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Low-energy chaos in the Fermi–Pasta–Ulam problem

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Abstract. A possibility that in the FPU problem the critical energy for chaos goes to zero when the number of particles in the chain increases is discussed. The distribution for long linear waves in this regime is found and an estimate for the new border of the transition to energy equipartition is given.

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From 1955 the Fermi-Pasta-Ulam (FPU) problem [1] initiated much research and became a cornerstone in modern statistical mechanics [2, 3]. The absence of energy equipartition in the system of coupled nonlinear oscillators observed numerically in [1] pushed forward the investigations of chaos as well as the analysis of completely integrable systems (see [3] and references therein).

The first explanation of the striking result [1] was proposed by Chirikov and Izrailev [4] on the basis of the Chirikov criteria of overlapping resonances [5]. According to [4] it is necessary to exceed some critical energy value to obtain an overlapping of the resonances, chaos and energy equipartition over linear modes. According to [4], in the case of low-mode excitation (nonlinear sound waves), the critical energy increases with the number of oscillators in the chain (or energy per oscillator is constant). Below this energy it was argued that the resonances are not overlapped and the motion is close to an integrable one. Since some of the initial conditions in [1] were below this border the energy equipartition was absent [4]. The results of [4] were confirmed in the series of analytical and numerical researches [6] where the authors also analysed the dependence of the Lyapunov exponents on the energy. However, these researches showed that the relaxation to an equilibrium distribution could be very long at small energies which makes it difficult to study the transition from global chaos to integrable case.

In this paper the condition of resonance overlapping for long (sound) waves in the limit of small energy is analysed. For long waves the dispersion law is very close to linear. Due to that, for the system with a finite but large number of oscillators N there are some terms in the nonlinear part of the Hamiltonian which are in the resonance even for very low energies. Such resonances not being considered in [4] give a sharp decrease of the chaos border in energy which goes to zero with the increase of the number of particles in the lattice. In this sense the long-wave chaos can exist for arbitrarily small nonlinearity. The physical reason

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of this unusual phenomenon is connected with the linearity of unperturbed system. Due to that, for the sound dispersion law which is typical for long waves, the KAM theorem cannot be applied and chaos can appear for arbitrarily small nonlinear interaction. Such kinds of phenomena have already been studied in different dynamical systems with a few degrees of freedom [7–9]. In such a case the dynamics can be described by a renormalized Hamiltonian independent on the strength of nonlinear interaction. In particular, the measure of chaotic component remains unchanged with the decrease of nonlinearity. In the FPU-problem a deviation of the dispersion law from the linear one gives rise to a critical chaos border which is, however, extremely low and decreases with the number of particles in the chain. The estimates for the chaos border allow us to understand under what conditions energy equipartition sets in. Since generally chaotic systems have a divided phase space with mixed chaotic and integrable components in this paper the energy equipartition is understood in the following sense. Namely, it means that the energy is distributed approximately homogeneously between all modes, however, it does not exclude that some relatively small group of modes may have an integrable dynamics.

We start our analysis from the α-FPU problem with cubic nonlinearity in the Hamiltonian:

$$H = \frac{1}{2}\sum_{n=0}^{N}[{p_n}^2 + (x_{n+1} - x_n)^2] + \frac{\alpha}{3}\sum_{n=0}^{N}(x_{n+1} - x_n)^3 \tag{1}$$

where the first sum gives the Hamiltonian H_0 of the linear waves and the second sum represents the interaction $H_{\rm int}$. The boundary conditions are fixed as $x_0 = 0$; $x_{N+1} = 0$. The eigenmodes (Q_k, P_k) of H_0 are connected with the coordinates x_n, p_k by the equations $x_n = \sqrt{2/(N+1)}\sum_k Q_k \sin(q_k n)$, $p_n = \sqrt{2/(N+1)}\sum_k P_k \sin(q_k n)$ with $q_k = \pi k/(N+1)$, $1 \leqslant k \leqslant N$ [2]. In this representation H_0 can be written as $H_0 = \sum_k ({P_k}^2 + {\omega_k}^2 {Q_k}^2)/2 = \sum_k \omega_k I_k$ with the eigenfrequencies $\omega_k = 2\sin(q_k/2)$. The action-angle variables (I_k, θ_k) are connected with (P_k, Q_k) in the standard way [2].

It is convenient to write the total Hamiltonian in the action-angle variables (I_k, θ_k) of the linear problem. Taking into account that the nonlinear coupling is small, we can keep in $H_{\rm int}$ only the resonant terms corresponding to the resonant three-waves interaction. For long waves, this condition corresponds to $k_3 = k_2 + k_1$. All other terms can be eliminated by averaging over fast oscillations with frequencies of ω_k. After this procedure we obtain the averaged Hamiltonian:

$$\bar{H} = \sum_k \omega_k I_k + \frac{\alpha}{2\sqrt{N+1}}\sum_{k_1,k_2,k_3}(\omega_{k_1}\omega_{k_2}\omega_{k_3} I_{k_1} I_{k_2} I_{k_3})^{1/2}\cos(\theta_{k_3} - \theta_{k_2} - \theta_{k_1})\delta_{k_3,k_1+k_2} \tag{2}$$

which can be written as $\bar{H} = H_0 + \bar{H}_{\rm int}$. Here the bar denotes averaging over fast oscillations with $\omega_k \geqslant \omega_1 = \pi/(N+1)$. The term fast means that $\omega_1 \gg \delta\omega$ where $\delta\omega$ is the typical nonlinear frequency $\delta\omega \sim \partial\bar{H}_{\rm int}/\partial\theta \sim \alpha(E_0/N)^{1/2}\omega_k$. For a few low modes excited around a given k-value, we obtain $\delta\omega \sim \alpha(E_0/N)^{1/2}k/N$ where E_0 is the initial energy. Following [4], where the β-FPU model with quartic nonlinearity had been studied, we can find the chaos border from the condition of the overlapping resonances $\delta\omega \sim \Delta\omega$ where $\Delta\omega \approx \omega_1 \approx \pi/N$ is the distance between the main resonances in (1). According to this condition the global chaos appears for $\tilde{\alpha} = \alpha {E_0}^{1/2} > \tilde{\alpha}_{CHI} \sim \sqrt{N}/k$.

The Hamiltonian $\bar{H}$ has additional integral of motion $E_S = \pi\sum_k k I_k/(N+1) \approx E_0$. For long sound waves ($k \ll N$) we can use approximate expression for the dispersion law $\omega_k = q_k - q_k^3/24$ in H_0 while in the term with $\bar{H}_{\rm int}$ it is sufficient to use $\omega_k = q_k$. By using the new resonant phases $\phi_k = \theta_k - q_k t$ we can transform (2) into the new resonant

Hamiltonian:

$$H_R = -\sigma \sum_{k=1}^{M} k^3 I_k + 2\mu \sum_{k_1=1}^{M} \sum_{k_2=1}^{M-k_1} (k_1 k_2 k_{k_2+k_1} I_{k_1} I_{k_2} I_{k_2+k_1})^{1/2} \cos(\phi_{k_2+k_1} - \phi_{k_2} - \phi_{k_1}) \tag{3}$$

where $\sigma = \pi^3/(24(N+1)^3)$, $\mu = \pi^{3/2}\alpha/(4(N+1)^2)$ and M is the maximal number of harmonics. It is convenient to introduce the new dimensionless time $\tau = \mu t\sqrt{E_S(N+1)/\pi}$ in which the dynamics is described by the renormalized resonant Hamiltonian

$$H_{\mathrm{RN}} = -\nu \sum_{k=1}^{M} k^3 J_k + 2 \sum_{k_1=1}^{M} \sum_{k_2=1}^{M-k_1} (k_1 k_2 (k_2+k_1) J_{k_1} J_{k_2} J_{k_2+k_1})^{1/2} \cos(\phi_{k_2+k_1} - \phi_{k_2} - \phi_{k_1}) \tag{4}$$

with one dimensionless parameter

$$\nu = \frac{\sqrt{\pi}\sigma}{\mu\sqrt{(N+1)E_S}} = \frac{\pi^2}{6\alpha\sqrt{E_S}(N+1)^{3/2}}. \tag{5}$$

The new actions J_k are connected with the old ones by the relation $I_k = E_S J_k (N+1)/\pi$. They are now normalized by the condition $\sum_{k=1}^{M} k J_k = 1$.

Let us analyse now the dynamics of system (4). If initially only few modes are excited around a k-value then the distance between the resonances is $\Delta\omega \approx \nu k^3$ while the width of the resonance is $\delta\omega \sim k^{3/2} {J_k}^{1/2} \sim k$. From these estimates it is clear that the resonances are overlapped [5] for $\nu < \nu_{cr} \sim 1/k^2$ and then chaos arises. In the original variables this means that the chaos border is given by

$$\alpha\sqrt{E_S} > \tilde{\alpha}_s \approx \frac{k^2}{N^{3/2}} \qquad \text{or} \qquad \nu < 1/k^2. \tag{6}$$

This border, which takes into account the degenerate sound resonances $k_3 = k_2 + k_1$, decreases with the growth of N and is N^2 times below the border of global chaos $\tilde{\alpha}_{CHI}$. In the case of the excitation of low modes with $k \sim 1$ the critical energy above which the motion is chaotic is $E_c \sim 1/(\alpha^2 N^3)$. Therefore, chaos arises at zero temperature $T = E_0/N$.

For a better understanding of the properties of system (4) a numerical investigation of its dynamical motion was carried out. The initial conditions were usually fixed as three excited modes with $J_1 = J_2 = J_3 = \frac{1}{6}$ and different phases ϕ. The calculations of the maximal Lyapunov exponent show that above the border (6) the motion is characterized by the positive exponent λ_{RN} that indeed demonstrates the existence of chaos in this regime. Below the border the maximal Lyapunov exponent is zero (except exponentially narrow chaotic layers). A typical example of the dependence of λ_{RN} on the renormalized time τ is presented in figure 1. The energy distribution $E_k = k J_k$ over linear modes is shown in figure 2. To suppress the fluctuations, the values of E_k were averaged over time τ in the time interval [1000–2000]. Below the chaos border (6) the number of excited modes remains the same as for the initial distribution. In contrast, above this border the energy is distributed over some finite width Δk which is much larger than the initial width. For the high values of $k \gg \Delta k$ the distribution decays in an exponential way. In the whole interval of k the energy distribution E_k can be fitted by the effective distribution:

$$f_k = \frac{A}{l(\exp(k/l - \gamma) + 1)} \tag{7}$$

where the length l determines the effective number of excited modes, γ is some constant which mainly effects the shape of the distribution for small k and A is determined by γ via the normalization condition $\sum E_k \approx \int f_k \,\mathrm{d}k = 1$. For the case of figure 2, the optimal value is $\gamma = 2.65$. It is interesting to note that the fitting (7) describes quite well the

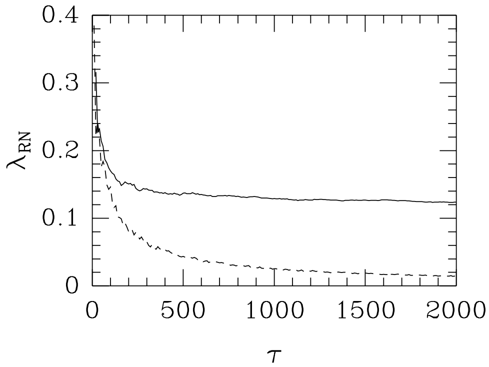

Figure 1. Maximal Lyapunov exponent $\lambda_{\rm RN}$ in (4) as a function of time τ: full curve: $\nu = 0.01$, $H_{\rm RN} = 0.544$, $\lambda_{\rm RN} > 0$; broken curve: $\nu = 1$, $H_{\rm RN} = -5.45$, $\lambda_{\rm RN} \to 0$ (values of $\lambda_{\rm RN}$ are multiplied by 5). For figures 1–4 only three modes were initially excited with $J_1 = J_2 = J_3 = \frac{1}{6}$.

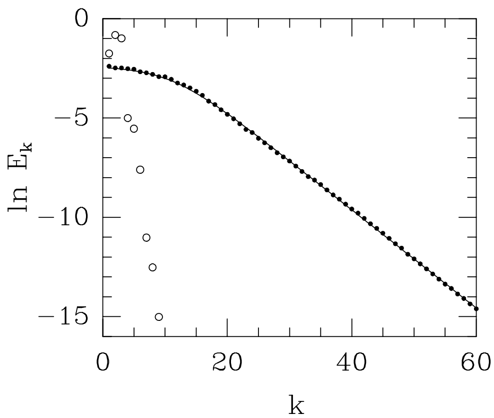

Figure 2. Averaged energy distribution $E_k = kJ_k$ over linear modes k: full circles correspond to the case of the full curve in figure 1 and open circles correspond to the case of the broken curve in figure 1. The full curve gives the fitting distribution (7) with $l = 4.05$; $\gamma = 2.65$, $A = 0.3678$.

distribution E_k in the large interval $0.03 < \nu < 0.0005$ with the same γ and different l. This fact is demonstrated in figure 3 where six distributions are superimposed in the rescaled variables lE_k and k/l. The fitting (7) allows us to determine the dependence of the length l on ν. This dependence is presented in figure 4 and is approximately given by the equation $l = 0.42/\sqrt{\nu}$. The same functional dependence on ν takes place for the quantity $1/E_1$ which characterizes the width of the distribution Δk for small k. The existence of the same scaling on ν for l and $1/E_1$ confirms once more that the distribution E_k has only one scaling parameter l.

The obtained scaling of l from ν can be understood on the following grounds. The nonlinear resonance width in (4) is $\delta\omega \sim \partial H_{\rm RN}/\partial J_k \sim k^{3/2}\sqrt{J_k}k^{1/2}$ with $k \sim l$. The last term $k^{1/2}$ gives the result of summation over k terms with random phases contributing in $\delta\omega$. A typical distance between the resonances is $\Delta\omega \sim \nu k^3$. The number of excited modes is determined by the chaos border given by the resonance overlapping: $\delta\omega > \Delta\omega$. According to this estimate the number of excited modes is $\Delta k \sim l \sim 1/\sqrt{\nu}$ that is in agreement with the numerical dependence from figure 4 and the previous estimate (6). Using the expression for ν we can find the effective number of excited linear modes expressed via the original variables:

$$\Delta k \sim l \sim (\alpha^2 E_0 N^3)^{1/4}. \tag{8}$$

From this expression it follows that for fixed α and E_0 the number of excited modes is quite large but still $\Delta k/N \ll 1$.

In the same way we can obtain an estimate for the maximal Lyapunov exponent $\lambda_{\rm RN}$

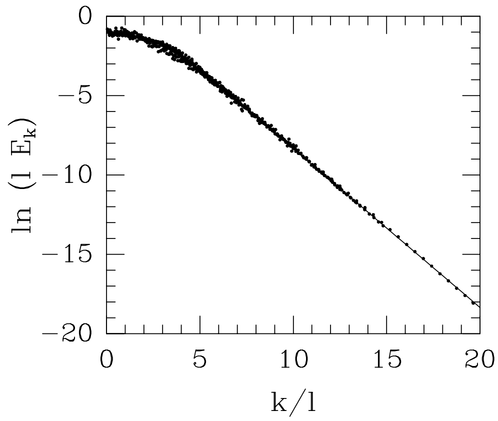

Figure 3. Normalized energy distribution lE_k as function of k/l for the six different values of ν from figure 4 (points). The full curve gives the fitting (7) with γ and A from figure 2.

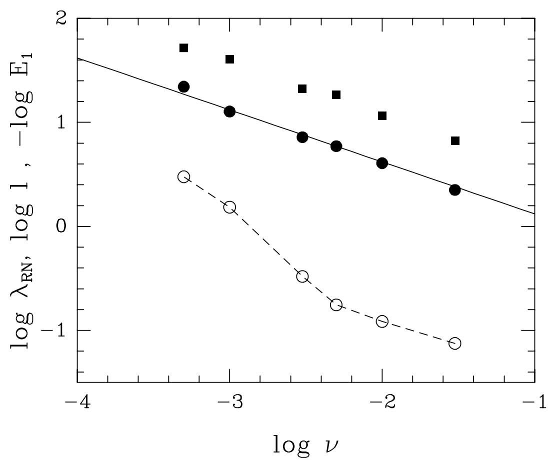

Figure 4. Dependence on ν for: length l obtained from distributions of figure 3 (points); average energy of first mode E_1 (squares); λ_{RN} (open circles). The straight line shows the theoretical dependence $l \sim 1/\sqrt{\nu}$.

in the renormalized Hamiltonian (4). Indeed, $\lambda_{\mathrm{RN}} \sim \delta\omega \sim k^{3/2}\sqrt{kJ_k}$ with $k \sim l$ and $\lambda_{\mathrm{RN}} \sim k \sim 1/\sqrt{\nu}$. Using the relation between the time t for the original system (1) and the time τ in the renormalized Hamiltonian (4) we obtain the estimate for the maximal Lyapunov exponent Λ in the system (1):

$$\Lambda = \frac{\pi\alpha\sqrt{E_S}\lambda_{\mathrm{RN}}}{4(N+1)^{3/2}} \sim \frac{\alpha^{3/2}{E_0}^{3/4}}{N^{3/4}}. \tag{9}$$

The numerical data for the dependence of λ_{RN} on ν are presented in the figure 4. Unfortunately, in the given interval of ν the variation of λ_{RN} is not quite monotonic and further numerical investigations are required for the verification of the theoretical dependence $\lambda_{\mathrm{RN}} \sim 1/\sqrt{\nu}$ (see the discussion below). Let us mention that the sign of ν in (4) is not important and the results are qualitatively the same for $\nu < 0$ when the absolute value of ν should be used in the estimates.

The comparison of Λ with the distance between main resonances $\Delta\omega$ shows that for sufficiently large N the nonlinear resonance width $\delta\omega \sim \Lambda$ becomes larger than $\Delta\omega \sim 1/N$.

The condition $\Lambda > \Delta\omega$ shows that the main resonances in (1) will be overlapped for

$$\alpha\sqrt{E_0} > \tilde{\alpha}_{eq} \approx 1/N^{1/6}. \tag{10}$$

Above this border the nonresonant terms neglected in the derivation of (2) give the overlapping of the main resonances and for $\alpha E_0 > 1/N^{1/3}$ the equipartition over all linear modes modes can be expected. So, in the limit of large N the equipartition can appear at zero energy and zero temperature. The time required to reach the equipartition is inversely proportional to Λ. Here it is important to note that chaos only appears for $\Lambda > 0$, however, $\Lambda > 0$ does not imply ergodicity and is not directly related with the properties of probability distribution in the k-space.

It is interesting to note that some conditions of [1] considered usually as integrable (figure 1 in [3]) have $\nu \approx 0.13$. Direct computation in (4) for this ν value with corresponding initial conditions gives, however, $\lambda_{\mathrm{RN}} = 0$. This makes the question arise about a more exact determination of the border of chaos $|\nu_{cr}|$.

Let us now briefly discuss the properties of chaos in the β-FPU model with quartic interaction $H_{\mathrm{int}} = \beta\sum_n (x_{n+1} - x_n)^4/4$. As in the α-case we should keep only the resonant terms for four waves with $k_1 + k_2 = k_3 + k_4$. The resonance nonlinear width can be estimated in the same way as in [4, 2] $\delta\omega \sim \beta E_0 \omega_k/N$. The overlapping of the main resonances happens for $\beta E_0 > N/k$ [4, 2]. However, for the resonant Hamiltonian, only the deviation of ω_k from the sound law $\pi k/N$ is important, so the distance between the resonances can be estimated as $\Delta\omega \sim k^3/N^3$†. This gives the border of slow chaos $\beta E_0 > k^2/N$ which is much below the standard border [4, 2]. Above this border the number of excited low linear modes is $k \approx \Delta k \sim \sqrt{\beta E_0 N}$ and the maximal Lyapunov exponent is $\Lambda \sim (\beta E_0/N)^{3/2} \sim \delta\omega$. The overlapping of the main resonances takes place for $\Lambda > 1/N$ or $\beta E_0 > N^{1/3}$. Above this border all linear modes are excited leading to energy equipartition. In a difference from the α-model this border grows with N but the critical temperature $T = E_0/N$ still goes to zero.

The above theoretical estimates were based on the comparison of the splitting between linear modes and nonlinear spread width. As in the case of the Chirikov criteria such an approach cannot exclude a possibility that the system under investigation is completely integrable or is very close to some of them. This point is very crucial for the α-FPU problem since at low energy it is very close to the Toda lattice (see [2]). Due to that generally we should expect that in contrast to the above estimates and numerical data the dynamics of α-FPU problem will be integrable. To understand this apparent contradiction with the numerical data additional simulations had been carried out. Namely, the total number of harmonics M has been increased up to $M = 120$ for the parameters of figure 1(a). While the simulations become very heavy in such a case they give approximately $\ln\tau/\tau$ decay of λ_{RN} up to $\lambda \approx= 0.02$ at maximally reached $\tau = 400$. This indicates that in a real system with very large M the Lyapunov exponent will be zero. At the same time such a change of M did not affect the averaged energy distribution (see figure 2). For a better check of this point a number of numerical simulations with the original Hamiltonian (1) have been done with N up to 151 and the initial conditions corresponding to figure 1(a) with fixed $\nu = 0.01$. For $N = 61$ the renormalized Lyapunov exponent (see (9)) was stabilized around $\lambda_{\mathrm{RN}} \approx 0.13$ (the time $t_{\max}$ in the simulations was $t_{\max} \approx 9 \times 10^5$); for $N = 101$ the exponent was also stabilized around $\lambda_{\mathrm{RN}} \approx 0.065$ ($t_{\max} \approx 9 \times 10^6$). However, in both of these cases the averaged energy distribution E_k significantly increased at high modes as opposed to

† Here for $\Delta\omega$ we used the estimate k^3/N^3 which is correct for the majority of k. But for some k values (e.g. near $k_1 = k_2 = k_3 = k_4$) this distance is k^2/N^3 that gives a wider spreading with $\Delta k \sim \beta E_0 N$, $\Lambda \sim (\beta E_0)^2/N$ and equipartition border $\beta E_0 \sim 1$. However, the chaos originating from these resonances should be much slower.

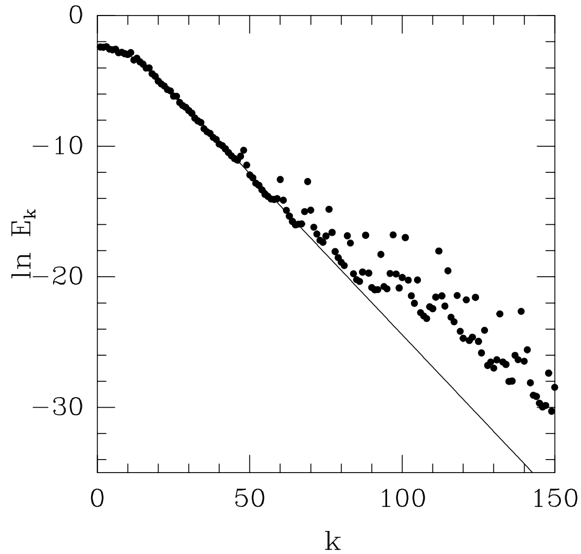

Figure 5. Same as in figure 2 obtained from the Hamiltonian (1) (see text).

figure 2. For $N = 151$ during all $t < t_{max} \approx 6 \times 10^6$ the value of λ_{RN} was decreasing as $\ln \tau/\tau$ reaching $\lambda_{RN} \approx 0.04$ at t_{max}. At the same time the averaged distribution E_k was practically the same as in figure 2 (see figure 5). These additional data show that in the low-energy limit the dynamics of the α-model is not chaotic ($\lambda_{RN} = 0$) as it can be expected from the comparison with the Toda lattice, despite the fact that the energy distribution (see (7)) is correctly given by the above estimates derived from the renormalized Hamiltonian. The reason why the renormalized dynamics is so sensitive to the maximal value of M is still not quite clear. It is possible that the important effects of coupling to high modes can be understood from a nonlinear wave equation in the continuous limit (see [10]). Very recently, the properties of the Lyapunov exponent in the system (1) with N up to 128 were studied [11].

The situation for the β-model can be more interesting. Indeed, apparently this model is not close to any integrable system and the above renormalization approach and estimates should give correct chaos borders. The picture of low-energy chaos developed here is qualitatively close to the one in [12]. However, additional investigations of this regime are still highly desirable. They should clarify some uncertainties in the estimate of $\Delta\omega\dagger$. Also the question of coupling to high modes can play a very crucial role [13].

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