POTENTIAL GRADIENT PARAMETRIZATION IN A LANGEVIN TYPE DISSIPATIVE DYNAMICS

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A parametrization of the conservative force in the dynamical coalescence and reseparation model is proposed. This model with one body dissipation formula, Yukawa plus exponential finite range potential, and shell effects included was recently adopted to follow Langevin trajectories for a collision of two very heavy nuclei which can end up as a compound system or reseparate. With our parametrization it is possible to speed up model calculations by a factor of 10 without loosing accuracy of trajectory integration. This can be of some importance in a case of Langevin trajectories calculation where many of them have to be traced in order to estimate probability for a process of interest, namely a fusion of two very heavy nuclei at beam energies close to the Coulomb barrier. Few examples of fusion excitation functions of heavy nuclei calculated with this faster version of the computer code are presented.

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1. Introduction

In recent years a large experimental effort undertaken in the GSI laboratory succeeded in a synthesis of new Superheavy Elements (SHE) with $Z = 110, 111, 112$ [1–3]. All these elements were created by cold fusion of different projectiles with a doubly magic nucleus ^{208}Pb as a target. Measured cross sections for production of an evaporation residue (ER) appeared here to be very small. For $^{278}112$ it is only 1 picobarn. Such cross section is in fact a product of two components: a cross section for formation of a compound nucleus $\sigma_{\rm CN}$ and a probability $P_{\rm ER}$ that the CN will not deexcite into fission channels. The $P_{\rm ER}$ probability can be deduced on a basis of

statistical models where inclusion of a fission barrier and binding energies of individual nucleons enables one to calculate competition between fission and evaporation residue channels [4]. On the other hand theory tells very little on values of σ_{CN} in the range of small collision energies characteristic for cold fusion. Coulomb repulsion in the entrance channel becomes here a serious restriction. After the fusion barrier is crossed structural effects are proved to play very important and even decisive role to prevent the system from disintegrating immediately through one of the fission channels. All the way to the CN the system evolves dynamically and converts its relative kinetic energy into the internal excitation. In the first stage it has to reach the fusion barrier. Where and how along this trajectory a decision is made by the system to fuse, and what is the minimal energy in the entrance channel necessary to cross the fusion barrier is so far not known.

On the microscopic level dynamics is governed by rearrangement of individual nucleons, and from the macroscopic point of view it implies that there is a coupling between collective degrees of freedom and thermal energy of the system, and such a coupling manifests itself as fluctuations of collective variables. It seems that the macroscopic dynamical model of Świątecki [5], and Błocki *et al.* [6], and very recently barrier and fusion probability fluctuations introduced to this model [7] are very well suited for the problem investigated here.

Evolution of the system on its way to fusion is described in a space of shape coordinates, and fluctuations are introduced by random Langevin forces [8]. Trajectories are computed numerically by integration of equations of motion, what consumes usually a lot of computer time. In this paper we propose to parametrize conservative forces, which considerably reduces the computer time.

The paper is organized as follows: in Section 2 we briefly recall main ingredients of the coalescence and reseparation model [6]. Section 3 explains new parametrization proposed for the gradient of the folding potential. Some comparisons with exact conservative force are also given. In this section excitation functions for few cases of interest are calculated with the parametrized version of the model. In Section 4 we conclude and summarize.

2. Dynamical model

In the model, shape of the fusing system is assumed to be axially symmetric and is parametrized by portions of two usually unequal spheres which are smoothly connected by a quadratic surface of revolution. For such shapes a classical collision trajectory is calculated in a space of coordinates: ρ, λ, Δ_A, where the first one gives information on a relative distance of these two spheres, the second one informs on a degree of window (neck) opening be-

tween spheres and the third one is related to asymmetry of these spheres (for exact definition see [9] or [10]). The starting point of each trajectory corresponds to two spheres separated by a distance at which a nuclear attractive force start to be important ($\rho \simeq 1.26$, $\lambda \simeq 0.0$, and Δ_A corresponds to the initial asymmetry in the entrance channel). Dynamics of the trajectory is governed by a conservative driving force which is calculated from the Yukawa plus exponential finite range interaction [11] and the Coulomb interaction, while energy dissipation is assumed as an one body in a form of the wall and wall-plus-window formula [12]. In order to follow dynamics of a collision in a more realistic way another variable, charge asymmetry, Δ_Z, was adopted in the model [8]. This means that the evolution in mass and charge of two colliding nuclei can now be traced independently. Finally, after the authors of Ref. [8], a contribution of shell effects has been added into the potential energy. These effects are especially important at the collision energies very close to the fusion barrier (low excitation energy case), and for closed shell nuclei, as suggested by Myers and Świątecki [13].

In a collision of two heavy ions one observes conversion of an initial relative kinetic energy into internal excitation energy. Due to a coupling between internal and macroscopic degrees of freedom, energy dissipation should be described by a mean frictional force (wall and window formula) and by fluctuating random forces known as Langevin forces [14]. These forces originate from thermal fluctuation effects. Correspondingly, to follow evolution of a system in a collision process, equations of motion of the Langevin type have to be solved [7,8]:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i} - \frac{\partial \Re}{\partial \dot{q}_i} + L_{q_i}(t)\,, \tag{1}$$

where $L = T - V$ is a Lagrangian (kinetic energy minus potential energy, $T-V$), $\Re$ is the Rayleigh dissipation function, and $L_{q_i}(t)$ ($q_i = \rho, \lambda, \Delta_A, \Delta_Z$) are the Langevin forces of a Gaussian type with zero average values. In a simplest case of zero angular momentum, trajectory of a collision is obtained by integrating numerically four equations of type (1).

In the integration procedure we use the Runge–Kutte fourth order method. It is important from the point of view of the computing time to find out which term in Eq. (1) is the most time consuming. It is especially crucial in the case of Langevin equations where in order to answer a question what is the probability of a given process, *e.g.* fusion, one needs to calculate many trajectories, especially at collision energies not too large comparing to the Coulomb barrier. In the space of shape coordinates used here it is not possible to write analytical formulas for the potential energy (three dimensional integral), for the kinetic energy (one dimensional integral), and for the dissipation function (one dimensional integral). That means, that at each point on a trajectory the computer code has to calculate numerically

all these integrals. We have checked that 90% of the processor time is used to compute each of the four components of the conservative force: $-\frac{\partial V}{\partial \rho}$, $-\frac{\partial V}{\partial \lambda}$, $-\frac{\partial V}{\partial \Delta_A}$, $-\frac{\partial V}{\partial \Delta_Z}$. It is so because, there is also no analytical formula for them, and algorithm, which computes these partial derivatives, has to calculate the potential energy 8 times in each time step.

3. Tabularization of the conservative force

To speed up calculations we propose here two methods.

i) The first (hybrid) method.

Each of the potential gradients is a function of four variables, *e.g.* $\partial V/\partial \rho \equiv F_\rho(\rho, \lambda, \Delta_A, \Delta_Z)$, and each of them has to be tabularized separately. We will explain our method on an example of F_ρ. The same will be true for three other gradients. In the first step a grid is created on the plane ρ, λ with a typical dimension 100×100. In each point on the grid F_ρ becomes a function of Δ_A, Δ_Z only. For instance $F_\rho(\rho, \lambda, \Delta_A, \Delta_Z) = f_\rho^{i,j}(\Delta_A, \Delta_Z)$, where indexes i, j denote ρ, λ on the grid, respectively, and Δ_Z, Δ_A are in the range $[-1, 1]$.

In fact, physical Langevin trajectories probe only a small part of the Δ_A, Δ_Z surface. They fluctuate around a line $\Delta_A = \Delta_Z$. Utilizing this fact one can rotate the Δ_A, Δ_Z surface by 45^0 to a set of new coordinates Δ'_A, Δ'_Z. On this new surface it is easy to select this part of the surface only which is interesting from the point of view of calculation (the Langevin trajectories). Now Δ'_A is in range $[-1, 1]$ while Δ'_Z changes from around $-.05$ to 0.05. We gain a lot by parametrizing only this part of the mass asymmetry and charge asymmetry surface which is physically interesting and with such a rotation this part is only one twentieth of the whole Δ_A, Δ_Z surface. Using now the Taylor expansion, we expand the $f_\rho^{i,j}(\Delta'_A, \Delta'_Z)$ function up to the second power in Δ'_Z and to the fourth power in Δ'_A with all mixing terms included. In this expansion we include additionally one term in the third power of Δ'_Z. Expansion is made around a point: $(\Delta'_A, \Delta'_Z) = (0, 0)$. This can be written formally as:

$$\begin{aligned} f_\rho(\Delta'_A, \Delta'_Z) \;=\; & f(0,0) + x_{0,1}\Delta'_Z + x_{0,2}\Delta'^2_Z + x_{0,3}\Delta'^3_Z + x_{1,0}\Delta'_A + x_{1,1}\Delta'_A\Delta'_Z \\ & + x_{1,2}\Delta'_A\Delta'^2_Z + x_{2,0}\Delta'^2_A + x_{2,1}\Delta'^2_A\Delta'_Z + x_{2,2}\Delta'^2_A\Delta'^2_Z + x_{3,0}\Delta'^3_A \\ & + x_{3,1}\Delta'^3_A\Delta'_Z + x_{3,2}\Delta'^3_A\Delta'^2_Z + x_{4,0}\Delta'^4_A + x_{4,1}\Delta'^4_A\Delta'_Z + x_{4,2}\Delta'^4_A\Delta'^2_Z, \end{aligned} \tag{2}$$

where $x_{m,n}$ (15 components) are the corresponding coefficients of the Taylor expansion and we treat them as unknowns. This equation is a linear one in $x_{m,n}$. To solve it, one has to calculate the potential gradient f_ρ for

sixteen points on the Δ'_A, Δ'_Z surface (sixteen not fifteen because there is a free term $f(0,0)$) thus receiving 15 linear equations which are solved with respect to $x_{m,n}$ numerically with a standard method. In such a way each of the gradients was parametrized. Typically, for one gradient $100 \times 100 \times 15$ numbers are necessary (equivalent of 600 Kb of computer memory, what is not so much comparing to the memory available in modern computers) and they are kept as matrices in the code.

Now, with such parametrization we no longer need to calculate three dimensional integrals in each step of integration along the trajectory, in order to compute any of the $\partial V/\partial\rho$, $\partial V/\partial\lambda$, $\partial V/\partial\Delta_A$, $\partial V/\partial\Delta_Z$ gradients. Instead, when a gradient is needed for a given (ρ, λ, Δ_A, Δ_Z) point, *e.g.* $\partial V/\partial\rho$, we locate first such a point on the ρ, λ grid then a linear interpolation is used to obtain corresponding coefficients $x_{m,n}$ of the parametrized gradient $\partial V/\partial\rho$ for a given ρ, λ, and finally by rotating Δ_A, Δ_Z by 45^0 and putting them into equation (2) the necessary gradient is obtained. In the same way all gradients can be calculated. To compare the quality of such parametrization with the originally calculated gradient, $\partial V/\partial\rho$, we have sampled the space (ρ, λ, Δ_A, Δ_Z) in a random way with 2×10^4 points. The result is presented in Fig. 1. For clarity the $\partial V/\partial\rho$ is drawn in six

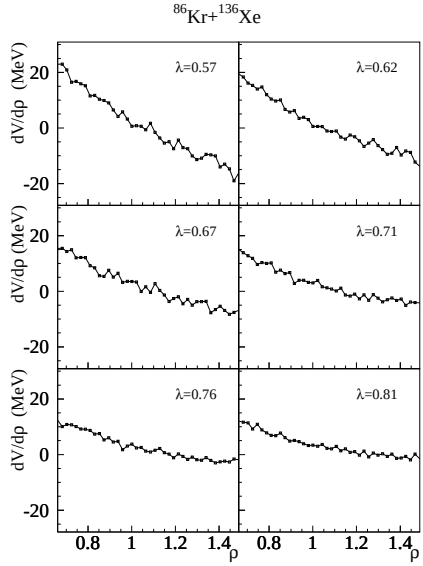

Fig. 1. Comparison, for different values of λ, between exactly calculated potential gradient $\partial V/\partial\rho$ (solid line), and the one calculated with the hybrid method (empty squares). Space $\rho, \lambda, \Delta_A, \Delta_Z$ was randomly sampled, and the grid in ρ, λ was 100×100.

different regions of λ as a function of ρ. Each point is a mean value over the randomly sampled Δ_A, Δ_Z space. As one can see, agreement between the exact gradient (full line), and that obtained from the grid (empty squares) is quite satisfactory.

ii) The second method.

Alternatively one can span the grid over a whole four dimensional space of ρ, λ, Δ'_A, Δ'_Z. For one gradient the grid is $30 \times 30 \times 30 \times 30$, what gives 8.1×10^5 values. They are kept in a matrix which occupies 3.24 Mb of the computer random access memory (RAM). Because there are four gradients one needs 12.96 Mb of RAM. Although in this case the needed amount of computer memory is large, it is still quite easy to have it with present day computers.

To compute in a dynamical calculations *e.g.* the $\partial V/\partial\rho(\rho, \lambda, \Delta'_A, \Delta'_Z)$ gradient the following interpolation procedure is applied. First we search for a position of the $(\rho, \lambda, \Delta'_A, \Delta'_Z)$ point on the grid. Suppose it has been found that $\rho \in [\rho^i, \rho^{i+1}]$, $\lambda \in [\lambda^j, \lambda^{j+1}]$, $\Delta_A \in [\Delta'^k_A, \Delta'^{k+1}_A]$, $\Delta_Z \in [\Delta'^l_Z, \Delta'^{l+1}_Z]$. For ρ^i, and also for ρ^{i+1} one can define a cell: $[\lambda^j, \lambda^{j+1}]$, $[\Delta'^k_A, \Delta'^{k+1}_A]$, $[\Delta'^l_Z, \Delta'^{l+1}_Z]$. For interpolation between points "i" and "i+1" one first make an interpolation inside each cell, and then a linear interpolation between two cells. The same method is applied for all gradients. As in the case of the first (hybrid) method we have sampled randomly the space (ρ, λ, Δ_A, Δ_Z) with 2×10^4 points, and used the same averaging procedure. Result of that test is depicted in Fig. 2 showing also a nice agreement with the gradient calculated in the exact way (using three dimensional integrals).

Using gradient parametrizations described above, we have performed a series of tests applying those gradients to the dynamical model represented by the set of coupled equations (see (1)). This was done in the following way: starting from the same initial conditions, *i.e.* the same system, energy, and angular momentum, dynamics of a collision was followed either using exact potential gradients (three dimensional integrals), or using the first or second grid method. In Fig. 3 two examples of dynamical trajectories are presented, both for central collisions ($L = 0\hbar$): the upper trajectory, leading to fusion, was calculated for the reaction ^{86}Kr+^{136}Xe, at a collision energy $E_L = 4.25$ MeV/u (Lab) and the lower one illustrates the coalescence and reseparation (the scission line is drawn as a dashed one) for the system ^{64}Ni+^{208}Pb at $E_L = 5.25$ MeV/u. Trajectories calculated by the original code are marked as empty squares, the solid line corresponds to the trajectory in which the potential gradient was calculated on the grid and the dotted line corresponds to the trajectory where the conservative force was calculated with a hybrid method. For ^{86}Kr+^{136}Xe our dynamics with parametrizations give a very good agreement with the dynamics of the original code. For the second

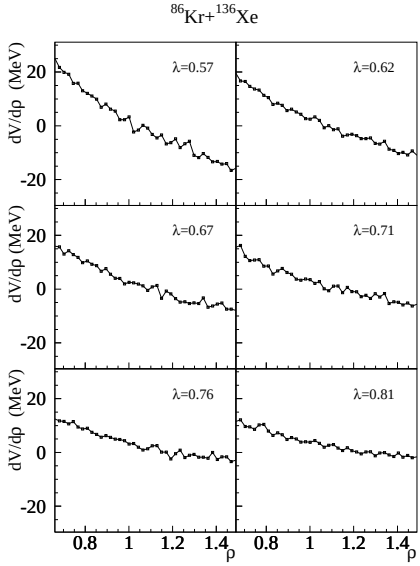

Fig. 2. Comparison, for different values of λ, between originally calculated potential gradient $\partial V/\partial\rho$ (solid line), and the one calculated with the second method (empty squares). Space $\rho, \lambda, \Delta_A, \Delta_Z$ was randomly sampled over the grid $30\times30\times30\times30$.

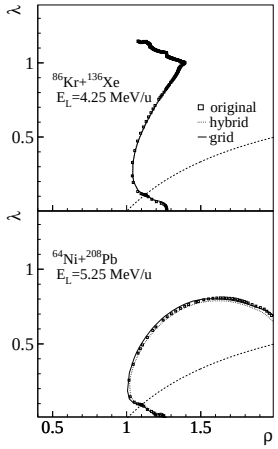

Fig. 3. For each of the reaction indicated in the figure three trajectories are presented. The empty squares correspond to trajectory calculated with the original code, dotted line represents trajectory calculated with the hybrid method: with 100×100 grid on the ρ,λ subspace, and the solid line represents trajectory calculated when a grid $30\times30\times30\times30$ spanned over the hole $\rho, \lambda, \Delta_A, \Delta_Z$ space was adopted.

case, ^{64}Ni+^{208}Pb, it seems that the potential gradient calculated on the grid reproduces the original dynamics better then the hybrid gradient. However, also in this case we consider that the agreement of our calculation with the original one is still satisfactory.

This faster version of the code, with thermal fluctuations included, enables one to calculate fusion excitation functions in the region of collision energies close to the interaction barrier of heavy nuclei, where many trajectories have to be calculated in order to collect a sufficient number of those leading to fusion. We present here two examples (Fig. 4) of such excitation functions calculated for fusion of ^{86}Kr+^{136}Xe and ^{86}Kr+^{123}Sb. In the

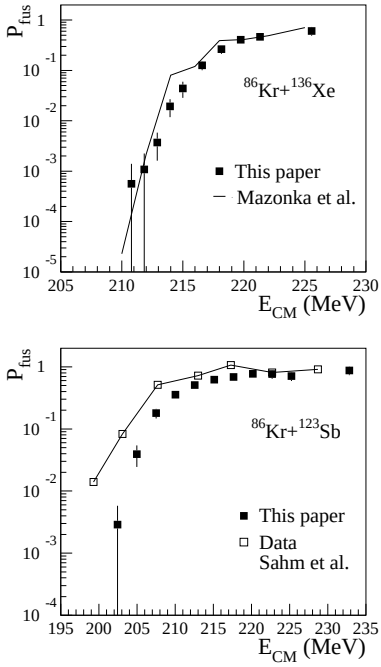

Fig. 4. The upper panel presents the comparison of the fusion excitation function (FEF) for the reaction ^{86}Kr+^{136}Xe calculated applying our potential gradient parametrization method to the dynamical model (full squares), and this based on the importance sampling method of paper [8] (solid line). In the lower panel experimental FEF (empty squares) from the reaction ^{86}Kr+^{123}Sb [15] are compared with present calculations based on the second method (full squares).

case of the first reaction which produces a compound nucleus ^{222}Th (upper panel in the figure) our calculations (full squares) are compared with these of ref. [8] (solid line) where the importance sampling method [7] was used in the dynamical model to calculate probability of very rare fusion

events at the lowest bombarding energies. As one can see these two methods are in reasonable agreement. Some discrepancies observed for E_{CM} smaller then 217 MeV can be due to statistical errors. In the lower panel of Fig. 4 comparison of our calculations is made with experimental ^{209}Fr fusion excitation function [15] (empty squares). As seen from Fig. 4 the experimental curve extends to lower bombarding energies and this part of excitation function is not reproduced by the model calculations. On the other hand fusion probabilities at higher incident energies (>212 MeV) are quite well reproduced by the model and in this energy range model seems to work reasonably well. Similar observation was made recently in Ref. [8]. Among factors which can be responsible for such disagreement one could point out Einstein–Smoluchowski relation implemented to the model. This theorem works at moderate excitation energies while at the lowest collision energies typical excitation energies are below 20 or even 10 MeV. For such low values of excitation energies Einstein–Smoluchowski relation probably needs some modifications as suggested by the nonperturbative transport theory [16]. Other possible sources of discrepancy are discussed in Ref. [8].

4. Summary and conclusions

It has been shown that the fusion process of two heavy nuclei has to be treated as a dynamical one, where thermal fluctuations coupled to macroscopic degrees of freedom (shape parameters) play important role in the case of fusion of heavy and super heavy nuclei [8], [14] *e.g.* they modify in a substantial way fusion excitation functions. Such a coupling can be taken into account by introducing a Langevin force, $L_{q_i}(t)$, to the deterministic dynamics.

In this paper we have presented a special parametrization of conservative force used in the model of Ref. [6]. Applicability of such parametrization has been presented in problems where one has to calculate many trajectories in order to get quantitative information on fusion excitation functions of heavy or superheavy nuclei. This approach takes advantage of large RAM memories of modern computers in tabularizing conservative force. Computation of such a force is the most time consuming task of the code. In this way we are able to gain a factor of 10 in the computer time.

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