Modelling of compound nucleus formation in fusion of heavy nuclei

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A new model that includes the time-dependent dynamics of the single-particle (s.p.) motion in conjunction with the macroscopic evolution of the system is proposed for describing the compound nucleus (CN) formation in fusion of heavy nuclei. The diabaticity initially keeps the entrance system around its contact configuration, but the gradual transition from the diabatic to the adiabatic potential energy surface (PES) leads to fusion or quasifission. Direct measurements of the probability for CN formation are crucial to discriminate between the current models.

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The understanding of new experimental results on fusion of heavy nuclei and the formation of superheavy elements (SHE) require modelling, not only of the initial capture process and the final CN de-excitation process, but also of the intermediate stage of evolution of the combined system from the contact configuration into the CN. The competition between fusion and quasifission (reseparation before CN formation) can inhibit fusion by many orders of magnitude, e.g. 1. Understanding this inhibition may be the key to forming more SHE. Nowadays, there is no consensus for the mechanism of the CN formation in fusion of heavy nuclei near the Coulomb barrier. Depending on the main coordinate for fusion, two sorts of models can be distinguished. In the first type, the fusion happens in the mass asymmetry coordinate \( \eta \), the fusion occurs along the radial coordinate using adiabatic PES obtained either with the liquid drop model or Strutinsky’s macroscopic-microscopic method. The competition between fusion and quasifission, which depends on the fluctuations 12, has only been included in recent models, e.g. 9, 10, 11. However, the experimental data are not always explained.

In the second type 13 (dinuclear system (DNS) model), the fusion happens in the mass asymmetry coordinate \( \eta = (A_1 - A_2)/(A_1 + A_2) \) where \( A_1 \) and \( A_2 \) are the mass numbers of the nuclei. The DNS nuclei remain at the touching configuration and exchange nucleons until either all nucleons have been transferred from the lighter to the heavier fragment (complete fusion), or the DNS decays before the CN formation (quasifission). The model assumes a sudden (double-folding in frozen density approximation) PES in the radial coordinate, while the PES behaves adiabatically along the fusion path in the \( \eta \) coordinate. Although the model has been used to explain many experimental evaporation residues (ER) cross sections, its theoretical foundation is not clear enough yet.

In this paper a new model is proposed for the CN formation, which is based on the following general ideas (which are well-established but have up to now not been used in combination in any of the current models of fusion): (i) Once the two nuclei are at the contact point, the system moves in a multidimensional space of collective coordinates \( q \) (shape parameters), (ii) this motion is governed by the master equation, and (iii) the nature of the s.p. motion is time-dependent, it is initially diabatic and then approaches the adiabatic limit due to residual two-body collisions. Consequently, the system moves in a time-dependent PES, \( V(q, t) \), which is initially diabatic and gradually becomes adiabatic. In the diabatic limit 14 (elastic nuclear matter), the nucleons do not occupy the lowest free s.p. energy levels as in the adiabatic case (plastic nuclear matter), but keep their quantum numbers and remain in the diabatic states during a collective motion of the system. This approach is realistic in the initial stage of collisions near the Coulomb barrier where the total excitation energy per nucleon \( E^* \gtrsim 0.03 \text{ MeV} \)

During the transition from the diabatic to the adiabatic limit, the nuclear matter is elastoplastic like glycerine. In contrast to the current models for CN formation, the present approach explicitly includes for the first time the time-dependent dynamics of the s.p. motion in conjunction with the macroscopic evolution of the system into the CN. In Refs. 6, 7, 9, 10 the ideas (i) and (ii) were applied, but the authors exclusively used adiabatic PES. In a recent paper 16, only idea (iii) was used to calculate the dynamical potential for the radial motion of the combined system, while in the past only the diabatic limit of the s.p. motion was used to study the initial capture process 17, 18. The ideas (i)-(iii) have solely been applied in combination to describe deep-inelastic reactions 19. The scenario presented here for the CN formation shows that following contact the diabaticity forms a valley in the PES where the system remains trapped around its touching configuration, but the gradual transition from the diabatic to the adiabatic PES allows the system to evolve in shapes leading to fusion or quasifission. The timescale for the decay to the adiabatic PES is crucial in determining the timescale of the transition to the compact fused system. The calculations are based on the master equation 20 and the diabatic two-center shell model (TCSM) 21 developed using the asymmetric TCSM (ATCSM) 22. The critical ingredients of the model are (i) temperature, (ii) diabatic...
PES, (iii) adiabatic PES, (iv) transition from diabatic to
adiabatic PES, and (v) shape parameters. The evaluation
of each will be described, then the results from the
model will be presented.

The time-dependent population probabilities $p$ for the
different configurations $q$ (shapes) of the system are so-
lutions of the master equation

$$
\dot{p}(q, t) = \sum_{q'} [\Lambda(q, q', t)p(q', t) - \Lambda(q', q)p(q, t)],
$$

(1)

where the macroscopic transition probabilities according to Ref. \[23\] are $\Lambda(q, q', t) = k_{0}\exp[V(q', t)/2T(q', t) - V(q, t)/2T(q, t)]$, justified by the assumption that the level density of the system determines the transition. The strength constant $k_0$ characterizes the global time scale and has a realistic value of $\sim 10^{22} \text{s}^{-1}$ \[24\]. The sum in Eq. \[1\] is extended only to the nearest configurations $q'$ (the collective coordinate space is discretized).

It is assumed that the system is initially at the con-
tact configuration $q_0$, where the s.p. occupation numbers obey a Fermi-distribution $n^F_\alpha(q_0, T_0)$ for a temperature $T_0$. Configurations other than $q_0$ are not populated at this time, and hence the initial condition for Eq. \[1\] is $p(q, 0) = \delta_0 q_0$. The temperature $T_0$ is related to the excitation of the system immediately after the capture process. This temperature can be estimated either as $T_0 \approx \sqrt{E_{c.m.} - V(q_0, 0)}/a$, where $E_{c.m.}$ is the total incident energy in the center of mass frame and $a = A/12$ \text{MeV}$^{-1}$ ($A$ is the total mass number of the system), if the initial radial kinetic energy is dissipated when the nuclei reach the contact point, or using a frictional model, e.g. \[10\], for the capture process. The local (at fixed $q$) temperature $T = \sqrt{E_{exc}/a}$ is defined by means of the local excitation energy

$$
E_{exc}(q, t) = a T_0^2 + \int_0^t \left( -\frac{d \Delta V_{\text{diab}}(q, t')}{dt'} \right) p(q, t') dt',
$$

(2)

which results from the decay of the diabatic part $\Delta V_{\text{diab}}$ of the potential $V$. $\Delta V_{\text{diab}}$ represents an energetic hin-
drance for the initial system to reach a configuration $q$,
if the nucleons follow diabatic levels during this process
(elastic response). The local excitation of the system is
cauised by the loss of its elasticity \[14\]. $\Delta V_{\text{diab}}$ is calculated as

$$
\Delta V_{\text{diab}}(q, t) \approx \sum_{\alpha} \varepsilon_{\alpha}^{\text{diab}}(q)[n_{\alpha}(q, t) - n^F_{\alpha}(q, T)],
$$

(3)

where $\varepsilon_{\alpha}^{\text{diab}}$ are the diabatic levels with occupations $n_{\alpha}(q, t)$ and $\alpha$ denotes the quantum numbers of these states. The diabatic levels $\varepsilon_{\alpha}^{\text{diab}}$ and their wave functions $\phi_{\alpha}^{\text{diab}}(r)$ are obtained with the maximum symme-
try method \[21\]. The dynamical PES is defined as $V(q, t) = V_{\text{adiab}}(q, T) + \Delta V_{\text{diab}}(q, t)$, where $V_{\text{adiab}}$ is the adiabatic PES which is calculated using Strutinsky's macroscopic-microscopic method \[22\]. The nuclear part of the macroscopic energy is obtained with the Yukawa-
plus-exponential method \[23\]. The diabaticity destroys the Fermi-distribution of the occupations, but the residual
two-body collisions gradually recover it. This process
is locally described by the relaxation equation \[24\]

$$
n_{\alpha}(q, t) = -\tau^{-1}(q, t)[n_{\alpha}(q, t) - n^F_{\alpha}(q, T)],
$$

(4)

where $\tau$ is an average relaxation time (in order to con-
serve the number of particles). The initial occupations $n_{\alpha}(q, 0)$ are the diabatic ones obtained from $n^F_{\alpha}(q_0, T_0)$. $\tau$ is defined as

$$
\tau^{-1}(q, t) = \frac{\sum_{\alpha} [n_{\alpha}(q, t) - n^F_{\alpha}(q, T)] \Gamma_{\alpha}(q, T)}{N_{\text{coll}} \hbar \sum_{\alpha} n_{\alpha}(q, t)},
$$

(5)

where $\Gamma_{\alpha}$ are the widths of the s.p. levels. The fac-
tor $N_{\text{coll}}$ is the average number of two-body collisions per nucleon to establish the equilibrium occupations $n^F_{\alpha}$. The value $N_{\text{coll}} = 3 \times 10^6$ will be used. The expression \[13\] follows the idea that the relaxation process becomes slower when the occupations approach $n^F_{\alpha}$. If the equilib-
rium was reached, the relaxation time would be infinite, i.e. the occupations would remain the same. The widths $\Gamma_{\alpha}$ are obtained with the parametrization given in Ref. \[27\]. Since the diabatic s.p. excitations occur around the Fermi surface, the values $\Gamma_{\alpha}^{-1} = 0.061 \text{MeV}^{-1}$ for half saturation density and $c = 20 \text{ MeV}$ will be used \[27\].

The collective coordinates $q$ are the shape parameters of the ATCSM \[22\]: (i) the elongation $\lambda = l/2R_0$, which measures the length $l$ of the system in units of the diam-
eter $2R_0$ of the spherical CN and describes the relative
motion, (ii) the deformation $\beta_1 = a_1/b_1$ of the fragments, defined by the ratio of their semiaxes, (iii) the neck coordi-
nate $\epsilon = E_0/E'$, defined by the ratio of the actual bar-
rier height $E_0$ to the barrier height $E'$ of the two-center oscillator, and (iv) the volume asymmetry of the nuclear shapes (equipotential shapes) $\xi = (V_1 - V_2)/(V_1 + V_2)$, where $V_1$ and $V_2$ are the volumes of the left and right regions divided by a plane at the necks between the frag-
ments. The collective coordinate space is divided into three regions: (i) compact shapes around the spherical shape (fusion region), (ii) elongated shapes outside the initial contact configuration and beyond the Coulomb barrier (quasifission region), and (iiii) intermediate shapes which could lead to fusion or quasifission. In the fusion region the physical mass asymmetry $\eta$ (defined like $\xi$ but in terms of the masses which are calculated using the micro-
scopic density distribution $\rho(r) = \sum_n n_{\alpha} |\phi_{\alpha}^{\text{diab}}(r)|^2$ ) reaches a minimal plateau, i.e. a maximal number of nu-
cleons move (their wave-functions spread) in the whole
volume of the system due to the decrease of the bar-
rier $E_0$ between the fragments. The fusion ($P_{\text{CN}}$) and quasifission ($P_{\text{QF}}$) probabilities are defined as the sum of the population probabilities $p$ in the fusion and quasifission regions, respectively. In addition the CN excitation
In the following the fragments are considered as spherical ($\beta_v = 1$) and the neck coordinate is fixed at $\epsilon = 0.75$. With this value of $\epsilon$ the Coulomb barrier of the diabatic potential for an initial system with $T_0 = 0$ MeV is close to the barrier of the double-folding potential. For computational reasons the calculations are done using the coordinates $\lambda$ and $\xi$ that are the relevant ones in the current models for CN formation. The non-linear set of equations are solved by successive iterations using a small time step $\Delta t = 10^{-23}$ s. The master equation is solved on a grid ($1 \leq \lambda \leq 1.8, |\xi| \leq 0.7$ where $\Delta \lambda = 0.02$ and $\Delta \xi = 0.1$) with appropriate boundary conditions to follow the continuous split of the initial population probabilities $p(\mathbf{q}, 0)$ into fusion and quasifission. Values of $|\xi| > 0.7$ are not included in the calculation because the TCSM used is not appropriate for large $\xi$. The fusion and quasifission processes are determined at the timescale $t_0$ when $P_{CN}(t_0) + P_{QF}(t_0) \approx 1$. The model will be applied to some (near) symmetric central ($l = 0$) collisions. In these calculations the excitation energy of the initial system at the contact configuration is 40 MeV.

Fig. 1 shows the dynamical PES for $^{110}\text{Pd} + ^{110}\text{Pd}$ (i) at the initial moment (diabatic PES, upper part) when the nuclei are at the contact configuration (square), (ii) at $t_0 = 4 \times 10^{-20}$ s (middle part), and (iii) the adiabatic PES (lower part). The PES is normalized with the macroscopic energy of the spherical CN. In Fig. 2, the distribution of the population probabilities $p(\lambda, \xi, t_0)$ on the PES of Fig. 1 (middle part) is presented. From these figures, it is observed that the diabaticity initially forms a valley confining the entrance system around its touching configuration as in the DNS model. Nevertheless, the gradual transition to the adiabatic PES leads to fusion mainly in the elongation $\lambda$ (relative distance) or the population of neighbouring configurations ending in the quasifission channel. In contrast to the DNS model, the diffusion along the $\xi$ coordinate, while the nuclei remain at the contact point ($\lambda = 1.5 - 1.6$), is strongly suppressed by a large diabatic hindrance. $P_{CN}$ and $P_{QF}$ are determined before the dynamical PES reaches the adiabatic one (comparing middle and lower parts in Fig. 1).

The competition between fusion and quasifission is regulated by the dynamical PES. The probability of configurations which stay close to that of the entrance channel and reseparate is very large, as can be seen from Fig. 2. This causes the fusion hindrance for $^{110}\text{Pd} + ^{110}\text{Pd}$ which is consistent with the experimental conclusions drawn in Ref. [1]. The final population probabilities in the fusion

![FIG. 1: Dynamical PES for $^{110}\text{Pd} + ^{110}\text{Pd}$: (upper part) at $t=0$ s (diabatic PES), the square denotes the contact configuration; (middle part) at $t_0 = 4 \times 10^{-20}$ s; and (lower part) the adiabatic PES. See text for further details.](image1)

![FIG. 2: Distribution of the population probabilities $p(\lambda, \xi, t_0)$ for $^{110}\text{Pd} + ^{110}\text{Pd}$ on the PES of Fig. 1 (middle part). The fusion region is $\lambda \leq 1.3$. See text for further details.](image2)

| Reaction | $P_{CN}$ | $t_0$ | $E_{CN}$ | $P_{CN}^{exp}$ |
|----------|----------|------|--------|----------------|
| $^{100}\text{Zr} + ^{100}\text{Hg}$ | $3 \times 10^{-1}$ | 5 | 40 | 2 |
| $^{100}\text{Mo} + ^{100}\text{Mo} \rightarrow ^{200}\text{Po}$ | $1.4 \times 10^{-1}$ | 4.5 | 40 | 2 |
| $^{110}\text{Pd} + ^{110}\text{Pd} \rightarrow ^{220}\text{U}$ | $1.7 \times 10^{-2}$ | 4 | 40 | 2 |
| $^{100}\text{Mo} + ^{110}\text{Pd} \rightarrow ^{210}\text{Ra}$ | $7.5 \times 10^{-2}$ | 4.3 | 40 | 2 |
| $^{96}\text{Zr} + ^{124}\text{Sn} \rightarrow ^{220}\text{Th}$ | $4.5 \times 10^{-2}$ | 4 | 40 | 2 |
The dependence of $P_{CN}$ on the excitation energy of the initial system at the touching point is rather weak, i.e., a saturation of the $P_{CN}$ practically occurs from $\sim 20$ MeV upwards.

In summary, a new realistic model for the CN formation in fusion of massive nuclei has been developed. It incorporates for the first time important physical effects which critically affect the evolution of the fusing system. The diabatic initially keeps the entrance system around its touching point, but the gradual transition from the diabatic to adiabatic PES leads to fusion (mainly in the relative distance) or quasifission. The dynamical PES regulates the competition between fusion and quasifission. The probabilities for CN formation in some (near) symmetric central collisions have been obtained and found to agree very well with the recent direct experimental determination for $^{90}\text{Zr}+^{124}\text{Sn}$. Direct measurements of the $P_{CN}$ like in Ref. [28] along with distributions of the quasifission fragments are crucial to discriminate between the current models for CN formation. To calculate ER cross sections the present approach should be combined with other models that describe the initial capture stage and the survival of the CN against fission. A TCSM more appropriate for reactions with large mass-asymmetry is being developed which should be useful in predicting production cross sections of SHE.

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