Photo made during the conference can be found on the web page (see album "Santa Barbara"):

http://picasaweb.google.com/felix.izrailev

Onset of chaos and thermalization in isolated quantum systems of interacting particles: Old and recent results

F. M. Izrailev

Instituto de Física, BUAP, Puebla, México

and

Michigan State University, USA

In collaboration with:

V. V. Flambaum, F. Borgonovi, L.F. Santos

Santa Barbara, August 20, 2012

Many-body chaos

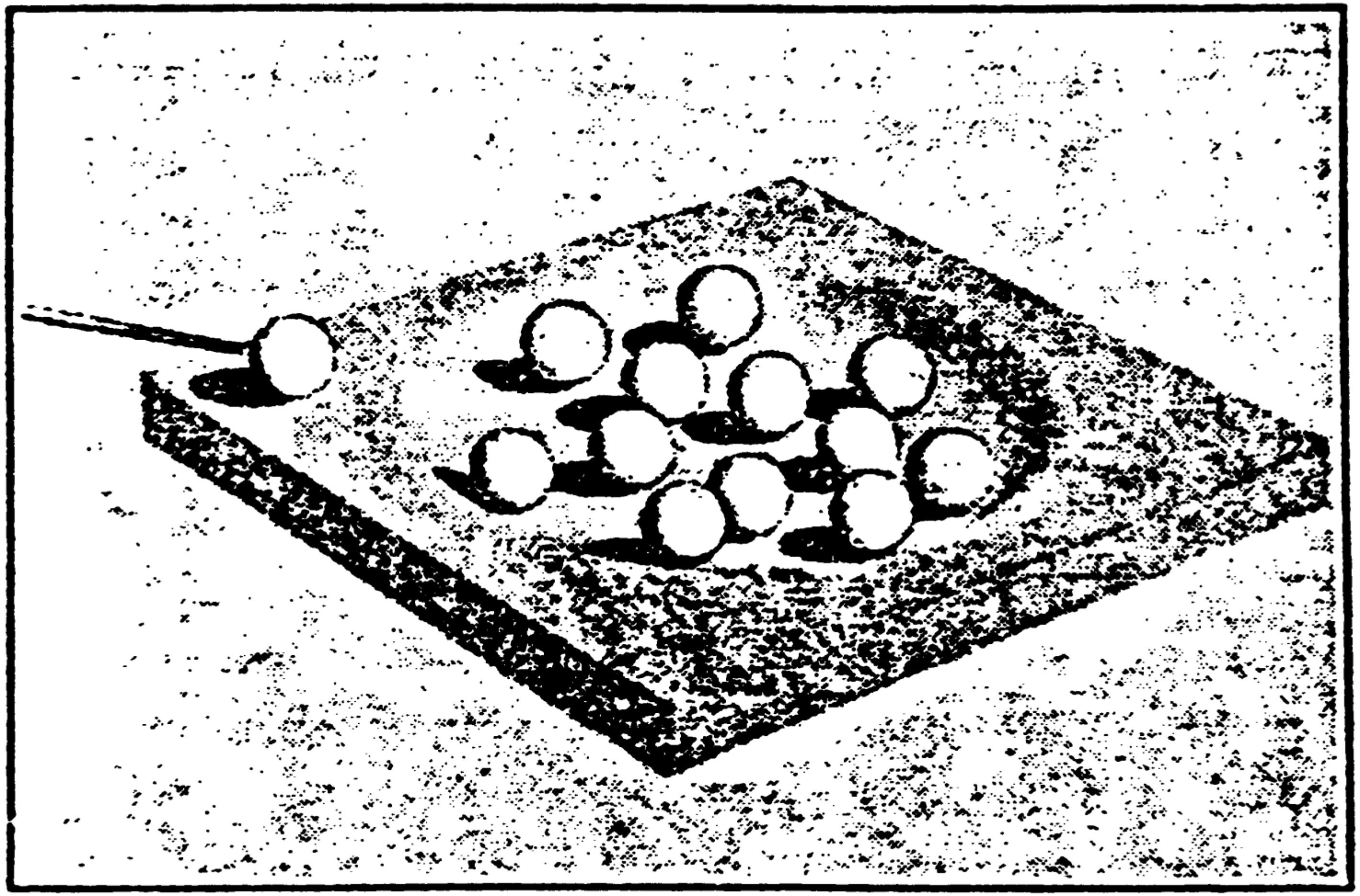


Fig. 35. Picture illustrating the compound nucleus idea, as presented by N. Bohr in 1936. In a neutron-nucleus collision the constituent nucleons are viewed as billiard balls and the nuclear binding as a shallow basin (taken from [112]).

Random Matrix Theory

E.Wigner (1955) : local statistical properties of spectra of complex quantum systems such as of heavy nuclei, are universal, and can be described by the RMT

The commonly used quantity is the level spacing distribution

Wigner surmise: $$p(s) = As^{\beta} \exp\left(-Bs^{2}\right)$$

E.Wigner (1957) : "The problem of the spacing of levels is neither a terribly important one nor have I solved it."

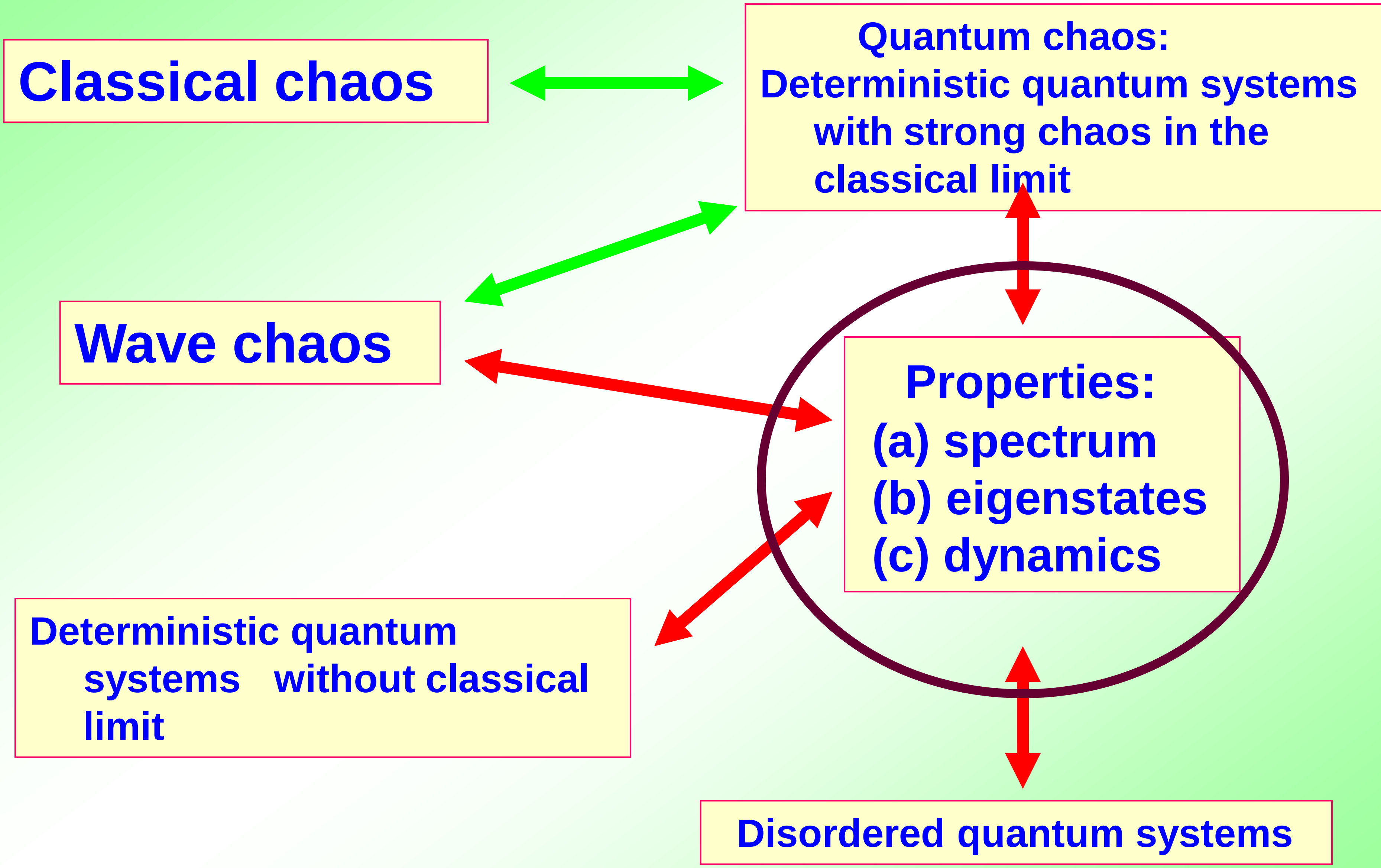
"Quantum chaos" in deterministic systems

S.W. McDonald and A.N. Kaufman, "Spectrum and Eigenfunctions for a Hamiltonian with Stochastic Trajectories", Phys. Rev. Lett. 42 (1979) 1189.

G.Casati, I.Guarneri, F.Valz-Gris, "On the connection between quantization of nonintegrable systems and statistical theory of spectra", Lett. Nuovo Cimento 28 (1980) 279.

M.V. Berry, "Quantizing a Classically Ergodic System: Sinai's Billiard and the KKR Method", Annals of Physics, 131 (1981) 163.

O.Bohigas, M.-J.Giannoni, C.Schmit, "Characterization of Quantum Chaotic Spectra and Universality of Level Fluctuation Laws", Phys. Rev. Lett. 52 (1984) 1.


Classical chaos
Quantum chaos:
Deterministic quantum systems with strong chaos in the classical limit
Wave chaos
Properties:
(a) spectrum
(b) eigenstates
(c) dynamics
Deterministic quantum systems without classical limit
Disordered quantum systems

Chaotic eigenstates

Volume 108A, number 2 PHYSICS LETTERS 18 March 1985

AN EXAMPLE OF CHAOTIC EIGENSTATES IN A COMPLEX ATOM

Boris V. CHIRIKOV

Institute of Nuclear Physics, 630090 Novosibirsk, USSR

Received 7 January 1985

Statistically processing a group of excited states with the total angular momentum and parity $J^{\pi} = 1^{+}$ in the cerium atom reveals that their eigenfunctions are random superpositions of some few basic states. A possible dynamical mechanism responsible for the formation of those chaotic states is briefly discussed.

M.Shapiro and G.Goelman, "Onset of Chaos in an Isolated Energy Eigenstate", Phys. Rev. Lett. 53 (1984) 1714.

Chaotic eigenstates as the condition for thermalization

L.D.Landau and E.M.Lifshitz:

† It may again be mentioned that, according to the fundamental principles of statistical physics, the result of the averaging is independent of whether it is done mechanically over the exact wave function of the stationary state of the system or statistically by means of the Gibbs distribution. The only difference is that in the former case the result is expressed in terms of the energy of the body, and in the latter case as a function of its temperature.

Statistical Physics, Vol.5 (Pergamon, Oxford, 1969)

J.M.Deutsch, "Quantum statistical mechanics in a closed system, Phys. Rev. A 43 (1991) 2046.

M.Srednicki, "Chaos and quantum thermalization", Phys. Rev. E 50 (1994) 888.

Chaos and thermalization in nuclei and atoms

M.Horoi, V.Zelevinsky, B.A.Brown, Phys. Rev. Lett. 74 (1995) 5194; V.Zelevinsky, M.Horoi, B.A.Brown, Phys. Lett. B 350 (1995) 141; V.Zelevinsky, B.A.Brown, M.Horoi, N.Frazier, Phys. Rep. 276 (1996) 85.

V.V.Flambaum, A.A.Gribakina, G.F.Gribakin, M.G.Kozlov, "Structure of compound states in the chaotic spectrum of the Ce atom: Localization properties, matrix elements, and enhancement of weak perturbations, Phys. Rev. A 50 (1994) 267.

in particular, the reduced density matrix operator was analyzed numerically for individual eigenstates, and compared with analytical average over number of chaotic states

Chaotic eigenstates in a gold atom

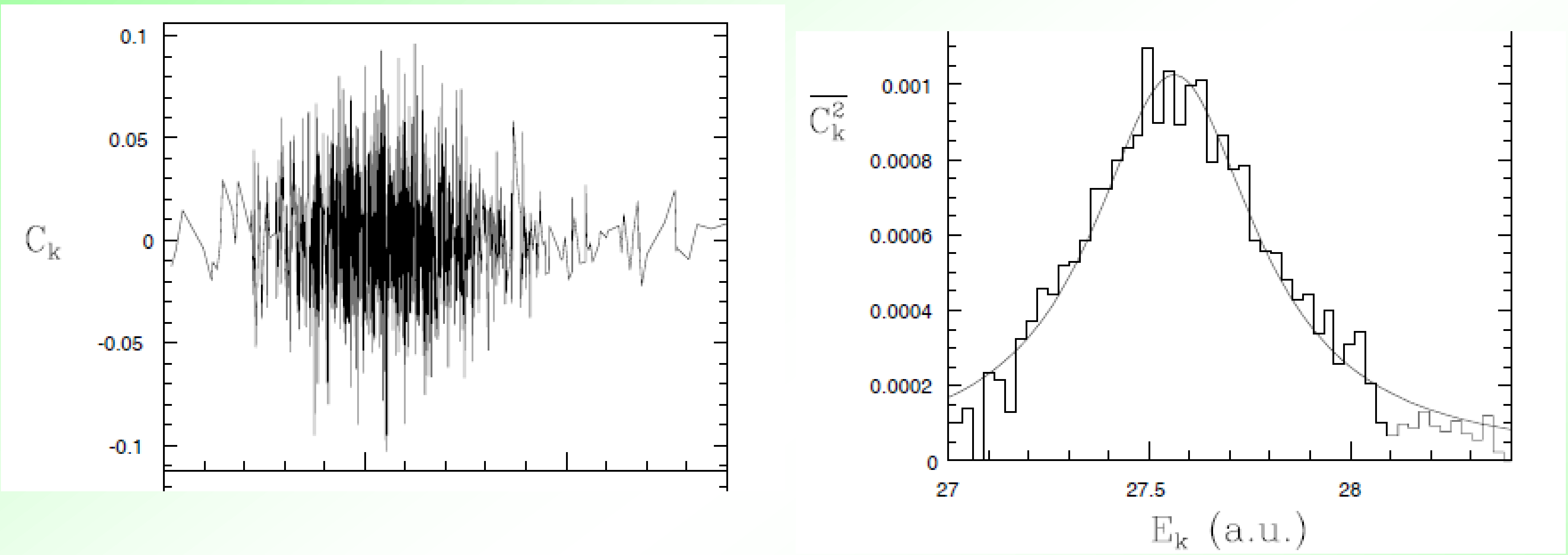


FIG. 3. Components of the 590th $J^\pi = \frac{13}{2}^-$ eigenstate from a two-configuration calculation (top), and a fit of $\overline{C_k^2}(E)$ by the Breit-Wigner formula (6) (bottom).

G.F.Gribakin, A.A.Gribakina, V.V.Flambaum,
arXiv:physics/9811010; Aust. J. Phys. 52 (1999) 443.

(problem of electron recombination)

Thermalization in an isolated gold atom

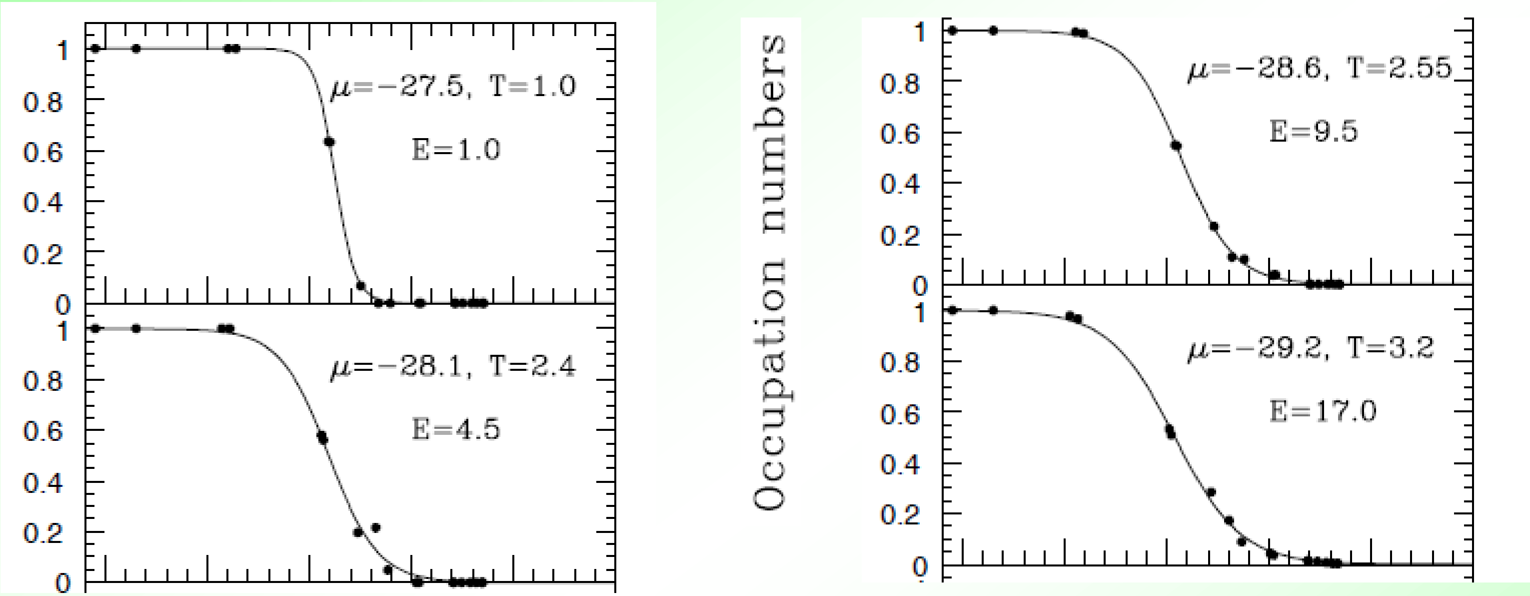


FIG. 7. Orbital occupation numbers in Au^{24+} calculated numerically from Eq. (7) at excitation energies $E = 1$, 4.5, 9.5, 17 and 27.5 a.u. (solid circles), and the Fermi-Dirac distributions (solid line) with temperature T and chemical potential μ chosen to give best fits of the numerical data.

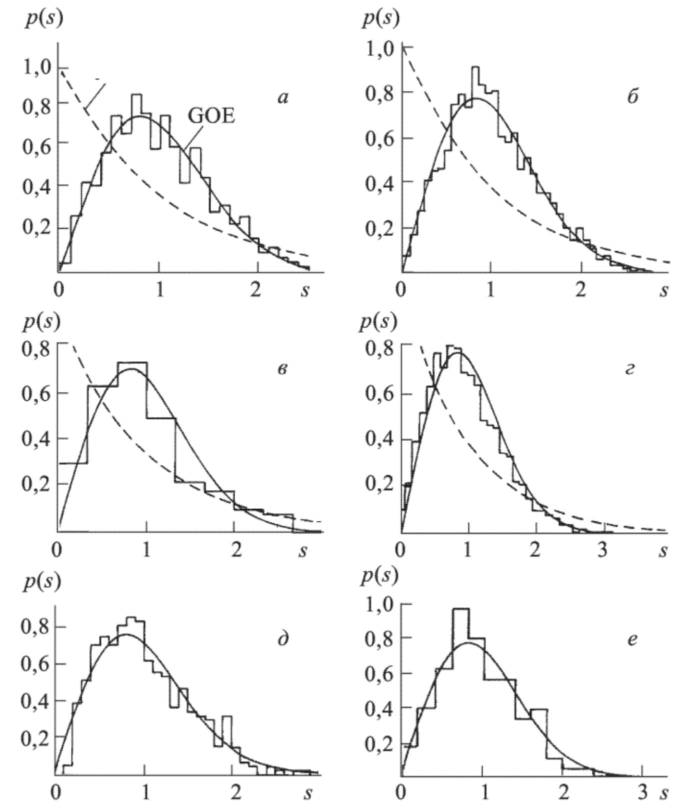
G.F.Gribakin, A.A.Gribakina, V.V.Flambaum,
arXiv:physics/9811010; Aust. J. Phys. 52 (1999) 443.

Universality of chaos

Sinai billiard

Excited molecule NO_2

Microwave billiard



H-atom in magnetic field

Acoustic modes in quartz

Spectra of vibrations of a plate

V.V.Flambaum and F.M.I., "Statistical theory of finite Fermi systems based on the structure of chaotic eigenstates", Phys. Rev. E 56 (1997) 5144; V.V.Flambaum, F.M.I., G.Casati, Phys. Rev. E 54 (1996) 2136.

" A type of "microcanonical" partition function is introduced and expressed in terms of the average shape of eigenstates $F(E_k, E)$ *where E is the total energy of the system. This partition function plays the same role as the canonical expression* $\exp\left(-E^{(i)}/T\right)$ *for open systems in a thermal bath…"*

The following problems have been considered:

(a) the distribution of occupation numbers and its relevance to the canonical and Fermi-Dirac distribution;
(b) criteria of equilibrium and thermalization;
(c) the thermodynamical equation of state and the meaning of temperature;
(d) the meaning of temperature, entropy and heat capacity;
(c) the increase of temperature due to the interaction…."

Two-Body Interaction Model

$$H = \sum_{k}^{m} \varepsilon_k a_k^+ a_k + \frac{1}{2} \sum_{kqpr} V_{kqpr} a_k^+ a_q^+ a_p a_r$$

$|k\rangle, |q\rangle, |p\rangle, |r\rangle$ single-particle states

V_{kqpr} two-body matrix elements (random or dynamical)

m number of single-particle states

n number of particles ("quaisi-particles")

ε_k energy of single-particle states

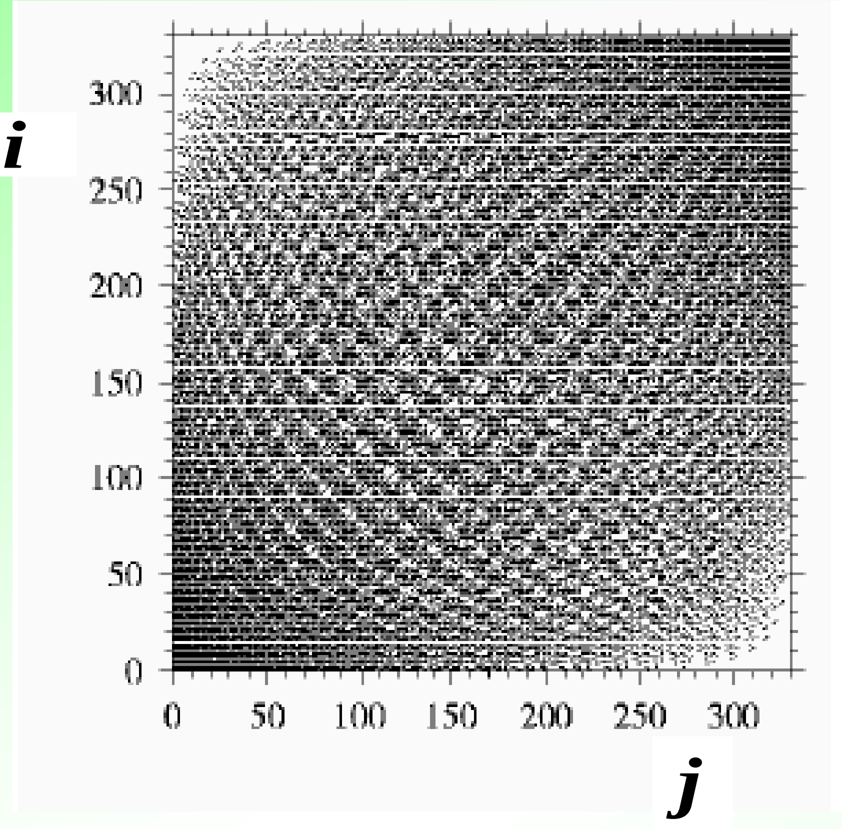
H is considered in the many-particle basis of

$$H_0 = \sum_{k}^{M} \varepsilon_k a_k^+ a_k$$

H_0 determines the basis in which the dynamics occurs

Many-body localization

H_{ij}



D - density of **all** many-body states

d_f - density of many-body states **directly connected** by the two-body interaction

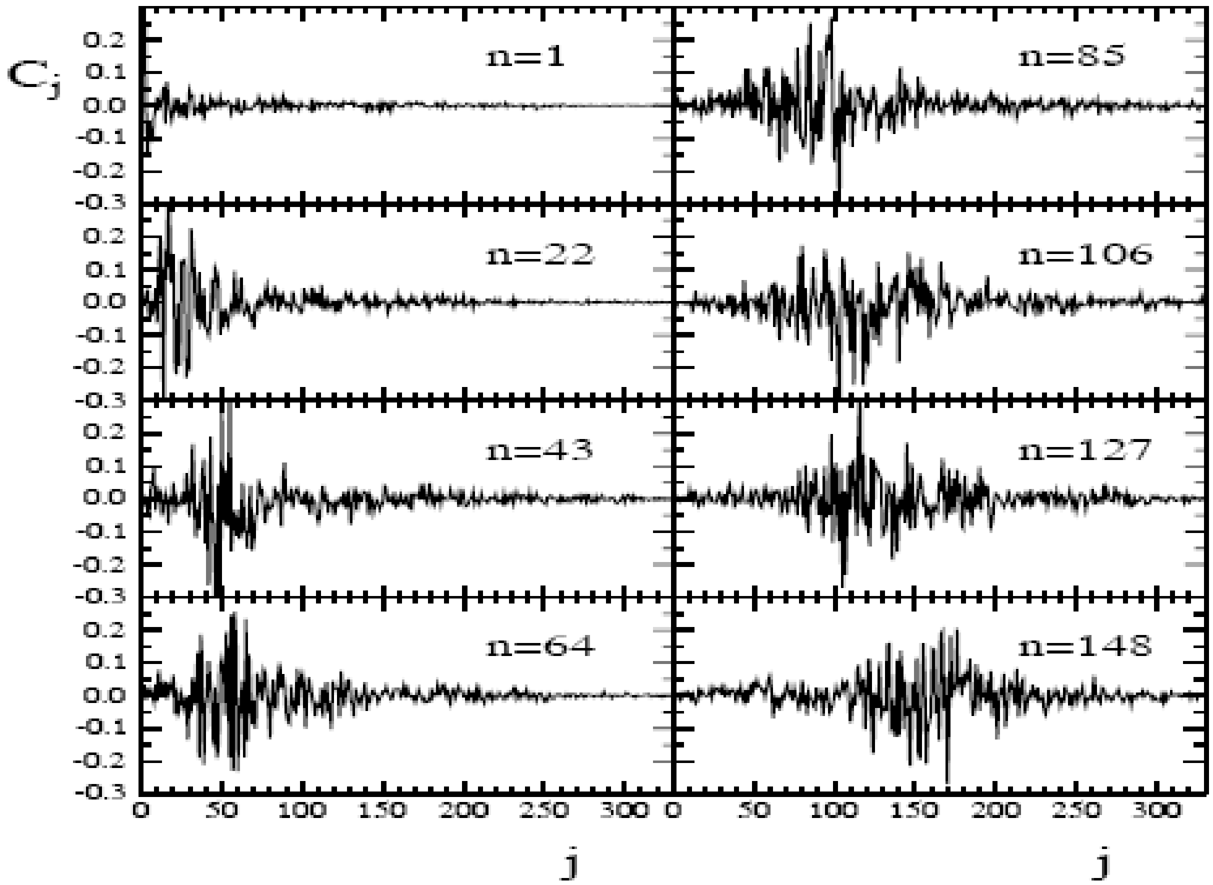
Onset of chaos: $V / d_f \geq 1$

B.Altshuler et. al (1997)

$$V > V_{cr} \approx 8 d_0 / [4n + n(n-1)(m-n-1)]$$

FIG. 1. Sparsity of the Hamiltonian matrix H_{n_1,n_2} for $n = 4$ particles, $m = 11$ orbitals. Black points are non-zero matrix elements.

Transition to “chaos”: chaotic eigenstates



Fermi-Dirac distribution

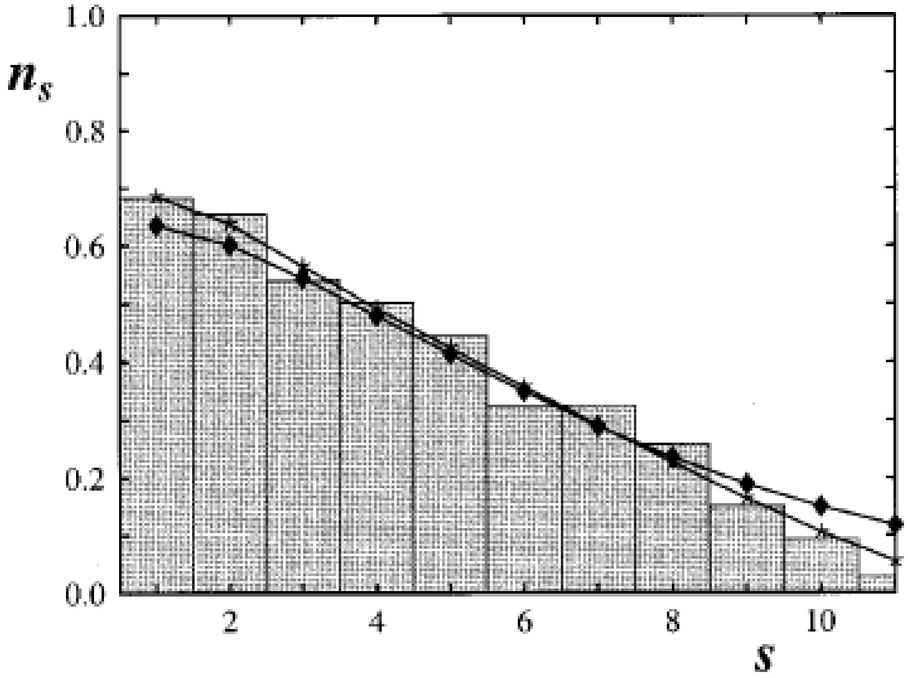


FIG. 1. Analytical description of the occupation numbers. Data are given for the two-body random interaction model (1) of $n=4$ Fermi particles distributed over $m=11$ orbitals with $V=0.20$ and

Circles: analytical description versus numerical data,

Diamonds: Fermi-Dirac with thermodynamical temperature

$$S_{\rm th} = \ln \rho(E) + {\rm const},$$

$$\frac{1}{T_{\rm th}} = \frac{dS_{\rm th}}{dE} = \frac{d\,\ln \rho}{dE}.$$

Shannon entropy of packets

$$S(t) = -\sum_n w_n(t) \ln w_n(t) \qquad w_n(t) = \left|C_n(t)\right|^2$$

"**Cascade model" (the flow of probability in the H_0 - space)**

V.V.Flambaum and F.M.I. – Phys. Rev. E 64 (2001) 036220

Result: $S(t) \approx \Gamma t \ln M$ **(for infinite number of states)**

for strong interaction $t_0 < t \le t_c$

M **is the number of directly coupled states**

Γ **is the width of the strength function**

One-Dimensional Bose System

$$H = \sum_{k=-M}^{M} \varepsilon_k \hat{n} + \frac{g}{2L} \sum \hat{a}_k^+ \hat{a}_q^+ \hat{a}_p \hat{a}_r \delta(k+q-p-r)$$

where L -- length of a ring; $n = \frac{N}{L}$ -- density of bosons

N -- number of bosons

$\hat{n}_k = \hat{a}_k^+ \hat{a}_k$ and $|k\rangle$ -- single-particle levels with $\varepsilon_k = \frac{4\pi^2 k^2}{L^2}$

G.P.Berman, F.Borgonovi, F.M.I., A.Smerzi – PRL 92 (2004) 030404

It is known that $n/g \to \infty$ corresponds to the mean-field regime and $n/g \to 0$ is the Tonks-Girardeau regime

- integrable system !

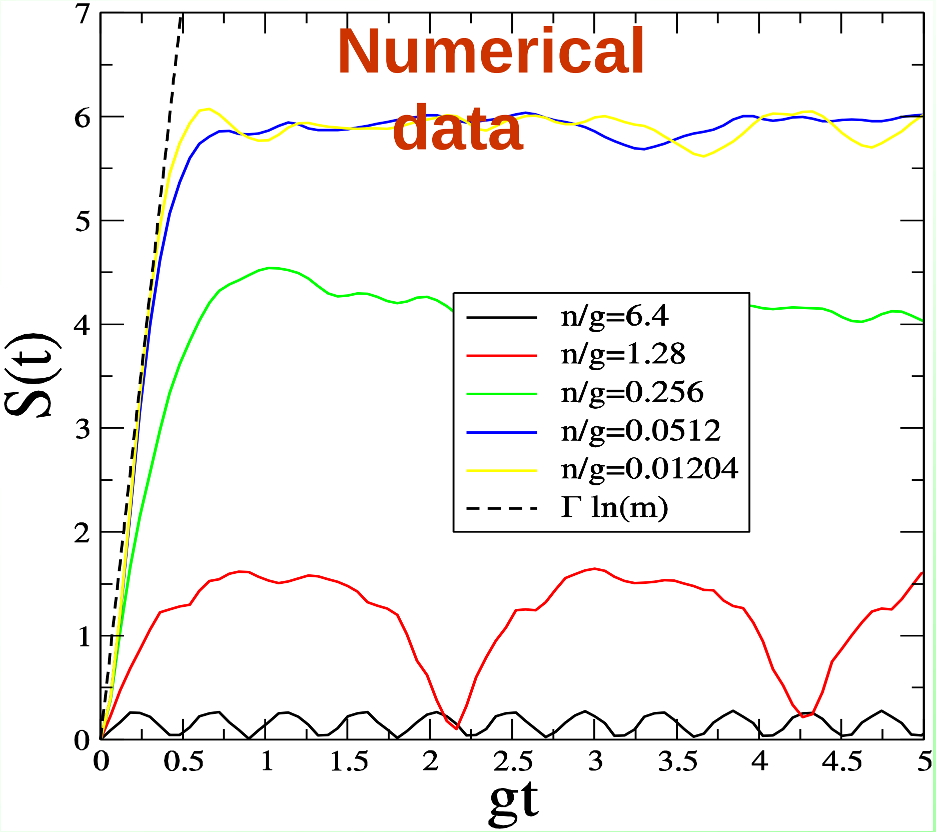
Transition occurs at $n/g \approx 1$

Transition from regular to irregular dynamics

At $t = 0$ all bosons occupy the level with $k = 0$

(ground state for $g = 0$)

What is going on after switching on the interaction $g \neq 0$ between bosons, for $t > 0$?



$m \equiv M$

Experimental setup is proposed to observe this transition

$$S(t) \approx \Gamma t \ln M$$

Chaos and relaxation dynamics in 1/2-spin models

model 1 integrable

$$H_1 = H_0 + \mu V_1,$$

$$H_0 = \sum_{i=1}^{L-1} J\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right),$$

$$V_1 = \sum_{i=1}^{L-1} J S_i^z S_{i+1}^z$$

model 2 non-integrable

$$H_2 = H_1 + \lambda V_2,$$

$$V_2 = \sum_{i=1}^{L-2} J\left[\left(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y\right) + \mu S_i^z S_{i+2}^z\right].$$

$$\lambda_{cr} \approx 0.5$$

- for transition from Poisson to Wigner-Dyson

L.F.Santos, F.Borgonovi, F.M.I., Phys. Rev. Lett. 108 (2012) 094102; Phys. Rev. E 85 (2012) 036209.

Emergence of chaotic states

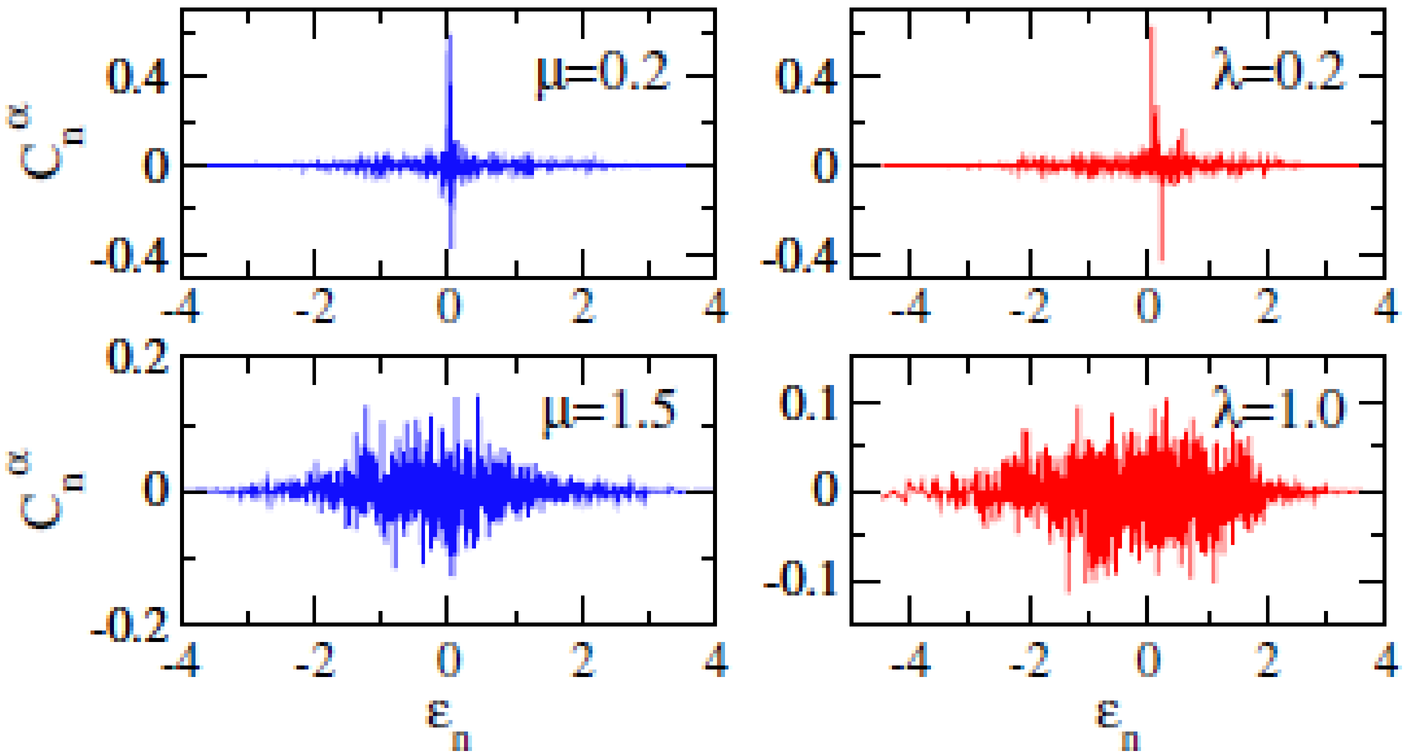


FIG. 2 (color online). Typical localized (top) and extended (bottom) eigenstates for model 1 (left) and model 2 (right).

$|\alpha\rangle$ **- basis of** H

$|n\rangle$ **- basis of** H_0

Structure of eigenfunctions

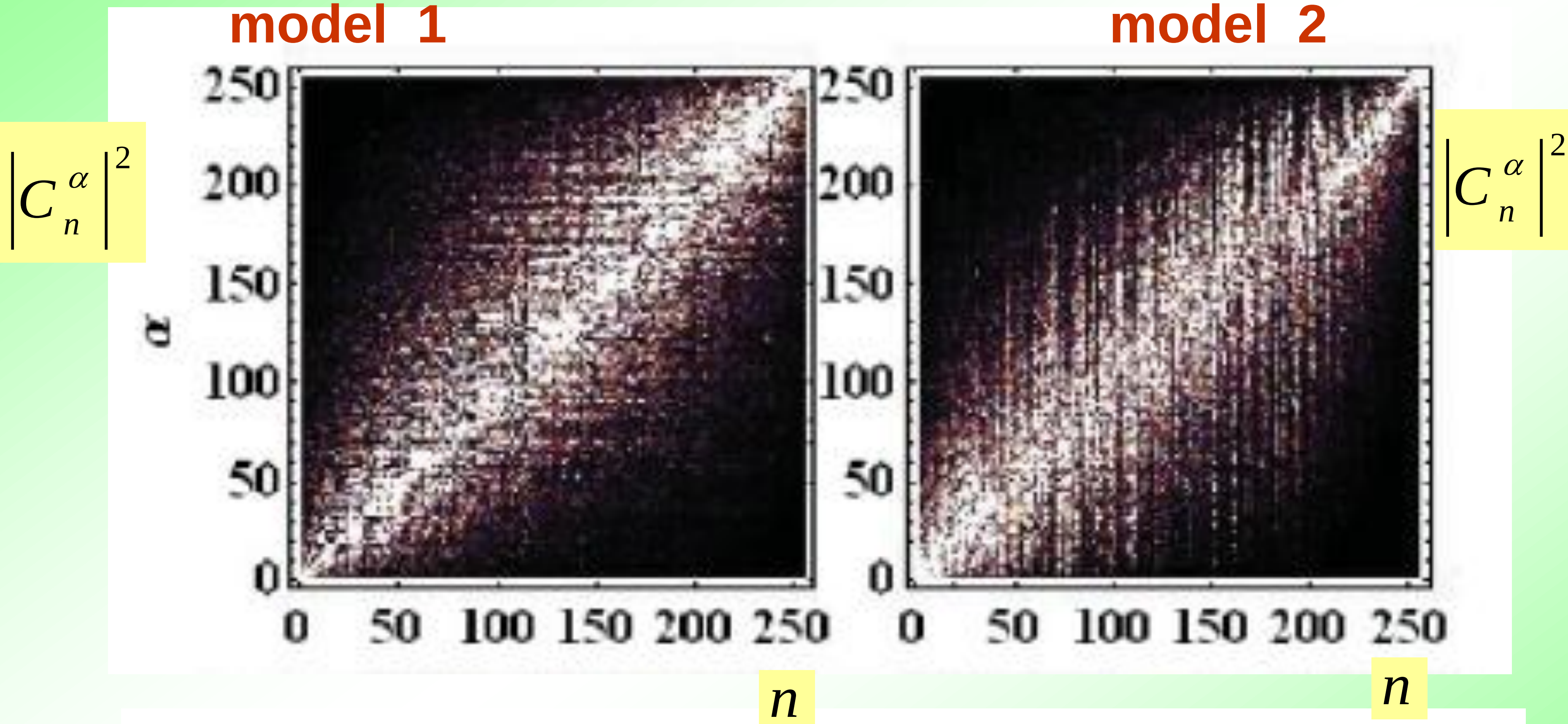


FIG. 8. Matrix of squared components of the eigenstates

Delocalization in energy shell

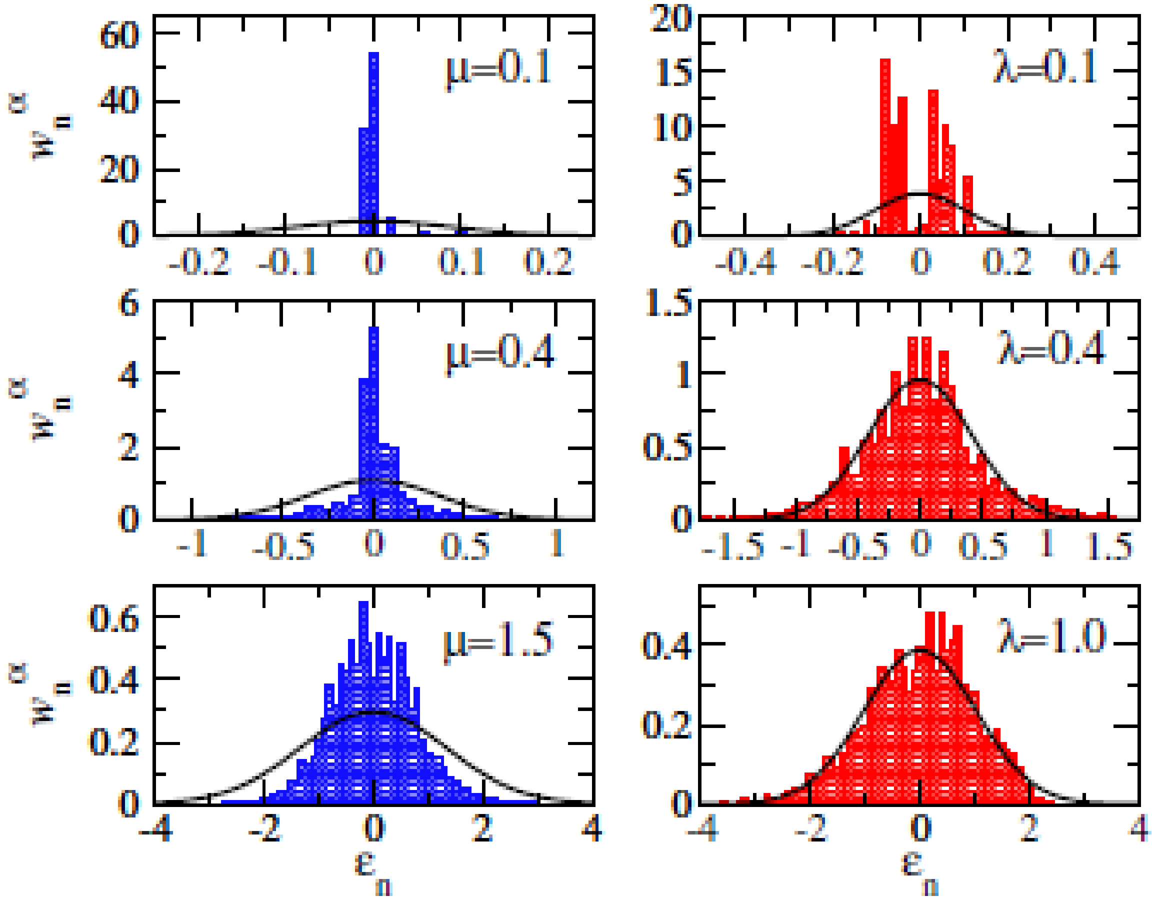


FIG. 4 (color online). Structure of eigenstates in the energy shells for model 1 (left) and model 2 (right) obtained by averaging over 5 states in the middle of the energy band. Solid curves correspond to the Gaussian form of the energy shell.

Strength function: from Breit-Wigner to Gauss

$$P_{n_0}(E) = \overline{\left| C_{n_0}^{\alpha} \right|^2} \rho(E)$$

BW is characterized by half-width: $\Gamma_{n_0} \approx 2\pi \overline{\left| H_{n_0 m} \right|^2} \rho_m$

Gauss is characterized by its variance: $\sigma_{n_0}^2 = \sum_{m \neq n_0} \left| H_{n_0 m} \right|^2$

Transition to chaos occurs when

$\Gamma \approx \sigma$ **!!**

Strength functions (LDOS)

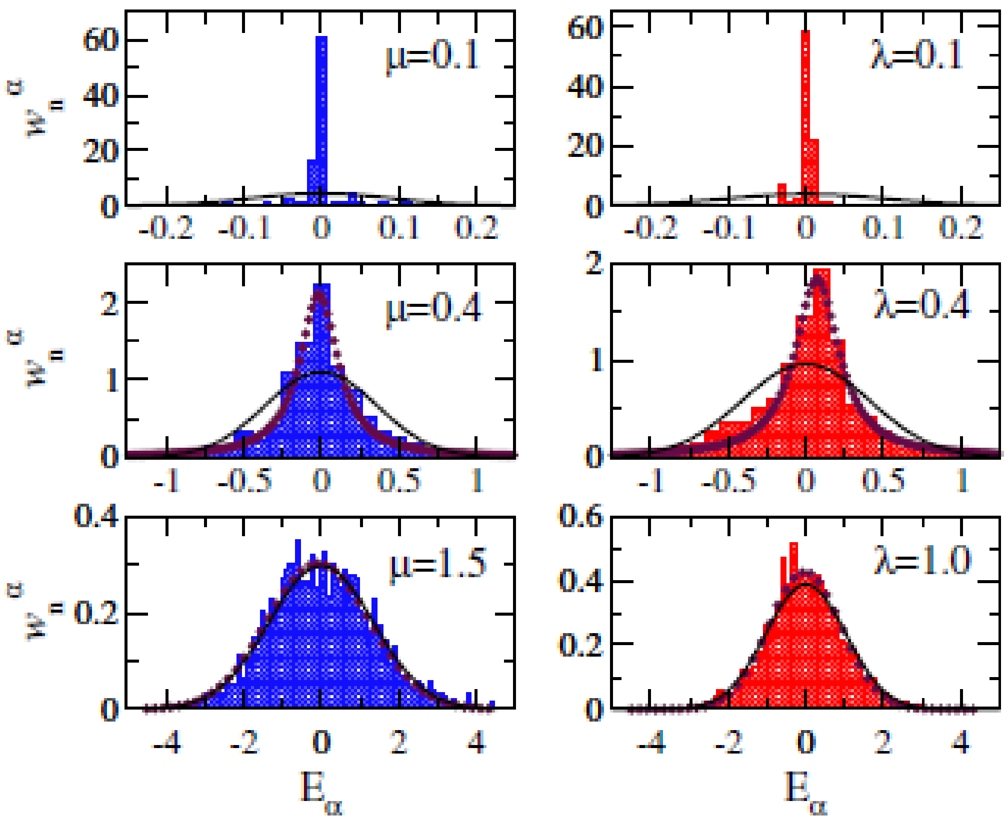


FIG. 3 (color online). Strength functions for model 1 (left) and model 2 (right) obtained by averaging over 5 close states in the middle of the spectrum. Middle panels: circles give a Breit-Wigner fit. Lower panels: circles stand for a Gaussian fit. In all panels, solid curves correspond to the Gaussian form of the energy shells.

Statistical relaxation – increase of entropy

$$S(t) = -\sum_n w_n(t) \ln w_n(t) \qquad w_n(t) = |C_n(t)|^2$$

according to statistical theory:

$$S(t) = -w_{n_0}(t) \ln w_{n_0}(t) - [1 - w_{n_0}(t)] \ln\left(\frac{1 - w_{n_0}(t)}{N_{pc}}\right)$$

Here $W_{n_0}(t)$ is the probability for the system to stay in the initial state $|n_0\rangle$ and N_{pc} is the average number of directly coupled states. We obtain N_{pc} numerically according to $N_{\text{pc}} = \langle e^S \rangle$, where the average $\langle . \rangle$ is performed over a long time after the saturation of the entropy.

Statistical relaxation – quench dynamics

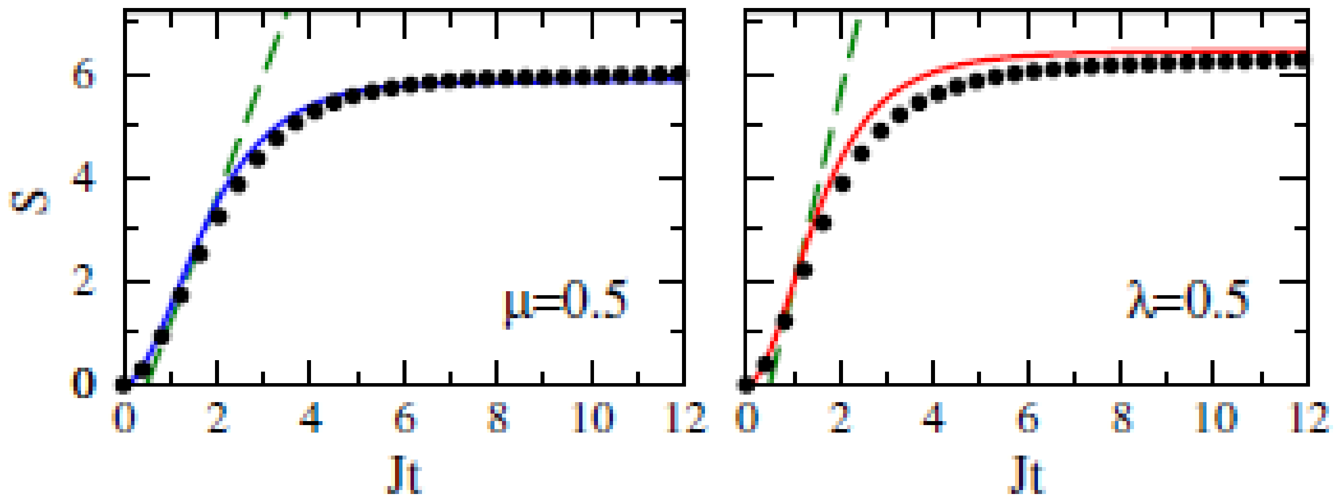


FIG. 5 (color online). Shannon entropy vs rescaled time for model 1 (left) and model 2 (right) for strong perturbation. Circles stand for numerical data, solid curves correspond to Eq. (3), and dashed lines show the linear dependence (4).

no difference between integrable and non-integrable models

smooth curves – analytical expressions

Chaos in integrable systems

B.V.Chirikov, "Transient Chaos in Quantum and Classical Mechanics", Foundation of Physics, Vol.16, No.1 (1986).

Abstract: "Bogolubov's classical example of statistical relaxation in a many-dimensional linear oscillator is discussed. The relation of the discovered relaxation mechanism to quantum dynamics as well as to some new problems in classical mechanics is considered."

N.N.Bogoliubov, "On Some Statistical Methods in Mathematical Physics", Academy of Sciences USSR Publishers, Kiev, 1945, p.115 (Russian); in: "Selected Papers" (Naukova Dumka, Kiev, 1970, Vol.2, p.77 (Russian).

Foundation of statistical mechanics

Two mechanisms of a statistical behavior (relaxation to a steady state distribution) in classical mechanics:

- **Thermodynamical limit** $N \to \infty$ **;**
- **Exponential instability plus boundary in phase space (** $\lambda > 0$ **) – "dynamical (deterministic) chaos"**

What is common for both mechanisms? – Infinite number of statistically independent frequencies in the time evolution of observables.

in quantum mechanics – only second mechanism

B.V.Chirikov, "Linear and nonlinear dynamical chaos", Open. Sys. & Informaion Dyn. 4 (1997) 241-280 .

"Linear chaos" in thermodynamical limit

Let us consider the function $$f(t)=\sqrt{\frac{2}{N}}\sum_{n=1}^{N}\cos(\omega_n t)$$

where the numbers ω_n **are linearly independent:**

$$k_1\omega_1+k_2\omega_2+k_3\omega_3+\cdots=0$$ **only if all integer numbers**

$$k_1=k_2=k_3=\cdots=0$$

Then, the relative time for $f_1 < f(t) < f_2$ **is** $$\frac{1}{\sqrt{2\pi}}\int_{f_1}^{f_2} e^{-\frac{y^2}{2}}\,dy$$

Infinite number of independent frequencies results in randomness !

Thank you for your attention!