Michigan State University

National Superconducting Cyclotron Laboratory

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MIHAI HOROI, VLADIMIR ZELEVINSKY, and B. ALEX BROWN

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Mihai Horoi[1,3], **Vladimir Zelevinsky**[1,2,4] and **B. Alex Brown**[1,2]

[1] *National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48824-1321, USA*

[2] *Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824-1116, USA*

[3] *Institute of Atomic Physics, Bucharest, Romania*

[4] *Budker Institute of Nuclear Physics, Novosibirsk 630090 Russia*

Abstract

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.

Chaotic dynamics is one of the most extensively developing subjects in physics. Although classical deterministic chaos is well understood [1,2] a rigorous definition of quantum chaos does not exist. The relation to the classical limit is straightforward in problems of the one-body type. Quantum billiards is the best known example. Classically, regular or chaotic features of motion are determined by the shape of boundaries. The corresponding quantum level statistics [3,4] display local correlations and fluctuations of Poisson or Wigner type. In many-body quantum systems a semiclassical picture arises in the mean field approximation when the system is modeled by a gas of independent quasiparticles and symmetry (lack of symmetry) of the mean field determines regularity (chaoticity) of single-particle motion. As the excitation energy and level density increase, the residual interactions between quasiparticles transform the stationary states into exceedingly complicated superpositions of the original "simple" configurations. Already at early stages of this process the local level statistics exhibit [5] features of chaos. The pattern of chaotic signatures mixed with the apparent failure of the independent quasiparticle model can be called "many-body chaos" [6].

In this paper we address the question of 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 [7,8]) 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 wave function at the same energy [9]. 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. To go beyond the perfect gas, we note that 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 [10]. As for the quantum case, already the pioneering paper on compound nucleus by Niels Bohr [11] contains on equal footing elements of both patterns, chaos and thermalization. In discussing properties of chaotic wave functions, Percival [12] assumes that all of them "look the same" and cover the entire available configuration space. According to Berry [13], in systems with the chaotic classical limit as a gas of hard spheres, the eigenfunctions should behave like random superpositions of plane waves. This conjecture is in fact equivalent to the microcanonical ensemble and leads [14] 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 of many-body dynamics where the interaction is reduced to exclusion of the inner volume of the spheres. However, it was shown long ago by van Hove [15] that the broader class of gas-like 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 molecular chaos (*Stosszahlansatz*). Self-sustained Fermi systems like nuclei behave, according to Landau-Migdal theory, analogously to the gas of interacting quasiparticles. The residual interaction cannot be reduced to rare pairwise collisions and is to be treated on exact quantum-mechanical basis. The generalization of the results derived for rigid spheres to the strongly interacting case is not known. We address this question by comparing the signatures of quantum chaos 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 [7,16] which has been tested earlier by numerous calculations of observables. Many-body basis states $|k\rangle$ were constructed with good total angular momentum J, its projection M, parity π and isospin T, T_3. Within this basis, the hamiltonian matrix has diagonal elements which are dominated by the one-body part and numerically are spread over the region from -120 to -60 MeV, and off-diagonal elements with an average value of about 0.5 MeV. Eigenvalues E_α for states with $J^\pi T$ equal to 0^+0 and 2^+0 (with model space dimensions $N = 839$ and $N = 3273$ respectively) clearly showed chaotic level statistics [8]. The amplitudes C_k^α of eigenfunctions

$$|J^\pi T;\alpha\rangle = \sum_k C_k^\alpha |J^\pi T;k\rangle \tag{1}$$

have, for a given $|\alpha\rangle$, 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 local chaos in the vicinity of energy E_α. In the extreme chaotic case N^α approaches the space dimension N manifesting total mixing and delocalization of eigenfunctions. We found $N^\alpha \approx 0.9N$ in the middle of the spectrum for realistic interaction and $N^\alpha \approx N$ for the degenerate model with no stabilizing influence of the mean field. Instead of N^α, it is also convenient to use the informational entropy [17]

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

as well as moments of the distribution function of the components C_k^α. All such characteristics 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 [8] that the mean field basis is preferential for such an analysis.

The same process of stochastization can be described in the 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 ("thermodynamical") characteristics are determined by the statistical weight $\Omega(E) = \rho(E)\Delta E$ the exact value of the uncertainty ΔE being not important as far as $\Delta E \ll E$. One can then define the thermodynamic entropy $S^{th}(E) = \ln\Omega(E)$ and temperature T according to

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

Of course, this description is basis-independent.

A system with a finite Hilbert space can be heated until the level density saturates at maximum entropy and infinite temperature (3). The local level density $\rho(E)$ for $N = 839$

states 0^+0 is presented as a histogram in Fig. 1 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 (3) is $T = \sigma_E^2/(E_0 - E)$. Similar results are valid for other $J^\pi T$ classes and the Gaussian fit parameters turn out to be the same. This means that one may speak about thermodynamic equilibrium. The right half of the spectrum is associated with decreasing entropy and negative temperature.

The Gaussian rather than semicircle $\rho(E)$ is expected [4] for a many-body system with two-body residual interaction. The transition from semicircle to Gaussian level density occurs [18] 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 [19] and analytically [20], 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 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 on Fig. 2 where the panels *a*,*b* and *c* correspond to $0^+0, 2^+0$ and 9^+0 ($N = 657$ states), respectively. Although the states within each $J^\pi T$ class are orthogonal and apparently have nothing in common, all classes exhibit an identical smooth behavior of occupation numbers. This is an additional evidence for an equilibrated system.

In the center of the spectrum all occupancies $f_{lj}^\alpha = n_{lj}^\alpha/(2j+1)$ become equal to each other the common value being 1/2 for our case of 12 particles in the *sd*-shell. It suggests that one can associate to each eigenstate $|\alpha\rangle$ an effective single-particle "temperature" T_{s-p}^α

defined by the Fermi distribution $f_{lj}^{\alpha} = \{\exp[(e_{lj} - \mu)/T_{s-p}^{\alpha}] + 1\}^{-1}$. T_{s-p}^{α} changes smoothly with E_α being the same for all complicated wave functions near E_α as it should be for an intensive thermodynamic quantity. It becomes infinite simultaneously with the thermodynamic temperature (3) when the memory of the initial single-particle energies e_λ is lost.

The microscopic mechanism of equilibration can be understood from the analysis of fragmentation of projected shell model states $|J^\pi T; k\rangle$. Applying the recipes of statistical spectroscopy of French and Ratcliff [21] one can explain the approximately constant occupation of the $s_{1/2}$ orbital as well as the smooth evolution of occupation factors for $d_{3/2}$ and $d_{5/2}$ orbitals as a function of excitation energy. The conclusion is that the thermodynamics of the system is determined mainly by the stabilizing action of the mean field, despite the strong mixing of configurations. An artificial reduction by a factor 10 of the diagonal matrix elements implies (Fig. 2*d*) constancy of occupation numbers, i.e. vanishing heat capacity. In this case one has an analog of a dense hot gas with a very short quasiparticle lifetime.

Using the occupancies f_{lj}^{α} of individual orbitals one can calculate the single-particle entropy of the quasiparticle gas [9] for each state $|\alpha\rangle$,

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

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

The column I of Fig. 3 shows the limit of a stable mean field and relatively weak interaction (the diagonal matrix elements are amplified by a factor 10). The thermodynamical entropy Ia is determined solely by the level density. It displays Gaussian behavior of a pure combinatorial nature typical for a slightly imperfect Fermi-gas in a finite number of states. It is quite similar to the single-particle picture I*c*. The informational entropy I*b* is very low; only in the middle region of enhanced level density does one see some effects of mixing.

The opposite case III corresponds to the strong residual interaction (as in Fig. 2*d* the diagonal matrix elements are reduced by a factor 10). Almost all states are totally mixed and the informational entropy III*b* is near its chaotic maximum [8] of $\exp(S^{\alpha})_{chaotic} = 0.48N = 404$ for this class of states. S^{α}_{s-p} is also constant (III*c*) on the maximum level corresponding to the equiprobable population of orbitals. Within the fluctuations, S^{α} and S^{α}_{s-p} coincide. However, the level density still has the Gaussian shape (IIIa) so that the system has normal thermodynamic properties. It means that in the absence of the mean field the response of the system to thermal excitation cannot be formulated in terms of quasiparticle degrees of freedom. Therefore the informational entropy calculated in the quasiparticle basis becomes irrelevant from thermodynamic viewpoint.

The realistic case of the mean field consistent with the empirical residual interaction is shown in column II. When the magnitudes are normalized to each other, all three entropies become identical within fluctuations. Therefore, using Eq.(3), we can identify the temperature scales as well. For example, in Fig. 4 we show the temperature which follows from Eq.(3) and Gaussian fit (Fig. 1) for $\rho(E)$, as compared to T^{α}_{s-p} extracted from the occupation factors of Fig. 2*a*-*c* with the use of the Fermi distribution which allows one to determine effective single-particle energies $e(lj)$. From the horizontal line corresponding to the $s_{1/2}$ orbital, it follows that the chemical potential $\mu \approx e(s_{1/2})$. The *d*-orbitals can be determined with respect to this level. In the α-scale of Fig. 2, the occupation numbers n_{λ} have, except for the edges, a constant slope $(dn_{\lambda}/d\alpha)_0$. Therefore one can use the middle point of infinite temperature and the Gaussian width σ_E to find

$$e_{\lambda} - \mu = 4\rho(E_0)\sigma_E^2 \frac{1}{2j_{\lambda}+1}(dn_{\lambda}/d\alpha)_0. \tag{6}$$

Numerical values $e(d_{5/2}) - \mu = -3.4$ MeV and $e(d_{3/2}) - \mu = 4.7$ MeV for the effective single-particle energies can be compared to the shell model spin-orbit splitting 7.2 MeV near the ground state.

Thus, we have studied the relation of the individual properties of the eigenstates to statistical features of the equilibrium thermal ensemble. For the self-consistent mean field and residual interactions, the thermodynamic entropy defined either via the global level density or in terms of single-particle occupation numbers behaves in the same way as the informational entropy of generic compound states. It allows one to conclude that (i) onset of "many-body" chaos is accompanied by the transition to thermodynamic equilibrium; (ii) average equilibrium properties of a heated many-body 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 [22]).

Let us stress the special role of the mean field representation [23] both for studying the degree of chaoticity of specific wave functions [8] and for the statistical description. With the artificially depressed or enhanced diagonal matrix elements, the level density still keeps the Gaussian shape so the thermodynamic entropy S^{th} is qualitatively the same as in the realistic case (Fig. 3a). 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}_{s-p}, going together, are different from the total 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. It means that, with no stable mean field, the quasiparticle "thermometer" cannot resolve the spectral regions with different temperatures.

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 non-complete 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 [9] over the ensemble. If the ensemble is generated by interaction with the environment, possible states of the entire system are $|k;\nu\rangle$ where ν characterizes 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 $S = -Tr(\mathcal{D} \ln \mathcal{D})$ 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 [23] (our "simple" states $|k\rangle$). Complicated stationary states $|\alpha\rangle$ mimic the "total" system (quasiparticles + interaction field). The ensemble average of $\mathcal{D}_{kk'} = \overline{C_k^\alpha C_{k'}^\alpha}$ is to be taken over several neighboring states $|\alpha\rangle$. If the amplitudes C_k^α 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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Figure captions

Figure 1. Level density $\rho(E)$ for $0^{+}0$ states; a histogram is compared with the Gaussian fit (dashed line).

Figure 2. Single-particle occupation numbers, Eq.(4), *vs* state number α for states $0^{+}0$ (panel *a*), $2^{+}0$ (panel *b*), and $9^{+}0$ (panel *c*). Panel *d* shows occupation numbers for $0^{+}0$ states for diagonal matrix elements reduced by a factor 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. At the middle of the spectrum all curves correspond to half-filled orbitals (occupation numbers 1, 2 and 3 respectively).

Figure 3. Entropy-like 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 thermodynamic entropy, informational entropy, Eq.(2), of individual states, and single-particle entropy, Eq.(5), of individual states calculated from the occupation numbers, respectively. The e^{S} values in panels *c* are in units of 10^{4}.

Figure 4. Temperature found from the Fermi-Dirac occupation numbers of Fig. 2*a*, points, and calculated from the global fit to the level density of Fig. 1, solid line.

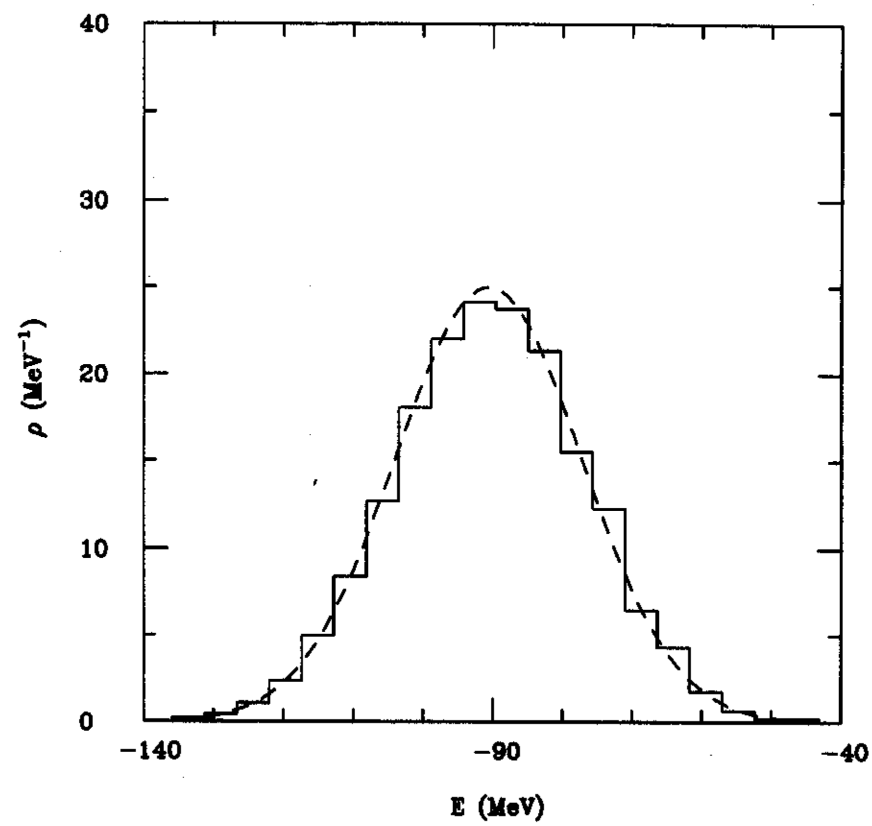
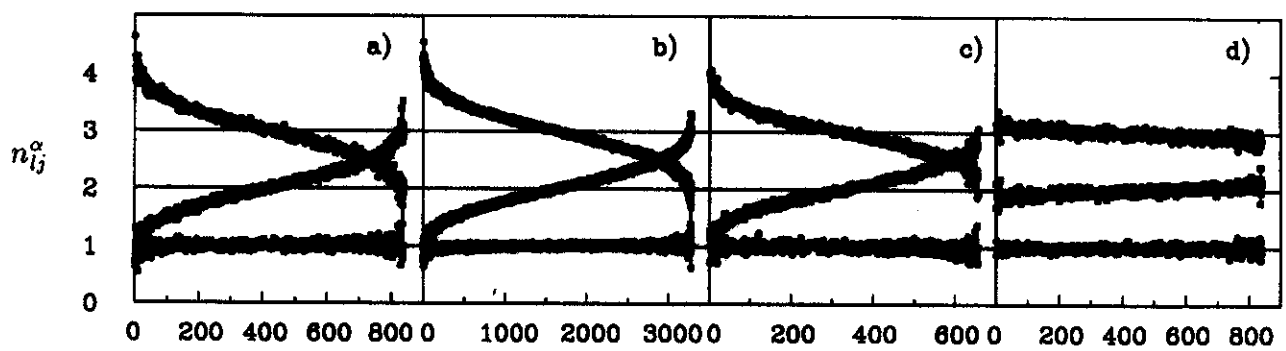


Figure 1:



a)
b)
c)
d)
n_{lj}^{α}
4
3
2
1
0
0 200 400 600 800
0 1000 2000 3000
0 200 400 600
0 200 400 600 800

Figure 2:

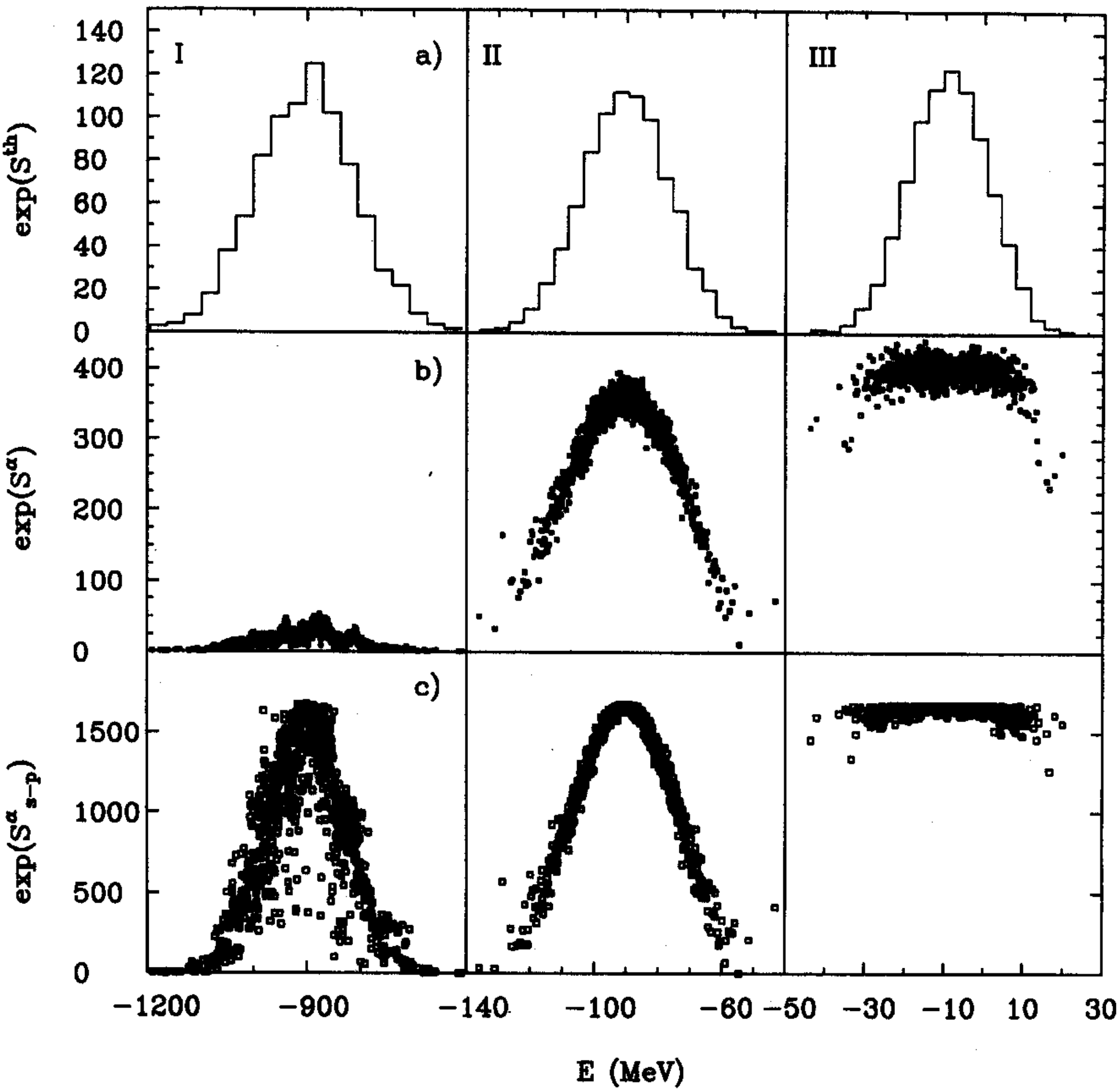


Figure 3:

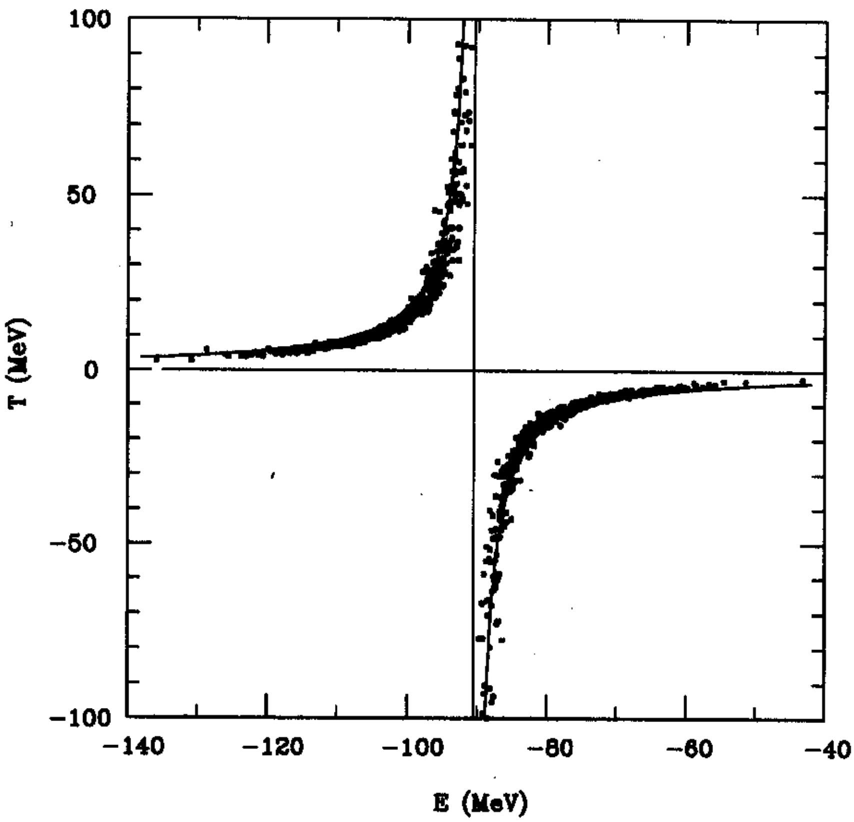


Figure 4: