Molecular dynamics approach:
from chaotic to statistical properties of compound nuclei

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ABSTRACT

Statistical aspects of the dynamics of chaotic scattering in the classical model of \( \alpha \)-cluster nuclei are studied. It is found that the dynamics governed by hyperbolic instabilities which results in an exponential decay of the survival probability evolves to a limiting energy distribution whose density develops the Boltzmann form. The angular distribution of the corresponding decay products shows symmetry with respect to \( \pi/2 \) angle. Time estimated for the compound nucleus formation ranges within the order of \( 10^{-21} \)s.

PACS: 05.45.+b; 05.60.+w; 24.10.-i; 24.60.Dr; 24.60.Lz

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In the description of compound nuclei molecular dynamical approaches [1] (MDA) generating chaotic behavior appear to provide an interesting alternative to quantum stochastic methods [2] based on the random matrix theory. Indeed, the resulting exponential decay of the classical survival probability reflects the presence of Ericson fluctuations [3] as can be seen [4] from the semiclassical energy autocorrelation function of an S-matrix element. The corresponding unitarity deficit [5] allows to determine [1] the probability for the compound nucleus formation. An important related issue which, however, finds no quantitative documentation in the literature so far is the problem of statistical properties of the objects to be interpreted as compound nuclei formed within the molecular dynamics frame. These properties are responsible for the decay characteristics such as energetic and angular distributions of the outgoing particles. The Boltzmann form of the energy distribution and the symmetry with respect to $\pi/2$ of the angular distribution are considered to constitute the most convincing signatures that memory is lost and a certain kind of equilibrium is reached [6].

Because of an explicitly dynamical character MDA offers a very attractive frame for addressing the related questions. In particular, does an ensemble of two colliding objects, each composed of a certain limited number of interacting constituents evolve to some limiting energy distribution? And, if so, under what conditions this happens, what is the distribution and what are the time scales involved? This question differs from the one asked in statistical mechanics where one assumes that at equilibrium the system will have the most probable distribution which results in the Boltzmann distribution, the density of which is $\exp(-E/T)$. For an isolated system of $n$ interacting particles obeying a nonlinear energy distribution law, Ulam conjectured [7], that no matter what the initial distribution of energy is we have convergence to the exponential distribution. This conjecture, based on the com-
puter experiments, was proved later on mathematically [8]. The case of interest for the present considerations corresponds, however, to open phase space phenomena [9] and the particles escape from the interaction region after some time depending on the initial conditions. Is there, then, enough time for the randomization to occur?

The model [10] specified as a classical limit of the time-dependent cluster theory [11] offers an interesting and realistic molecular dynamics scheme, and will be used here for addressing the above questions. A Van-der-Waals – type form of the effective interaction between the elementary constituents, the pointlike alpha particles in the present case, allows to assign a quite general meaning to the related analysis.

MDA study of the scattering processes is usually based on the concepts of the transport theory [12] which, for instance, allows to determine the classical survival probability $P_{ij}(E, t)$ for a system to remain in the interaction region with respect to a $j \rightarrow i$ transition. This is a quantity which, according to the semiclassical considerations determines, via the Fourier transform, the energy autocorrelation function $C_{ij}$ of an S-matrix element, $C_{ij}(\epsilon) = \langle S_{ij}^*(E)S_{ij}(E + \epsilon) \rangle_E$, and thus makes a link between the quantum and the classical picture. Chaotic scattering connected with the existence of only unstable periodic trajectories (hyperbolic chaotic scattering) results in an exponential decay: $P(E, t) \sim \exp(-\gamma t)$. The resulting autocorrelation function has a Lorenzian form: $C(\epsilon) \sim \hbar/(\epsilon + i\hbar\gamma)$, a characteristic of Ericson fluctuations observed in the decay of compound nuclei. Whether this automatically guarantees appearance of the other characteristics of the compound nucleus is, however, not immediately obvious. Actually, the literature presents schematic two dimensional studies of chaotic scattering on deformed nuclei [13] or on various three center potentials [14–16] which lead to the exponential decay of $P(E, t)$ but the angular distribution of outgoing trajectories is not symmetric with respect to $\pi/2$ angle.
Realistic MDA description of nuclei involves, however, many more degrees of freedom. In the model considered here both, the target nucleus and the projectile are composed of the interacting alpha particles each of them moving in the six-dimensional phase space. Furthermore, in order to simulate reality and for consistency with the transport theory the nuclei are defined as the statistical ensembles of elementary constituents. Each configuration in such an ensemble is constructed so as to ensure the proper binding energy of a nucleus and its internal linear and angular momenta zero. Consistently, for a nucleus composed of \( n \)-bodies any observable represented by a function \( f \) is evaluated by integrals

\[
\int dr_1 \ldots dr_n \int dp_1 \ldots dp_n \delta \left( \sum_{i=1}^{n} r_i \right) \delta \left( \sum_{i=1}^{n} p_i \right) \delta \left( \sum_{i=1}^{n} l_i \right) \\
\times \delta \left( E_B - \sum_{i=1}^{n} p_i^2 / 2m - V(r_1, \ldots, r_n) \right) f(r_1, \ldots, p_n),
\]

(1)

where \( r_i, p_i \) and \( l_i \) denote the position, momentum and angular momentum of \( i \)-th alpha particle with respect to the center of mass of the nucleus.

We begin by studying the time evolution of the energy distribution of particles for \(^{12}\text{C} + ^{12}\text{C} \) head on reaction and concentrate on the higher energy part because it eventually drives the decay. Each of the two colliding three \( \alpha \)-particle \(^{12}\text{C} \) nuclei is prepared at separation according to the above prescription. Firstly, \( 4 \cdot 10^5 \) scattering events involving various internal configurations of both nuclei have been generated on the computer. The time evolution is continued in each case till the resulting compound system does decay. Thus, for longer times the number of events which determine the energy distribution of individual particles decreases. As, however, is shown in Fig. 1 this process clearly establishes a limiting energy distribution \( \rho(E) \) comparatively soon, within the times of the order of \( 8 - 10 \cdot 10^{-22} \) s (counting of time begins at the closest approach distance). Before collision, the energy distribution of particles is the one representing ground states of the two nuclei at separation.
and is well localized. The initial relative motion boost shifts this distribution to positive energies. Early stage of the collision converts energy of the relative motion into an internal one and, therefore, $\rho(E)$ disperses in the direction of much higher energies. These high energy particles quickly escape the interaction region and for the remaining events $\rho(E)$ approaches an exponential form whose slope allows to define a temperature like parameter $T$. This, however, is not yet a limiting distribution. By preserving the exponential form $\rho(E)$ decreases the slope which reaches the limiting value corresponding to $T = 1.3\,\text{MeV}$ for times of the order of $10^{-21}\,\text{s}$ as can be seen from the time evolution of the parameter $T$ shown in the lower part of Fig. 1.

The observation of primary interest for our present discussion is that this time is strongly correlated with time the exponential decay of the survival probability sets in. This can be concluded from the upper part of Fig. 2 which shows the number of events $N(t)$ such that all the particles still remain in the interaction region up to time $t$. Another important and consistent result, extracted from these calculations and illustrated in the lower part of Fig. 2 is that the distribution of the kinetic energy of the escaping $\alpha$ particles collected from all the events entering the exponential region ($t > 8 \cdot 10^{-22}\,\text{s}$) is also exponential in energy. The slope parameter $T$ describing this distribution equals $1.5\,\text{MeV}$ and is thus larger than the one corresponding to the energy distribution inside the compound system as listed above. This seems to reflect the fact that the escape of more energetic particles from the compound nucleus is more probable due to the Coulomb barrier. Thus, the ‘temperature’ read over from the escaping particles exceeds the one inside the nucleus. The fast particles, escaping at an early stage of the collision (times up to $8 \cdot 10^{-22}\,\text{s}$) are Gaussian distributed similarly as they are inside the compound system (Fig. 1). Finally, we wish to mention, without explicitly demonstrating here
the result that for peripheral collisions of $^{12}\text{C} + ^{12}\text{C}$ in the decay channel to the same final configuration we identify the power-law decay of the survival probability which is typically connected with the existence of more solid structures (KAM surfaces) in the underlying phase-space [16]. No universal limiting energy distribution exists in this case.

Our study of the statistical properties of a compound nucleus was based so far essentially on investigation of the temporal aspects of chaotic motion. More severe test may come from the analysis of spatio-temporal aspects such as the angular distribution of the decay products. This particular characteristics is especially interesting in nuclear physics but the need for studying the spatio-temporal aspects of chaotic motion is identified [17] also from the more general perspective. In the present context we are mostly concerned with the conditions under which the compound system, in a sense, forgets the way it was formed and as a consequence decays symmetrically with respect to $\pi/2$ angle in the center of mass frame. In order to make such a study meaningful one needs to break the mass symmetry in the entrance channel. For that reason we still consider the same compound system as before (six $\alpha$-particles) but, this time, produced in the $\alpha + ^{20}\text{Ne}$ reaction. At 20 MeV for this initial configuration the probability for the compound nucleus formation is much smaller than for $^{12}\text{C} + ^{12}\text{C}$, therefore, we lower the energy to 15 MeV. The relevant results for two different angular momenta, $l = 0$ and $l = 5$ are shown in Fig. 3. Because of lower energy the dynamics is somewhat slower and, consequently, the initial stage of the reaction, before the exponential decay, takes about $5 \cdot 10^{-22}$s longer than previously. Still, one observes an impressive coincidence between the behavior of the survival probability and the form of angular distribution of the emitted $\alpha$ particles. Events surviving not longer than $11 \cdot 10^{-22}$s remember the initial direction of motion and the emission of the $\alpha$ particles occurs in the forward direction with much higher
probability. Larger fraction of such a type of events governs the dynamics for $l = 5$ than for the central collisions ($l = 0$), simply because the corresponding transmission coefficients [1] are smaller for more peripheral collisions. The angular distribution of all the events decaying after $t = 20 \cdot 10^{-22}$s shows symmetry with respect to $\pi/2$ angle for all angular momenta. The dip in the region of $\pi/2$ seen for $l = 5$ is the known effect connected with the collective rotation of the compound system. The angular distribution of cases decaying for the intermediate times between $11 \cdot 10^{-22}$ and $20 \cdot 10^{-22}$s also displays the intermediate shapes which reflects the fact that the transition is gradual. This distribution for $l = 5$ is, however, already closer to the symmetric one than for $l = 0$ because of a tendency to regular orbiting which reduces the number of particles emitted in forward direction already at this stage.

The many–body model of nuclear dynamics generating chaotic behavior is thus able to reproduce not only the probability of the compound nucleus formation [1] and the correlation width but also to account for more subtle effects connected with the decay such as energy and angular distribution of the emitted particles. The appearance of these characteristics is strongly correlated with an exponential time dependence of the survival probability. It is also interesting to notify that all those attributes of compound nuclei emerge already for the systems with a relatively small number of the constituents.

We thank Marek Ploszajczak for helpful discussions. This work was partly supported by KBN Grants No. 2 P302 157 04 and No. 2 0334 91 01.
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Figure captions

1. **Upper part**: Energy distribution of particles for $^{12}$C + $^{12}$C head on reaction at 20 MeV incident energy: before collision (full circles – solid line is to guide the eye), at the initial stage ($t = 0$ in our time scale) – when the relative momentum of the two $^{12}$C becomes zero (squares – solid line represents Gaussian fit), at $t = 6 \cdot 10^{-22}$s (triangles – long dashed line represents exponential fit), at $t = 16 \cdot 10^{-22}$s (diamonds – short dashed exponential fit), and at $t = 24 \cdot 10^{-22}$s (open circles – dash-dotted exponential fit).

**Lower part**: Corresponding time dependence of the parameter $T$ describing the slope of the exponential fits the high energy distribution of particles.

2. **Upper part**: A number of two body events $N$ living until a given time and leading to an $\alpha$-particle emission after $^{12}$C + $^{12}$C head on collision at 20 MeV incident energy. Straight line represents exponential fit for times longer than $7 \cdot 10^{-22}$s.

**Lower part**: Corresponding energy spectra of emitted $\alpha$-particles, collected for shorter ($t \leq 8 \cdot 10^{-22}$s – circles) and longer ($t > 8 \cdot 10^{-22}$s – triangles) times of life of the composite system (cf. upper part) in 0.5 MeV. Solid line represents Gaussian fit to the former and dashed line – exponential fit to the latter.

3. Relative number of events before $\alpha$-particle emission from the composite system living up to a time $t$ (on the left) and the yield of the outgoing $\alpha$-particles (on the right) from the $\alpha + ^{20}$Ne head on reaction, $l = 0$ (upper part) and $l = 5$ (lower part) at 15 MeV incident energy as a function of the scattering angle. Triangles represent $\alpha$-particles escaped before $t = 11 \cdot 10^{-22}$s and circles those escaped after $t = 20 \cdot 10^{-22}$s. Full line in $l = 0$ part represents mean value of the yield. Distributions for the intermediate times are indicated by
squares. Error bars correspond to the statistical uncertainty (square root of the number of events).
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