynamical wavepacket width, as additional degree of freedom which before was scarcely considered in the QMD model, can enhance the fluctuation and accelerate the incident energy dissipation in the target-projectile approaching process. As a result, the fusion barrier is strongly reduced and it is easier to run towards equilibrium in calculations with dynamical width.

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