Chaos vs Thermalization in the Nuclear Shell Model

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Generic signatures of quantum chaos found in realistic shell model calculations are compared with thermal statistical equilibrium. We show the similarity of the informational entropy of individual eigenfunctions in the mean-field basis to the thermodynamical entropy found from the level density. Mean occupation numbers of single-particle orbitals agree with the Fermi-Dirac distribution despite the strong nucleon interaction.

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Chaotic dynamics is one of the most extensively developing subjects in physics. Near the ground state a many-body quantum system is modeled by a gas of quasiparticles, and symmetry (lack of symmetry) of the mean field determines regularity (chaoticity) of single-particle motion ("one-body chaos"). As the excitation energy and level density increase, the residual interactions transform the stationary states into complicated superpositions of quasiparticle configurations. Already at early stages of this process the local level statistics exhibit [1–3] features of chaos. The pattern of chaotic signatures mixed with the apparent failure of the independent quasiparticle model can be called "many-body chaos" [4].

In this Letter we study the relation between the complicated structure of eigenstates and the general principles of statistical mechanics. Having at our disposal exact eigenfunctions of a model Fermi system with strong interactions (the nuclear shell model [5,6]), we compare their statistical properties with those of the equilibrium thermal ensemble.

The statistical approach implies that the observables are insensitive to the actual microscopic state of the system. Averaging over the equilibrium ensemble should give the same outcome as an expectation value for a typical single stationary state at the same energy [7]. Being in a certain sense a definition of equilibrium, this requires the similarity of the generic wave functions in a given energy region. Perfect gases give the simplest example of many-body systems where such properties of stationary states are evident. However, the above description also fits the notion of stochastic dynamics. In the classical case, the correspondence between statistical equilibrium and chaotic trajectories exploring the whole energy surface is taken almost for granted by many authors, see, for example, [8]. As for the quantum case, already the pioneering paper on compound nucleus by Bohr [9] contains on equal footing elements of both patterns, chaos and thermalization. The definition of chaotic wave functions by Percival [10] assumes that all of them "look the same" and cover the entire available configuration space. According to Berry [11], in systems with the chaotic classical limit such as a gas of hard spheres, the eigenfunctions behave like random superpositions of plane waves. This conjecture is in fact equivalent to the microcanonical ensemble and leads [12] to the standard (Maxwell-Boltzmann, Bose-Einstein, or Fermi-Dirac) momentum distribution for individual particles.

One can argue that the gas of hard spheres is a specific case where the interaction is reduced to exclusion of the inner volume of the spheres. However, it was shown by van Hove [13] that the broader class of gaslike systems displays quantum ergodicity; a random initial wave function evolves with time into a state which gives the same values of observables as the microcanonical ensemble. The assumption of randomness or phase incoherence is similar to Berry's conjecture or even to Boltzmann's *Stosszahlansatz*. In self-sustained Fermi systems like nuclei, the residual interaction cannot be reduced to rare pairwise collisions, and the generalization of the results derived for rigid spheres is not known. We address this question by comparing the signatures of quantum chaos and complexity in the nuclear shell model with the pattern of thermal equilibrium.

The actual computations were performed for 12 particles in the *sd* shell with the Wildenthal interaction [5,14] which has been tested by numerous calculations of observables. Many-body basis states $|k\rangle$ were constructed with good total angular momentum J, M, parity π, and isospin T. In this basis, the Hamiltonian has diagonal elements which are dominated by the one-body part and numerically are spread from -120 to -60 MeV, and two-body off-diagonal elements with an average value of about 0.5 MeV.

We studied earlier [6] the signatures of quantum chaos both in energy eigenvalues and in complexity of eigenvectors. Eigenvalues E_α for states with $J^\pi T = 0^+0$ and 2^+0 (with model space dimensions $N = 839$ and $N = 3273$, respectively) showed perfect agreement with chaotic level statistics. The amplitudes C_k^α of eigenfunctions

$$|J^\pi T;\alpha\rangle = \sum_k C_k^\alpha |J^\pi T;k\rangle \qquad (1)$$

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have, for a given $|\alpha\rangle$ (except for the edges of the spectrum), Gaussian distribution with zero mean value and variance $\overline{(C_k^\alpha)^2} = 1/N^\alpha$. The localization length N^α gives a measure of complexity of the eigenstates at energy E_α. In the extreme chaotic case N^α approaches the dimension N, manifesting total mixing and delocalization of eigenfunctions ($N^\alpha \approx 0.9N$ in the middle of the spectrum for the realistic interaction and $N^\alpha \approx N$ for the degenerate model with no stabilizing influence of the mean field). The informational entropy,

$$S^\alpha = -\sum_k (C_k^\alpha)^2 \ln[(C_k^\alpha)^2], \tag{2}$$

as well as moments of the distribution function of the components C_k^α, show that, as the excitation energy increases, the eigenfunctions become more complex and the maximum of complexity is reached in the middle of the spectrum. Our measures of complexity are basis dependent. We argued [6,15] that the mean-field basis is preferential for such an analysis.

The same process of stochastization can be described in the basis-independent thermodynamic language. A closed equilibrated system with a sufficiently high number of degrees of freedom is excited into an energy interval $(E, E + \Delta E)$ where the density of states with given values of exact integrals of motion ($J^\pi T$ in our case) is $\rho(E)$. The average ("thermodynamic") characteristics are determined by the statistical weight $\Omega(E) = \rho(E)\Delta E$, the exact value of the uncertainty ΔE being not important as long as $\Delta E \ll E$. Assuming that equilibrium can be described by the microcanonical ensemble, the statistical weight determines the thermodynamic entropy $S^{\text{th}}(E) = \ln \Omega(E)$ and temperature T according to

$$\frac{\partial S^{\text{th}}}{\partial E} = \frac{1}{T}. \tag{3}$$

For a subsystem of a large closed system, this leads [7] to the canonical or grand canonical ensembles. The thermodynamic description is known to be fruitful even for finite systems like nuclei [16] where the statistical ensembles are not strictly equivalent due to the pronounced role of fluctuations. The empirical nuclear level density can be satisfactorily modeled by that of Fermi gas or rather Fermi liquid.

In our system with a restricted Hilbert space, the level density $\rho(E)$ saturates at maximum entropy and infinite temperature (3). For $N = 839$ states 0^+0, it is presented as a histogram in Fig. 1(a) together with a Gaussian fit with the centroid at $E_0 = -90$ MeV and variance $\sigma_E = 13$ MeV. For such a fit, the temperature $T = \sigma_E^2/(E_0 - E)$ is shown by a solid line in Fig. 1(b). The right half of the spectrum is associated with decreasing entropy and negative temperature. Similar results are valid for other $J^\pi T$ classes, and the Gaussian fit parameters turn out to be the same. The Gaussian rather than semicircle $\rho(E)$ is expected [1] for a many-body system with two-body residual interactions. The transition from Gaussian to semicircle level density occurs

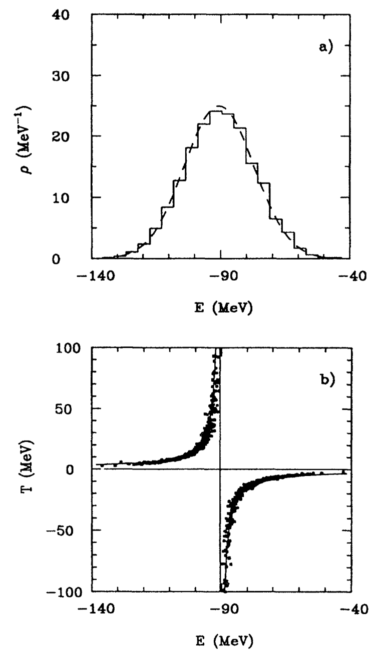

FIG. 1. Level density $\rho(E)$ for 0^+0 states (a); a histogram is compared with the Gaussian fit (dashed line); (b) temperature calculated from the global fit to the level density (solid line) and found from the occupation numbers of Fig. 2(a) (dots).

[17] when many-body forces are introduced, lifting the selection rules for interactions between configurations. On the other hand, the banded random matrix theory predicts, both numerically [18] and analytically [19], the semicircle density for a sufficiently wide band of nonzero matrix elements around the main diagonal. The realistic Hamiltonian matrix is banded in the basis of many-body configurations coupled via two-body forces. But the matrix is far from being random since its elements are linear combinations of only a few (63 in the *sd* shell) two-body matrix elements.

To compare the global thermodynamic behavior with the properties of individual eigenfunctions, we have calculated the evolution of single-particle occupation numbers (the isoscalar monopole component of the single-particle density matrix) n_λ^α of the orbitals $\lambda = (l, j)$ along the spectrum of stationary many-body states $|\alpha\rangle$, Eq. (1),

$$n_{lj}^\alpha = \frac{1}{2} \sum_{m\tau} \langle \alpha | a_{ljm\tau}^\dagger a_{ljm\tau} | \alpha \rangle. \tag{4}$$

The results are shown in Fig. 2 where the panels (a), (b), and (c) correspond to 0^+0, 2^+0, and 9^+0 ($N = 657$) states, respectively. All classes exhibit an identical smooth behavior of occupation numbers. It suggests that one can associate to each eigenstate $|\alpha\rangle$ a single-particle "temperature" T_{sp}^α defined by the (grand canonical) Fermi distribution $f_{lj}^\alpha = \{\exp[(e_{lj} - \mu)/T_{\text{sp}}^\alpha] + 1\}^{-1}$. In the center of the spectrum where one expects infinite temperature, all occupancies $f_{lj}^\alpha = n_{lj}^\alpha/(2j + 1)$ indeed become equal to each other, the common value being 1/2 for our case of

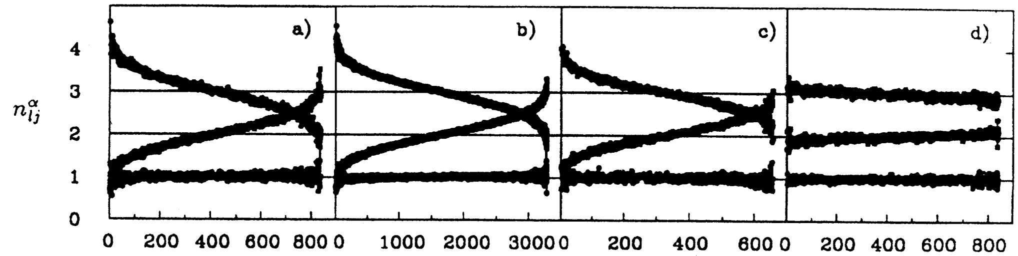

FIG. 2. Single-particle occupation numbers, Eq. (4), vs state number α for states 0^+0 (a), 2^+0 (b), and 9^+0 (c). (d) Occupation numbers for 0^+0 states for diagonal matrix elements reduced by a factor of 10. For all panels the three curves (sets of points) refer to $s_{1/2}$, $d_{3/2}$, and $d_{5/2}$ orbitals, from bottom to top.

12 particles in the *sd* shell. The effective single-particle energies $e_{lj} - \mu$ obtained from the slopes of the lines in Fig. 2 are -3.4, 0.0, and 4.7 MeV for $d_{5/2}$, $s_{1/2}$, and $d_{3/2}$ orbitals, respectively (for comparison, the shell model spin-orbit splitting near the ground state is 7.2 MeV). One can then extract the $T_{\rm sp}^\alpha$ for each level $|\alpha\rangle$, Fig. 1(b) (dots), and check that, despite the strong interaction, the "single-particle thermometer" on average measures the same temperature as obtained from the level density.

These results imply that the system can be considered as an equilibrated Fermi liquid and its properties can be expressed in terms of occupation numbers for a gas of interacting quasiparticles. The microscopic mechanism of equilibration can be understood from the fragmentation of projected shell model states $|J^\pi T; k\rangle$. Applying the recipes of statistical spectroscopy [20], one can explain the approximately constant occupation of the $s_{1/2}$ orbital and the smooth evolution of occupation factors for $d_{3/2}$ and $d_{5/2}$ orbitals as a function of excitation energy. The thermodynamics of the system is determined mainly by the stabilizing action of the mean field. An artificial reduction by a factor of 10 of the diagonal matrix elements implies [Fig. 2(d)] constancy of occupation numbers (vanishing heat capacity).

Using the occupancies f_{lj}^α of individual orbitals, one can calculate the single-particle entropy of the quasiparticle gas [7] for each state $|\alpha\rangle$,

$$S_{\rm sp}^\alpha = -\sum_{lj\tau}(2j+1)[f_{lj}^\alpha \ln f_{lj}^\alpha + (1-f_{lj}^\alpha)\ln(1-f_{lj}^\alpha)]. \tag{5}$$

Now we have three, apparently different, entropylike quantities: thermodynamic entropy $S^{\rm th}(E) \sim \ln\rho(E)$, informational entropy S^α (2), and single-particle entropy $S_{\rm sp}^\alpha$ (5), the latter two for individual eigenstates. In Fig. 3 we juxtapose the energy behavior of $\exp(S)$ for different physical situations, I, II, and III (columns). Rows (a), (b), and (c) present $S^{\rm th}$, S^α, and $S_{\rm sp}^\alpha$, respectively, for 0^+0 states.

The column I of Fig. 3 shows the limit of a relatively weak off-diagonal interaction (the diagonal matrix elements are amplified by a factor of 10). The thermodynamic entropy I(a) displays Gaussian behavior of a combinatorial nature typical for a slightly imperfect Fermi gas in a finite number of states. Within the fluctuations related to the transition from the microcanonical to grand canonical ensemble, it is quite similar to the single-particle picture I(c). The informational entropy I(b) is low; only at high level density does one see some effects of mixing. This is an equilibrium picture of almost noninteracting particles where the degree of complexity given by the informational entropy is only weakly correlated with thermalization. Using the language of kinetic theory, collisions (mixing) are necessary for equilibration, but the equilibrium properties do not depend on the collision rate.

The opposite case III corresponds to a strong off-diagonal interaction [as in Fig. 2(d), the diagonal matrix elements are reduced by a factor of 10]. Almost all states are strongly mixed and the informational entropy III(b) is near its chaotic maximum [6] of $\exp(S^\alpha)_{\rm chaotic} =$

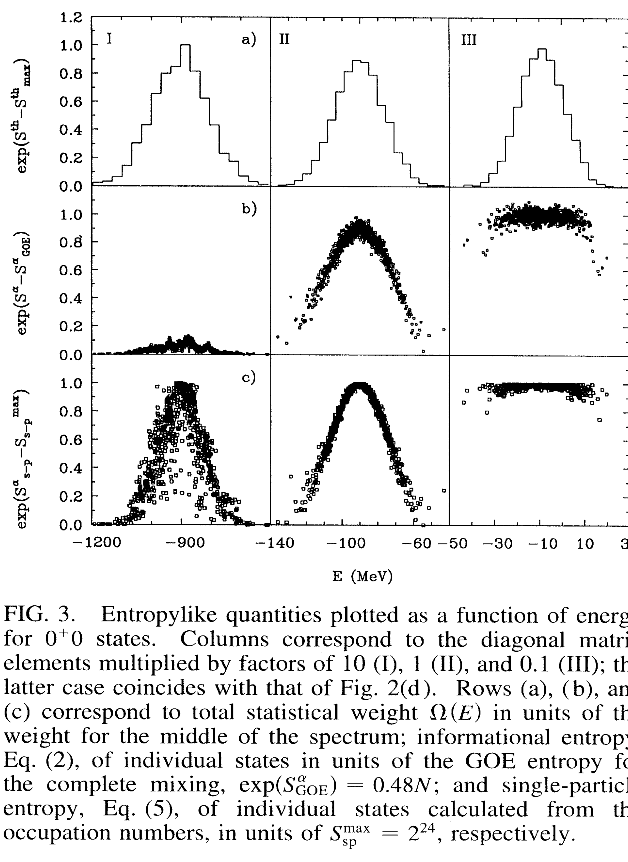

FIG. 3. Entropylike quantities plotted as a function of energy for 0^+0 states. Columns correspond to the diagonal matrix elements multiplied by factors of 10 (I), 1 (II), and 0.1 (III); the latter case coincides with that of Fig. 2(d). Rows (a), (b), and (c) correspond to total statistical weight $\Omega(E)$ in units of the weight for the middle of the spectrum; informational entropy, Eq. (2), of individual states in units of the GOE entropy for the complete mixing, $\exp(S_{\rm GOE}^\alpha) = 0.48N$; and single-particle entropy, Eq. (5), of individual states calculated from the occupation numbers, in units of $S_{\rm sp}^{\rm max} = 2^{24}$, respectively.

$0.48N = 404$ for 0^+0 states. S^α_{sp} [III(c)] is also at the maximum level corresponding to the equiprobable population of orbitals. Within the fluctuations, S^α and S^α_{sp} coincide. However, as seen from III(a), the system has normal thermodynamic properties governed by the level density. Therefore, in the absence of the (diagonal) mean field, the response to thermal excitation cannot be expressed in terms of quasiparticles. In both cases, I and III, the informational entropy becomes irrelevant for thermodynamics, although it still characterizes the degree of complexity of eigenstates in the mean-field basis.

The case of the realistic mean field and empirical residual interaction is shown in column II. When the magnitudes are normalized, all three entropies are identical within fluctuations except for the edges of the spectrum. Near the ground state the Fermi surface is already smeared due to the two-body correlations. Even for the low-lying states, the single-particle occupation numbers and informational entropy show deviations from the frozen Fermi gas. The difference between low thermodynamic temperature and single-particle temperature as measured, for instance, in particle knockout experiments near the ground state was discussed in [15]. For the majority of states and for the mean field consistent with residual interactions, the thermodynamic entropy defined either via the global level density or in terms of occupation numbers behaves similar to the informational entropy.

One can conclude that (i) equilibrium heating is strongly correlated with the evolution of "many-body" chaos and increase of complexity of individual eigenstates; and (ii) equilibrium properties of a heated system with strong interactions can still be described in terms of quasiparticles and their effective energies in the appropriate mean field (this opens the way for explicit calculation of matrix elements between compound states [21]).

Let us stress the special role of the mean-field representation [15] both for studying the degree of chaoticity of specific wave functions [6] and for the statistical description. With the artificially depressed or enhanced diagonal matrix elements, the level density and the thermodynamic entropy S^{th} are qualitatively the same as in the realistic case [Fig. 3(a)]. However, with no mean field [Fig. 3(III)] the increase of complexity measured by the S^α and the mixing of quasiparticle configurations measured by the S^α_{sp}, going together, are different from the heating measured by the level density and the "normal" entropy S^{th}. The interaction is too strong, and the mixing does not depend on the actual level spacing. Almost all wave functions "look the same" regardless of level density, and the quasiparticle "thermometer" cannot resolve the spectral regions with different temperatures. In this case the microcanonical description is the only possible.

Finally we would like to give a more formal argument in favor of the direct correspondence between chaos and thermalization. The general description of a quantum system with noncomplete information uses the density matrix $\mathcal{D}$ which has, in an arbitrary many-body basis $|k\rangle$, matrix elements $\mathcal{D}_{kk'} = \overline{C_k C^*_{k'}}$ where the amplitudes are averaged [7] over the ensemble. If the ensemble is generated by interaction with the environment, the states of the entire system are $|k;\nu\rangle$, where ν labels the states of the environment compatible with the state $|k\rangle$ of the subsystem under study. Then $\mathcal{D}_{kk'} = \sum_\nu C_{k\nu} C^*_{k'\nu}$. The corresponding statistical entropy $S = -\text{Tr}(\mathcal{D}\ln\mathcal{D})$ is basis independent and equals zero for pure states of the isolated subsystem. For canonical equilibrium ensembles, S coincides with the thermodynamic entropy. Let us consider a gas of quasiparticles in the ensemble generated by the residual interaction. This makes sense only after proper separation of global smooth dynamics from quasirandom incoherent processes. Such a separation defines the optimal basis, namely that of the self-consistent mean field [15] (our "simple" states $|k\rangle$). Compound states $|\alpha\rangle$ mimic the "total" system (quasiparticles + interaction field). The ensemble average of $\mathcal{D}_{kk'} = \overline{C^\alpha_k C^\alpha_{k'}}$ is to be taken over neighboring states $|\alpha\rangle$. If the amplitudes C^α_k are uncorrelated and all neighboring states $|\alpha\rangle$ are similar, only diagonal elements of $\mathcal{D}_{kk'}$ survive, and we come to the informational entropy (2).

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