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Microscopic Calculations of Low-Energy Fission within the Constrained Molecular Dynamics (CoMD) Model: Preliminary Results

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Abstract

The investigation of the mechanism of nuclear fission is a topic of current experimental and theoretical interest. In this work, we initiated a systematic study of low and intermediate energy fission calculations using the Constrained Molecular Dynamics (CoMD) code. The code implements an effective interaction with a soft isoscalar part and with several forms of the density dependence of the nucleon symmetry potential. In addition, CoMD imposes a constraint in the phase space occupation for each nucleon restoring the Pauli principle at each time step of the evolution of the nuclear system. In this work, we present results for the reactions p (27 MeV) + 232 Th and p (63 MeV) + 232 Th and compare them with recent experimental data. It appears that the CoMD code is able to describe the complicated many-body dynamics of the fission process especially for the higher-energy fission reaction. Proper adjustment of the parameters of the effective interaction and further improvements of the code are necessary to achieve a satisfactory quantitative description of low-energy fission where shell effects play a definitive role.

The microscopic description of the mechanism of nuclear fission is a topic of intense nuclear research. Understanding of nuclear fission, apart from the theoretical many-body point of view, is of practical importance for energy generation, isotope production, as well as for the transmutation of nuclear waste. Furthermore, nuclear fission is essentially the process that defines the upper limit of the periodic table of the elements and plays a vital role in the production of heavy elements via the astrophysical r-process.

Motivated by the present state of affairs regarding fission research, we initiated a systematic study of low and intermediate energy fission using the Constrained Molecular Dynamics (CoMD) code of A. Bonasera and M. Papa [1, 2]. The code implements an effective interaction with a nuclear-matter compressibility of K=200 (soft EOS) with several forms of the density dependence of the nucleon symmetry potential. In addition, CoMD imposes a constraint in the phase space occupation for each nucleon, restoring the Pauli principle at each time step of the collision. Proper choice of the surface parameter of the effective interaction has been made to describe fission.

In the calculations of the present work, the CoMD code was used with its standard parameters. A symmetry potential proportional to the nuclear density was chosen and the surface term of the potential was set to zero. For a given reaction, a total of approximately 5000 events were collected. For each event, the impact parameter of the collision was chosen in the range $b = 0-6$ fm, following a triangular distribution. Each event was followed up to 15000 fm/c and the phase space coordinates were registered every 50 fm/c. At each time step, fragments were recognized and their properties were reported. Thus, information on the evolution of the fissioning system and the properties of the resulting fission fragments were obtained.

In this presentation, we discuss preliminary results of fission for the reactions p $(27 \text{ MeV}) + {}^{232}\text{Th}$ and $p (63 \text{ MeV}) + {}^{232}\text{Th}$. The calculated mass distributions are compared with the experimental data of [3] in Fig. 1.

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In the experimental data of the reaction p $(27 \text{ MeV}) + {}^{232}\text{Th}$ (full points in Fig. 1a), we observe the asymmentric nature of the fission of ²³²Th. In contrast, the CoMD calculations result in a symmetric distribution with a flat top. The main reason is that the nucleon-nucleon interaction in the CoMD model does not include spin dependence, and thus the resulting mean field potential has no spin-orbit contribution. Consequently, the model cannot reproduce the correct shell effects necessary to describe the asymmetric lowenergy fission of ²³²Th.

When the proton energy increases, it is expected that the shell effects will fade and the fissioning system will preferentially undergo symmetric fission. In Fig. 1b, the mass yields for the same reaction at proton energy 63 MeV is presented. The experimental mass yield becomes more symmetric at this energy and the calculated yield curve is in better agreement with the data.

Figure 1: (Color online) Mass distributions (cross sections) of fission fragments from a) p (27 MeV) + 232 Th and b) p (63 MeV) + 232 Th. Full (grey) points: experimental data [3]. Open points (connected with the full line): CoMD calculations.

From the CoMD calculations to date and comparisons with available data, we see that this microscopic dynamical code is able to describe the many-body dynamics of the fission process. However, further improvements are necessary to achieve a satisfactory quantitative description of the the rich body of available experiment data of low and intermediate energy fission, which is one of the goals of our upcoming work.

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- [2] M. Papa et al, J. Comp. Phys. 208, 403 (2005).
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