# Molecular-dynamics approach: From chaotic to statistical properties of compound nuclei

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(Received 27 April 1994; revised manuscript received 9 November 1994)

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, characterized by the positive Lyapunov exponents and the fractal dimensions, 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 the $\pi/2$ angle. The time estimated for the compound nucleus formation ranges within the order of $10^{-21}$ s.

PACS number(s): 24.60.Lz, 24.60.Dr, 05.45.+b, 05.60.+w

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 us 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 computer 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 specified in Ref. [10] offers an interesting and realistic MDA scheme and will be used here for addressing the above questions. This model was invented to describe the breakup processes and can be considered as a classical counterpart of the time-dependent cluster theory [11]. Thus, the elementary constituents are the pointlike alpha particles and the corresponding two-body potential has a van der Waals-type form which in the present case can be parametrized as follows:

$$\begin{aligned} V(r) &= a_0/r + a_1 \exp[-(r-a_2)^2/{a_3}^2] \\ &\quad + a_4 \exp[-(r-a_5)^2/{a_6}^2] \quad \text{for } r > r_{\min}, \\ V(r) &= a_7 + a_8 (r - r_{\min})^2 \quad \text{otherwise}, \end{aligned} \tag{1}$$

with parameters $a_1 = -5.673\,\text{MeV}$, $a_2 = 3.781\,\text{fm}$, $a_3 = 1.23\,\text{fm}$, $a_4 = 1.6\,\text{MeV}$, $a_5 = 4.351\,\text{fm}$, $a_6 = 0.896\,\text{fm}$, and $a_0$ is the Coulomb parameter. The core parameters $a_7 = -3.164\,\text{MeV}$ and $a_8 = 4.004\,\text{MeV/fm}^2$ ensure continuity of the potential and its derivative at $r_{\min} = 3.6355\,\text{fm}$. The above interaction is derived from the adiabatic time-dependent Hartree-Fock approximation and thus incorporates globally the effects of quantum statistics. In order to make a clear point on the role of deterministic chaotic dynamics no stochastic force of Ref. [10] is included in the present analysis.

MDA study of the scattering processes is usually based on the concepts of the transport theory [12] which, for instance, allows us to determine the classical survival probability $P_{ij}(E,t)$ for a system to remain in the interaction region with respect to a $j \to i$ transition. This

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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:

$$P(E,t) \sim \exp(-\gamma t). \tag{2}$$

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 the $\pi/2$ angle and the corresponding energy may remain even a constant. A 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 [1, 10] so as to ensure the proper binding energy of a nucleus and its internal linear and angular momenta zero.

We begin by studying the time evolution of the energy distribution of particles for $^{12}C + ^{12}C$ head-on reaction and concentrate on the higher energy part because it eventually drives the decay. First, $4 \times 10^5$ scattering events involving various internal configurations of both nuclei have been generated. The time evolution is continued in each case until the resulting compound system does not 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–$10\times10^{-22}$ s (measurement 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. The 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 from the interaction region and for the remaining events $\rho(E)$ approaches an exponential form whose slope allows us to define a temperaturelike 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 $10^{-21}$ s as can be seen from the time evolution of the parameter $T$ shown in the lower part of Fig. 1. Independent estimates [17] predict the minimum number of collisions for a compound system to reach equilibrium to be three. Then assuming that the time between subsequent collisions equals the traversal time through the system, for our energy of 20 MeV one essentially obtains the same value of $10^{-21}$ s. At the same time the distribution of the kinetic energy alone also reaches the limiting value but the corresponding slope parameter $T = 1.6\,\text{MeV}$, as it is indicated by the dotted line in Fig. 1. The difference in $T$ reflects the fact that this is a strongly interacting quasibound system. Consequently, some particles with large kinetic energy may enter the region of significant attraction which lowers their total energy and changes the corresponding slope of $\rho(E)$ towards the smaller $T$. It is also interesting to notice that, as the direct calculation shows, out of the initial 20 MeV of energy, on the average, about 14.5 MeV is deposited in the kinetic energy. Since the

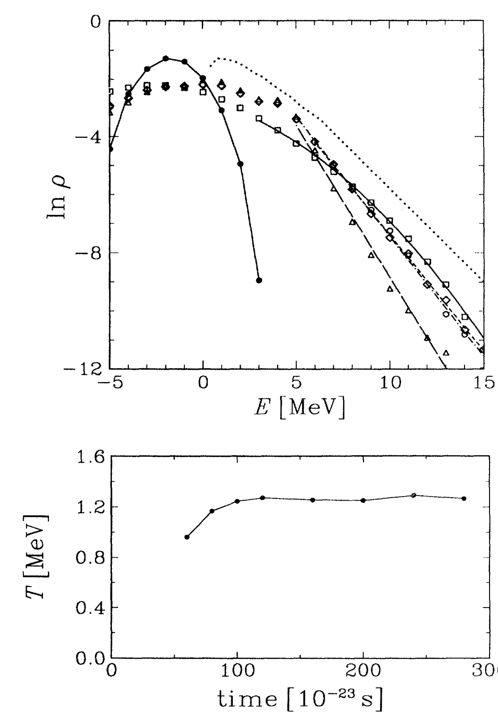


FIG. 1. Upper part: Energy distribution of particles for $^{12}C + ^{12}C$ head-on reaction at 20 MeV incident energy: before collision (solid circles—solid line is to guide the eye), at the initial stage ($t = 0$ in our time scale) —when the relative momentum of the two $^{12}C$ becomes zero (squares—solid line represents Gaussian fit), at $t = 6 \times 10^{-22}$ s (triangles—long dashed line represents exponential fit), at $t = 16 \times 10^{-22}$ s (diamonds—short dashed line represents exponential fit), and at $t = 24 \times 10^{-22}$ s (open circles—dash-dotted line represents exponential fit). Dotted line indicates the limiting distribution of the kinetic energy. Lower part: Corresponding time dependence of the parameter $T$ describing the slope of the exponential fits to the high energy distribution of particles.

kinetic energy enters the Hamiltonian in the separable form one may expect the equipartition theorem [18] to hold for that fraction of energy. Bearing in mind that our problem involves 18 degrees of freedom one obtains $T = 1.6\,\text{MeV}$ almost exactly.

The observation of primary interest for our present discussion is that the time of approaching the above equilibrium values 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 $t$. Such an exponential decay is characteristic of the hyperbolic chaotic scattering where delay of the scattering trajectories in the interaction region is connected with the existence of only unstable periodic trajectories. Under this condition the decay rate in Eq. (2) is predicted [16, 19] to be described by

$$\gamma = \Sigma_i \lambda_i (1 - D_i), \tag{3}$$

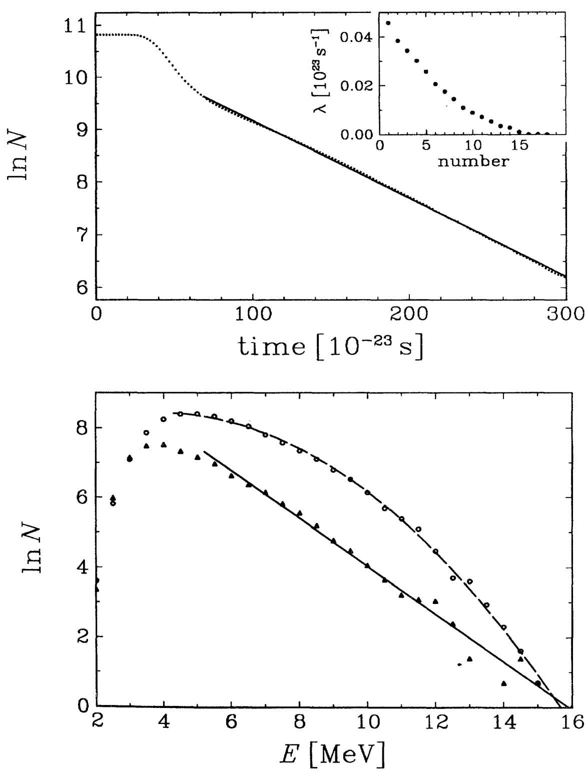

FIG. 2. Upper part: A number of two-body events $N$ living until a given time and leading to an $\alpha$-particle emission after $^{12}C + {}^{12}C$ head-on collision at 20 MeV incident energy. Straight line represents exponential fit for times longer than $7\times10^{-22}$ s. Inset shows the spectrum of positive Lyapunov exponents. Lower part: Corresponding energy spectra of emitted $\alpha$ particles, collected for shorter ($t \leq 8\times10^{-22}$ s—circles) and longer ($t > 8 \times 10^{-22}$ s—triangles) times of life of the composite system (cf. upper part) in 0.5 MeV. Solid line represents Gaussian fit to the former; dashed line—exponential fit to the latter.

where $\lambda_i$ and $D_i$ denote the positive Lyapunov exponents and the partial fractal dimensions, respectively. All positive $\lambda_i$ for our 18-dimensional problem, calculated according to the prescription of Ref. [20], are shown in the inset to the upper part of Fig. 2. There exist no well-defined methods to calculate the partial fractal dimensions $D_i$ for multidimensional problems. Because more particles are involved and any of them can escape from the interaction region, typical $D_i$ in the present case is, however, expected to be significantly closer to unity than the fractal dimension ($\sim 0.65$) corresponding to the simplified version of the same model [16] in the region of hyperbolic instabilities. In fact, a simple estimate based on the scaling relation between the difference in initial impact parameter for a pair of the scattering events and the resulting fraction of events uncertain in the decay mode or emission angle (uncertainty exponent technique [21]) gives a value of 0.9. This, most probably, does not correspond precisely to any of the $D_i$ but provides a reasonable indication for some average value. Via Eq. (3), the above values of $\lambda$ and $D$ give an estimate which agrees with $\gamma \approx 0.015$ as extracted from the time dependence of the survival probability shown in Fig. 2. This provides direct evidence that in the classical limit the physics of compound nuclei is governed by the positive Lyapunov exponents and the structure of instabilities is fractal.

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 ($t > 8 \times 10^{-22}$ s) is also exponential in energy. The slope parameter $T$ describing this distribution equals 1.5 MeV and is thus larger than the one corresponding to the total energy distribution inside the compound system but somewhat smaller than the one describing kinetic energy. The later effect is natural and reflects the existence of attraction in the two-body interaction. The former partly originates from the fact that the escape of more energetic particles from the compound nucleus is more probable due to the Coulomb barrier. The fast particles, escaping at an early stage of the collision (times up to $8 \times 10^{-22}$ 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 $^{12}C + {}^{12}C$ 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. A more severe test may come from the analysis of spatio-temporal aspects such as the angular distribution of the decay products. This particular characteristic is especially interesting in nuclear physics but the need for studying the spatio-temporal aspects of chaotic motion is identified [22] 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 the $\pi/2$ 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 $\alpha + {}^{20}\mathrm{Ne}$ reaction. At 20 MeV for this initial configuration the probability for the compound nucleus formation is much smaller than for ${}^{12}\mathrm{C} + {}^{12}\mathrm{C}$; 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 $5 \times 10^{-22}$ 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 $11 \times 10^{-22}$ s remember the initial direction of motion and the emission of the $\alpha$ particles occurs in the forward direction with much higher probability. A 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 $t = 20 \times 10^{-22}$ s shows symmetry with respect to the $\pi/2$ 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 $11 \times 10^{-22}$ and $20 \times 10^{-22}$ 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.

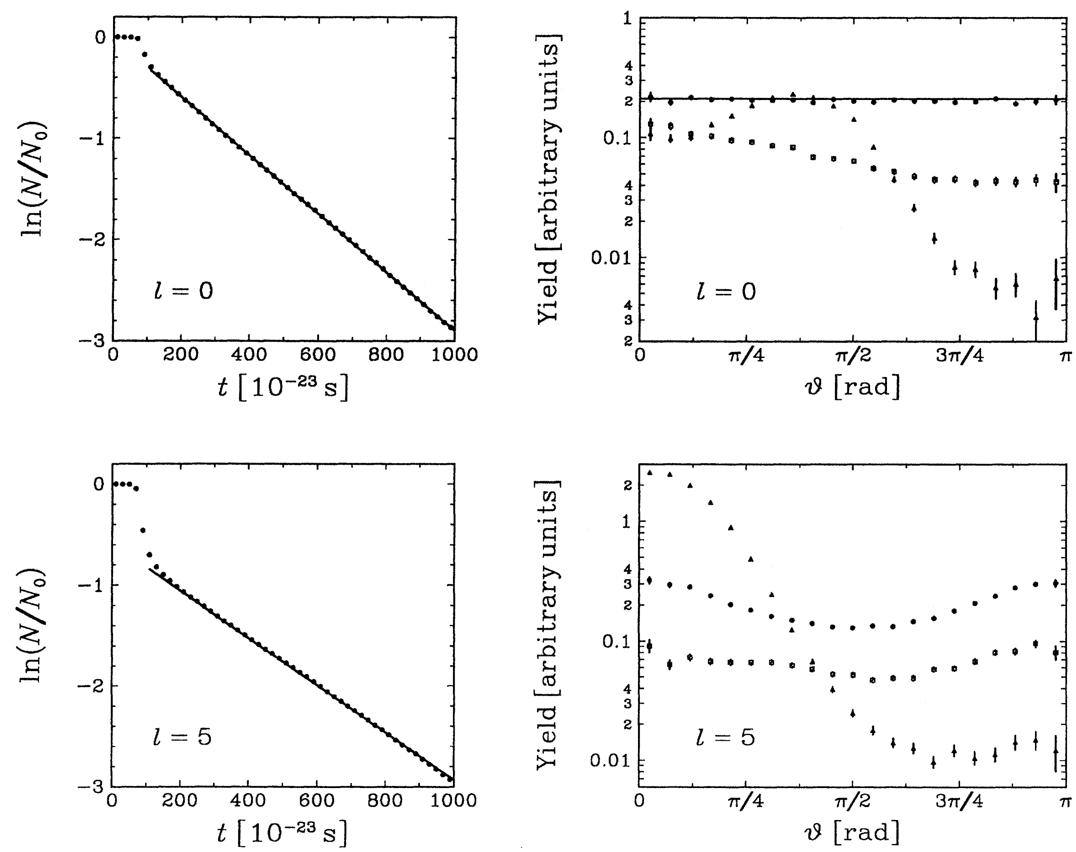


FIG. 3. Relative number of events before $\alpha$-particle emission from the composite system living up to a time $t$ (on the left) and the yield of the outgoing $\alpha$ particles (on the right) from the $\alpha + {}^{20}\mathrm{Ne}$ head-on reaction, $l = 0$ (upper part) and $l = 5$ (lower part) at 15 MeV incident energy as a function of the scattering angle. Triangles represent $\alpha$ particles escaped before $t = 11 \times 10^{-22}$ s and circles those escaped after $t = 20 \times 10^{-22}$ 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).

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. This, in turn, reflects the fact that the underlying dynamics is connected with those regions of the phase space which are characterized by the existence of unstable periodic trajectories only. It is the presence of these trajectories which leads to an exponential time delay. The number of such trajectories increases exponentially with energy. The exponential energy distribution of the emitted particles and the total energy conservation thus imply that the survival and energy spectrum of the residual system should also be governed by the unstable periodic trajectories. This time, however, they are connected with the phase space of the residual nucleus and are expected [23] to prescribe the corresponding density of states. This sets a parallel to the quantum mechanical picture: probability for a particle emission is proportional to the density of states in the residual nucleus. One may then conclude that appearance of the above attributes of compound nuclei demands the presence of hyperbolic instabilities in the residual nucleus. This is a stronger condition than the one encountered in the schematic models mentioned above where chaos is generated by the coupling between the projectile and the target. It is, however, interesting to note that all the conditions for a compound nucleus formation can be fulfilled in the systems with a relatively small number of 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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