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Modeling of compound nucleus formation in the fusion of heavy nuclei

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A new model that includes the time-dependent dynamics of the single-particle motion in conjunction with the macroscopic evolution of the system is proposed for describing the compound nucleus 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 leads to fusion or quasifission. Direct measurements of the probability for compound nucleus 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 modeling, not only of the initial capture process and the final compound nucleus (CN) deexcitation 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., Ref. [1]. Understanding this inhibition may be the key to forming more SHE. Nowadays, there is no consensus [2] 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 [3–12], the fusion occurs along the radial coordinate using either adiabatic potential energy surface (PES) obtained with Strutinsky's macroscopic-microscopic method or liquid drop PES. The competition between fusion and quasifission, which depends on the fluctuations [13], has only been included in recent models, e.g., Ref. [9–12]. However, the experimental data are not always explained. In the second type [14,15] [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 η 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 $\mathbf{q}$ (shape parameters), (ii) this motion is governed by the master equation, and (iii) the nature of the single-particle (sp) motion is time dependent, it is initially diabatic and then approaches the adiabatic limit due to residual two-body collisions. The diabatic sp motion arises from the coherent character of the coupling between the intrinsic and collective degrees of freedom and the dissipation is caused by the residual two-body collisions [16]. The adiabatic limit refers to the case when the occupation of the sp energy levels obeys an equilibrated Fermi distribution with a finite temperature. The thermal effect on the sp energies may be neglected at low temperature ($T=1-2$ MeV), so diabatic and adiabatic limits essentially correspond to two extreme situations for the occupations of the zero temperature sp energy levels. For practical purposes two types of sp energy levels can be distinguished, namely, the adiabatic and diabatic levels. These levels differ only in the area of avoided crossings of adiabatic states [17], i.e., the diabatic states are defined with real crossings. In the diabatic limit [16] (elastic nuclear matter), the nucleons do not occupy the lowest free sp 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. Another way of saying this is that the probability for Landau-Zener promotion of the nucleons at the avoided crossings of adiabatic sp levels is near the unity. This approach is realistic in the initial stage of collisions near the Coulomb barrier where the total excitation energy per nucleon $E^*\gtrsim 0.03$ MeV [18,19]. During the transition from the diabatic to the adiabatic limit, the nuclear matter is elastoplastic like glycerine. As a result of (iii), the system moves in a time-dependent PES defined below, $V(\mathbf{q},t)$, which is initially diabatic and gradually becomes adiabatic. In contrast to the current models for CN formation, the present approach explicitly includes for the first time the time-dependent dynamics of the sp motion in conjunction with the macroscopic evolution of the system into the CN. In Refs. [6,7,10,11] the ideas (i) and (ii) were applied, but the authors exclusively used either adiabatic PES or liquid drop PES. In a recent paper [19], 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 sp motion was used to study the initial capture process [20,21].

The ideas (i)–(iii) have solely been applied in combination to describe deep-inelastic reactions [22]. 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 time scale for the decay to the adiabatic PES is crucial in determining the time scale of the transition to the compact fused system. The calculations are based on the master equation [23] and the diabatic two-center shell model (TCSM) [17] developed using the asymmetric TCSM (ATCSM) [24]. 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 $\mathbf{q}$ (shapes) of the system are solutions of the master equation

$$\dot{p}(\mathbf{q},t) = \sum_{\mathbf{q}'} [\Lambda(\mathbf{q},\mathbf{q}',t)p(\mathbf{q}',t) - \Lambda(\mathbf{q}',\mathbf{q},t)p(\mathbf{q},t)], \quad (1)$$

where the macroscopic transition probabilities according to Ref. [25] are $\Lambda(\mathbf{q},\mathbf{q}',t)=\kappa_0 \exp[V(\mathbf{q}',t)/2T(\mathbf{q}',t)-V(\mathbf{q},t)/2T(\mathbf{q},t)]$, justified by the assumption that the level density of the system determines the transition. The strength constant κ_0 characterizes the global time scale and has a realistic value of $\sim 10^{22}$ s^{-1} [26]. The sum in Eq. (1) is extended only to the nearest configurations $\mathbf{q}'$ (the collective coordinate space is discretized). It is assumed that the system is initially at the contact configuration $\mathbf{q}_0$ where the sp occupation numbers obey a Fermi distribution $n^F_\alpha(\mathbf{q}_0,T_0)$ for a temperature T_0. Configurations other than $\mathbf{q}_0$ are not populated at this time, and hence the initial condition for Eq. (1) is $p(\mathbf{q},0)=\delta_{\mathbf{q},\mathbf{q}_0}$. The temperature T_0 is related to the excitation of the system immediately after the capture process. This temperature can be estimated either as $T_0 \approx \sqrt{[E_{\mathrm{c.m.}}-V(\mathbf{q}_0,0)]/a}$, where $E_{\mathrm{c.m.}}$ is the total incident energy in the center of mass frame and $a=A/12$ 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., Ref. [11], for the capture process. The local (at fixed $\mathbf{q}$) temperature $T=\sqrt{E_{exc}/a}$ is defined by means of the local excitation energy

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

which results from the decay of the diabatic part ΔV_{diab} of the potential V. ΔV_{diab} represents an energetic hindrance for the initial system to reach a configuration $\mathbf{q}$, if the nucleons follow diabatic levels during this process (elastic response). The local excitation of the system is caused by the loss of its elasticity [16]. ΔV_{diab} is calculated as

$$\Delta V_{diab}(\mathbf{q},t) \approx \sum_\alpha \varepsilon^{diab}_\alpha(\mathbf{q})[n_\alpha(\mathbf{q},t) - n^F_\alpha(\mathbf{q},T)], \quad (3)$$

where $\varepsilon^{diab}_\alpha$ are the diabatic levels with occupations $n_\alpha(\mathbf{q},t)$ and α denotes the quantum numbers of these states. The diabatic levels $\varepsilon^{diab}_\alpha$ and their wave functions $\phi^{diab}_\alpha(\mathbf{r})$ are obtained with the maximum symmetry method [17]. Following Ref. [17], the dynamical PES can be defined in general as $V(\mathbf{q},t)=V_{adiab}(\mathbf{q},T)+\Delta V_{diab}(\mathbf{q},t)$, where V_{adiab} is the temperature-dependent adiabatic PES which is the sum of the liquid drop energy and the microscopic shell and pairing corrections obtained with Strutinsky's method [27]. The nuclear part of the liquid drop energy is obtained with the Yukawa-plus-exponential method [28]. It is important to note that the diabatic contribution (3) is initially maximal, but gradually decreases when the actual sp occupations approach the Fermi distribution. The dynamical PES describes a continuous transition from the initial diabatic potential to the asymptotic adiabatic one. 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 [29]

$$\dot{n}_\alpha(\mathbf{q},t) = -\tau^{-1}(\mathbf{q},t)[n_\alpha(\mathbf{q},t) - n^F_\alpha(\mathbf{q},T)], \quad (4)$$

where τ is an average relaxation time (in order to conserve the number of particles). The initial occupations $n_\alpha(\mathbf{q},0)$ are the diabatic ones obtained from $n^F_\alpha(\mathbf{q}_0,T_0)$. τ is defined as

$$\tau^{-1}(\mathbf{q},t) = \frac{\sum_\alpha [n_\alpha(\mathbf{q},t) - n^F_\alpha(\mathbf{q},T)]\Gamma_\alpha(\mathbf{q},T)}{N_{coll}\,\hbar \sum_\alpha n_\alpha(\mathbf{q},t)}, \quad (5)$$

where Γ_α are the widths of the sp levels. The factor N_{coll} is the average number of two-body collisions per nucleon to establish the equilibrium occupations n^F_α. The value $N_{coll}=3$ [18] will be used. The expression (5) follows the idea that the relaxation process becomes slower when the occupations approach n^F_α. If the equilibrium was reached, the relaxation time would be infinite, i.e., the occupations would remain the same. The widths Γ_α are obtained with the parametrization given in Ref. [27]. Since the diabatic sp excitations occur around the Fermi surface, the values $\Gamma_0^{-1}=0.061$ MeV^{-1} for half saturation density and $c=20$ MeV will be used [27].

The collective coordinates $\mathbf{q}$ are the shape parameters of the ATCSM [24]: (i) the elongation $\lambda=l/2R_0$, which measures the length l of the system in units of the diameter $2R_0$ of the spherical CN and describes the relative motion, (ii) the deformation $\beta_i=a_i/b_i$ of the fragments, defined by the ratio of their semiaxes, (iii) the neck coordinate $\epsilon=E_0/E'$, defined by the ratio of the actual barrier 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 fragments. 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 (quasifis-

sion region), and (iii) intermediate shapes which could lead to fusion or quasifission. In the fusion region the physical mass asymmetry η [defined like ξ but in terms of the masses which are calculated using the microscopic density distribution $\rho(\mathbf{r})=\Sigma_\alpha n_\alpha|\phi_\alpha^{diab}(\mathbf{r})|^2$] reaches a minimal plateau, i.e., a maximal number of nucleons move (their wave-functions spread) in the whole volume of the system due to the decrease of the barrier E_0 between the fragments. The fusion (P_{CN}) and quasifission (P_{QF}) probabilities are defined as the sum of the population probabilities p in the fusion and quasifission regions, respectively. In addition the CN excitation energy E_{CN} is defined as the average of the excitation energies (2) of the different shapes in the fusion region.

In the following the fragments are considered as spherical ($\beta_i=1$) and the neck coordinate is fixed at $\epsilon=0.75$. With this value of ϵ 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 [19]. For computational reasons the calculations are done using the coordinates λ and ξ that are the relevant ones in the current models for CN formation, e.g., as in Refs. [11,15]. The nonlinear set of equations (1)–(5) are solved by successive iterations using a small time step $\Delta t=10^{-23}$ s. The master equation (1) is solved on a grid ($1\leqslant\lambda\leqslant 1.8, |\xi|\leqslant 0.7$ 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 [24] is not appropriate for large ξ. The fusion and quasifission processes are determined at the time scale t_0 when $P_{CN}(t_0)+P_{QF}(t_0)\simeq 1$. 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. The effect of rotation of the combined system on its evolution can also be included in the model. However, as it is well established experimentally and theoretically, this effect is weak in fusion of a heavy system due to its large moment of inertia. The experimental spin distribution [30] shows that the main contribution to the ER cross sections results from low partial waves. The repulsive potential energy gained by diabatic effects is much larger than the centrifugal energy that the system can gain by rotation. The inclusion of the rotation of the system may lead to the loss of transparency of the main features of the model, i.e., diabatic effects.

Figure 1 shows the dynamical PES for ^{110}Pd+^{110}Pd (i) at the initial moment (diabatic PES, upper part) when the nuclei are at the contact configuration (square), (ii) at $t_0=4\times10^{-20}$ 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 [14]. Nevertheless, the gradual transition to the adiabatic PES leads to fusion mainly in the elongation λ (relative distance) or the population of neighboring configurations ending in the quasifission channel. In contrast to the DNS model, the diffusion along the ξ coordinate, while the nuclei remain at the

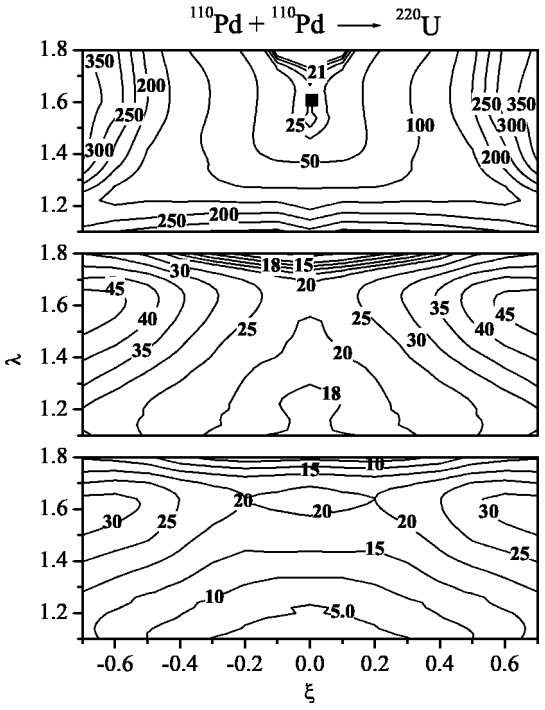

FIG. 1. Dynamical PES for ^{110}Pd+^{110}Pd: (upper part) at $t=0$ s (diabatic PES), the square denotes the contact configuration; (middle part) at $t_0=4\times10^{-20}$ s; and (lower part) the adiabatic PES. See text for further details.

contact point ($\lambda=1.5-1.6$), is strongly suppressed by a large diabatic hindrance. Calculations performed in Ref. [11] with the fluctuation-dissipation approach using liquid drop PES have also shown that the mass-asymmetry path does not contribute significantly to the CN formation. 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

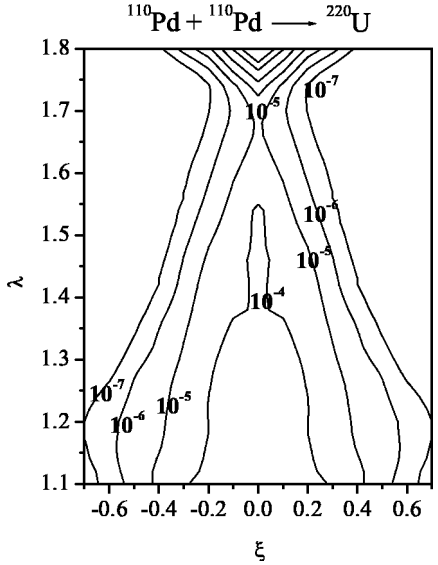

FIG. 2. Distribution of the population probabilities $p(\lambda,\xi,t_0)$ for ^{110}Pd+^{110}Pd on the PES of Fig. 1 (middle part). The fusion region is $\lambda\leqslant 1.3$. See text for further details.

TABLE I. P_{CN}, t_0 (10^{-20} s) and E_{CN} (MeV) for some (near) symmetric central collisions. The P_{CN} values are compared to direct experimental $P_{CN}^{\text{expt.}}$ [31].

Reaction	P_{CN}	t_0	E_{CN}	$P_{CN}^{\text{expt.}}$
$^{90}\text{Zr}+^{90}\text{Zr}\rightarrow{}^{180}\text{Hg}$	3×10^{-1}	5	40	
$^{100}\text{Mo}+^{100}\text{Mo}\rightarrow{}^{200}\text{Po}$	1.4×10^{-1}	4.5	40	
$^{110}\text{Pd}+^{110}\text{Pd}\rightarrow{}^{220}\text{U}$	1.7×10^{-2}	4	40	
$^{100}\text{Mo}+^{110}\text{Pd}\rightarrow{}^{210}\text{Ra}$	7.5×10^{-2}	4.3	40	
$^{96}\text{Zr}+^{124}\text{Sn}\rightarrow{}^{220}\text{Th}$	4.5×10^{-2}	4	40	5×10^{-2}

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], namely, that the fusion hindrance is primarily caused by reseparation shortly after passage of the Coulomb barrier. The final population probabilities in the fusion region ($\lambda\leqslant1.3$ in Fig. 2) are very small, and as a result of the expression (2), E_{CN} is practically the same as the excitation energy of the initial system at the contact point, i.e., 40 MeV. The scenario seen so far is the same for other systems studied. Table I shows P_{CN}, t_0, and E_{CN} calculated for some (near) symmetric reactions. The values of the model parameters are the same for all the reactions. The decrease of the P_{CN} values from $^{90}\text{Zr}+^{90}\text{Zr}$ to $^{110}\text{Pd}+^{110}\text{Pd}$ is observed along with an increase of the quasifission probability beyond 90%. This is because (i) the repulsive character of the diabatic PES increases with increasing mass number A of the combined system and (ii) the valley of the diabatic PES becomes more shallow with increasing A. Consequently the time scale t_0 of the fusion and quasifission processes decreases with increasing A. The P_{CN} for $^{96}\text{Zr}+^{124}\text{Sn}$ agrees very well with the recent direct experimental measurement [31]. The $P_{CN}^{\text{expt.}}$ includes the contribution of higher partial waves l, i.e., $l>0$, although the main contribution results from low l for heavy systems at this energy. The P_{CN} obtained with the DNS model for this reaction [14] also agrees well with that experiment, while P_{CN} for, e.g., $^{110}\text{Pd}+^{110}\text{Pd}$, is about one order of magnitude smaller than the present P_{CN} (see Table I). The fluctuation-dissipation model in Ref. [7] predicts P_{CN} values that are much larger than the present ones, i.e., about one order of magnitude larger for $^{110}\text{Pd}+^{110}\text{Pd}$ and $^{100}\text{Mo}+^{110}\text{Pd}$. Direct experimental measurements of P_{CN} as in Ref. [31] are crucial to discriminate between the current models for CN formation. The dependence of P_{CN} on the parameter Γ_0^{-1} is strong for the heaviest systems studied, i.e., changing the latter from 0.061 MeV^{-1} to 0.03 MeV^{-1}, causes the P_{CN} decrease by about one order of magnitude due to the faster transition to the adiabatic PES, whereas the effect on the time scale t_0 is rather weak. The time scale t_0 is mainly determined by the quasifission process that occurs near the contact configuration of the initial system, where the diabatic effects are small. 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 diabaticity 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 $^{96}\text{Zr}+^{124}\text{Sn}$. Direct measurements of the P_{CN} as in Ref. [31] 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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