Rotational and Vibrational Excitations of Colliding Nuclei in a Three-Stage Classical Molecular Dynamics Simulation

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Introduction

For nuclei with significant static deformation the reorientation of the deformed nucleus plays a key role in near-barrier collisions [1-3]. Using a ***C**lassical **R**igid **B**ody **D**ynamics* (CRBD) model for ^{24}Mg + ^{208}Pb system it is shown [2] that due to the Coulomb reorientation of the deformed nucleus, the isotropy of the initial orientations is modified. It is also shown that the extent of reorientation of the deformed nucleus depends not only on the initial orientation of the axis of symmetry of the deformed nucleus but it also depends strongly on the collision energy.

Due to the rigid-body constraint in the CRBD-model the two colliding nuclei, however, can not come very close together and the transfer of energy from the relative motion to internal excitation is explicitly neglected. This leads to no bound state formation of the two colliding nuclei in most of the cases. In such cases, however, passing over the barrier is assumed to be resulting in fusion. Fusion cross sections are calculated using the Wong's formula with energy and orientation dependent barrier parameters [3].

It is desirable that fusion cross section calculations must take into account subsequent capture of the two nuclei in a potential well behind the fusion barrier. This in-effect can modify the curvature of the barrier (ω_B) even if the barrier-height (V_B) and barrier-radius (R_B) may not get modified substantially. Modification of ω_B can also affect fusion cross sections.

In ***C**lassical **M**olecular **D**ynamics* (CMD) approach [4], on the other hand, all the degrees of freedom are explicitly included through the classical equations of motion for all the nucleons. Thus, allowing for the transfer of energy between the relative motion and the intrinsic degrees of freedom. When the two nuclei cross over the barrier, due to dissipation of energy from the relative motion, the two excited nuclei can get trapped in a well or a pocket behind the fusion barrier resulting in a bound or a fused system. In ref. [5] such an approach was used to calculate fusion cross sections for ^{24}Mg + ^{208}Pb system.

Because of the importance of the long-rage reorientation effect, the CRBD calculations are initiated at large initial separation of R_{cm} = 2500 fm. However, initiation of CMD at such distances (as in ref. [5] also) results in large computational time and accumulation of numerical errors. Therefore, in the present paper we propose a ***3**-**S**tage **C**lassical **M**olecular **D**ynamics* (3S-CMD) model for simulation of heavy-ion collisions. We present some initial simulation results which overcome the above problems and also explicitly take into account the long-rage reorientation effect.

Calculation Details

Heavy-ion collision simulation in the present classical approach (3S-CMD) is carried out in the following three-stages:

(1) **Rutherford Trajectory Calculation:** The two nuclei, assumed to be charged point particles, are brought along their Rutherford trajectories [4] with given collision energy (E_{cm}) and impact parameter (b) up to R_{cm} = 2500 fm.

(2) **CRBD model Calculation:** The two nuclei, assumed to be rigid bodies with their ground state configuration of nucleon positions, are then allowed to evolve further using the CRBD-model[2] by solving translational and rotational equations of motion for their centre of mass and the orientation angles of the their principal axes. The CRBD calculation is continued up to a relatively small separation of R_{cm}= 50 fm.

(3) **CMD Calculation:** The RB constraints are relaxed at about R_{cm}= 50 fm and trajectories of all the participating nucleons are computed using the coupled Newton's equations of motion for all the particles in a CMD approach [4].

Results & Discussions

Classical simulation of ^{24}Mg + ^{208}Pb system using 3S-CMD model described above is carried out. For comparison the CRBD model and CMD calculation are also carried out. The ground state configurations of ^{24}Mg and ^{208}Pb from ref. [2] are "hot" [6] and are dynamically "cooled" [4, 6] further, to remove all the initial internal excitations in order to explicitly look for internal excitations appearing due to the interaction of the colliding nuclei. All the simulations are for the same given arbitrary initial orientation of the two nuclei at b=0 and E_{cm}=120 MeV.

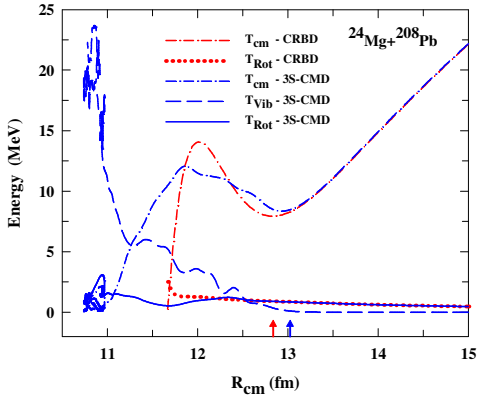

Fig.1 T_{cm}, T_{vib} & T_{rot} of ^{24}Mg+^{208}Pb in CRBD and 3S-CMD calculations. Arrows indicate location of the corresponding barrier top (fig.-2).

The total rotational energy (T_{rot}), total internal vibration excitation energy (T_{vib}), and total energy of the centre of masses (T_{cm}) at distances close to the barrier are shown in Fig.-1. This fig also shows T_{rot} and T_{cm} calculated in CRBD model. The two calculations of T_{rot} and T_{cm} match well with each other up to distances very close to the barrier top; thus justifying the use of CRBD model as 2nd stage in the 3S-CMD model. After crossing the barrier top, T_{vib} rapidly increases, draining the energy from the cm motion (T_{cm}) and resulting in a bound system.

The ion-ion potential near the barrier-top for 3S-CMD calculation and the CRBD model calculation are compared in Fig.-2. It is clear that the inside of the barrier is significantly modified by the CMD stage of 3S-CMD. For comparison, this fig. also shows CMD calculation initiated at R_{cm}= 50 fm with the same initial orientation but without any CRBD calculation stage (Rutherford trajectories are continued till this distance). This calculation does not match well with CRBD calculation or the 3S-CMD calculation.

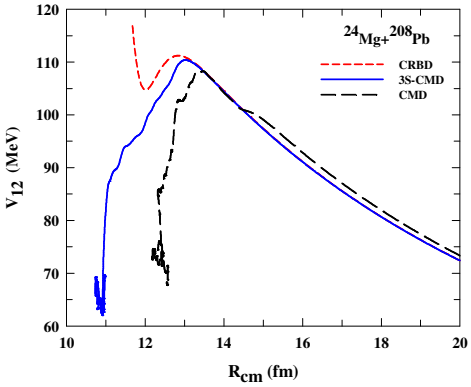

Fig.2 Ion-ion potential of ^{24}Mg+^{208}Pb for CRBD, 3S-CMD, and CMD calculations.

Conclusions

Since the rotational excitation or the reorientation effect is a long-range effect and the vibrational excitations take place only close to the barrier or inside of it, the three stage 3S-CMD model combining the CRBD calculation and the CMD calculation seamlessly in a single calculation is a very efficient and useful approach. It combines the benefits of both the approaches. It is also better than using the CRBD approach or the CMD approach alone. Detailed fusion cross section calculations are underway and will be presented.

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