Emergence of correlations in the process of thermalization of interacting bosons

F. M. Izrailev

Instituto de Física, BUAP, Puebla, México

and

Michigan State University, USA

In collaboration with:

F. Borgonovi, L.F. Santos, J.C. Molina-Victoria

Daejon, Sept. 3, 2018

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 as the condition for thermalization

R.V. Jensen and R. Shankar, "Statistical Behavior in Deterministic Quantum Systems with Few Degrees of Freedon", Phys. Rev. Lett. 54 (1985) 1879.

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.

Chaotic dynamics of systems of interacting particles

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$\hat{H}_0$ - "non-perturbed" part (describes the non-interacting particles/quasi-particles)

$\hat{V}$ - interaction between particles, or, with an external field

Many-body chaos – how to characterize?

Basic relations

$$H = H_0 + V$$

$$|\alpha\rangle = \sum_k C_k^\alpha |k\rangle \qquad |\alpha\rangle = \sum_k C_k^\alpha |k\rangle$$

$$H_0 |k\rangle = E_k^0 |k\rangle \qquad H|\alpha\rangle = E^\alpha |\alpha\rangle$$

Strength function (LDOS):

$$F^\alpha(E) = \sum_k |C_k^\alpha|^2 \delta(E - E_k^0)$$

F-function:

$$F_k(E) = \sum_\alpha |C_k^\alpha|^2 \delta(E - E^\alpha)$$

the *F−function*,

$$F^{\alpha}(E) = \sum_{k} |C_k^{\alpha}|^2 \delta(E - E_k^0), \qquad (6)$$

which is the energy representation of an eigenstate. From the components C_k^{α} one can also construct the *strength function* (SF) of a basis state $|k\rangle$,

$$F_k(E) = \sum_{\alpha} |C_k^{\alpha}|^2 \delta(E - E^{\alpha}) \qquad (7)$$

widely used in nuclear physics [20] and known in solid state physics as *local density of states*. The SF shows how the basis state $|k\rangle$ decomposes into the exact eigenstates $|\alpha\rangle$ due to the interaction V. It can be measured experimentally and it is of great importance since its Fourier transform gives the time evolution of an excitation initially concentrated in the basis state $|k\rangle$. Specifically, it

Structure of eigenfunctions

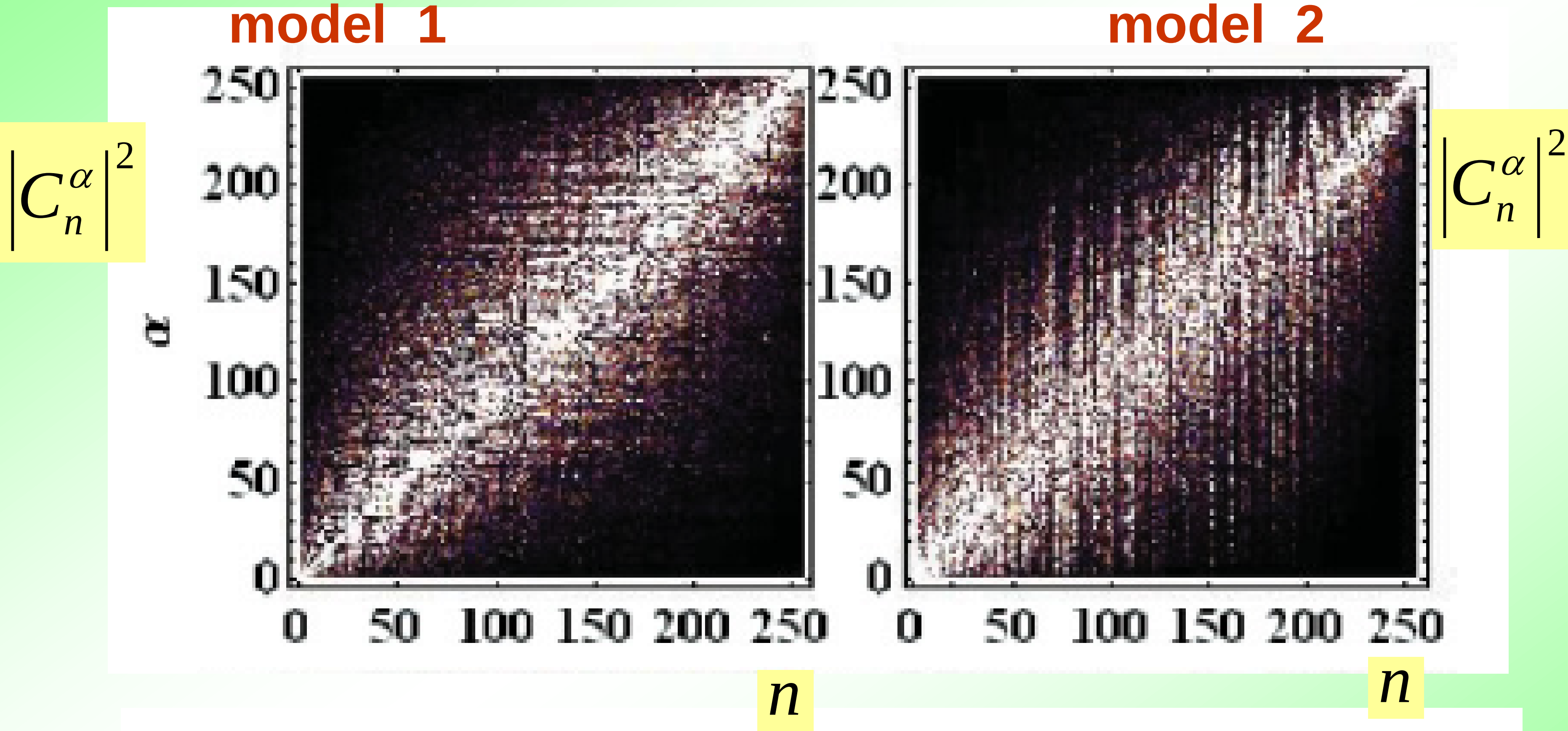
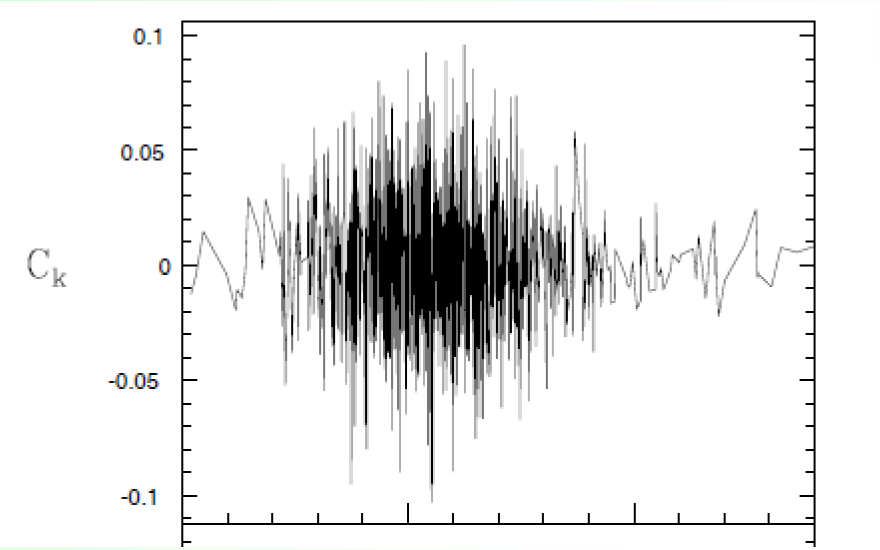


FIG. 8. Matrix of squared components of the eigenstates

Chaotic eigenstates in a gold atom



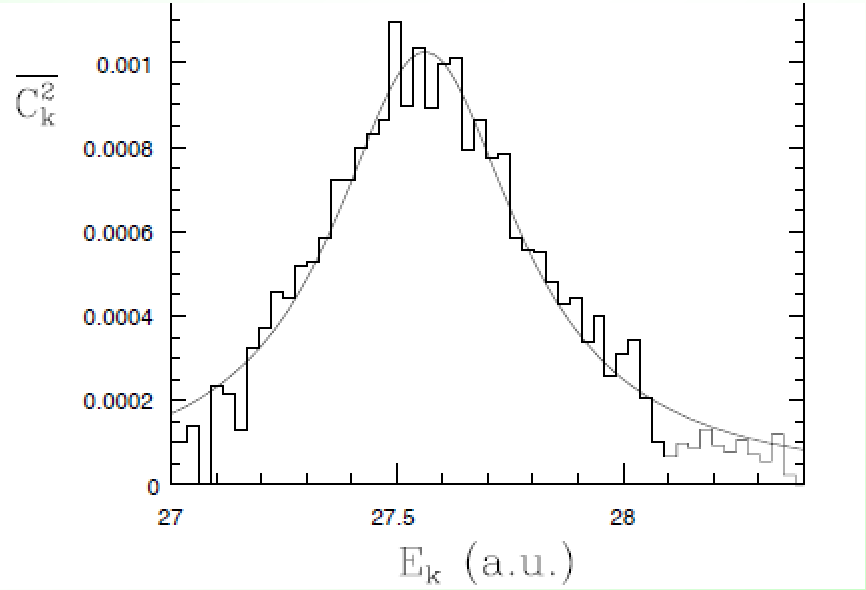


FIG. 3. Components of the 590th $J^\pi = \frac{13}{2}^-$ eigenstate from a two-configuration calculation (top), and a fit of $\overline{C_k^2}(E)$ by the Breit-Wigner formula (6) (bottom).

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

(problem of electron recombination)

Occupation number distribution

In order to define the temperature for each selected eigenstate $|\alpha\rangle$ let us consider its occupation number distribution (OND),

$$n_s^\alpha = \langle\alpha|\hat{n}_s|\alpha\rangle = \sum_k |C_k^\alpha|^2 \langle k|\hat{n}_s|k\rangle. \qquad (9)$$

As one can see, the OND (9) consists of two ingredients: the probabilities $|C_k^\alpha|^2$ and the occupation numbers $\langle k|\hat{n}_s|k\rangle$ related to the basis states of H_0. The latter are just integer numbers $0, 1, 2, ...N$ depending on how many bosons occupy the single-particle level s with respect to the many-body state $|k\rangle$. If the eigenstate $|\alpha\rangle$ of H con-

Thermalization in an isolated gold atom

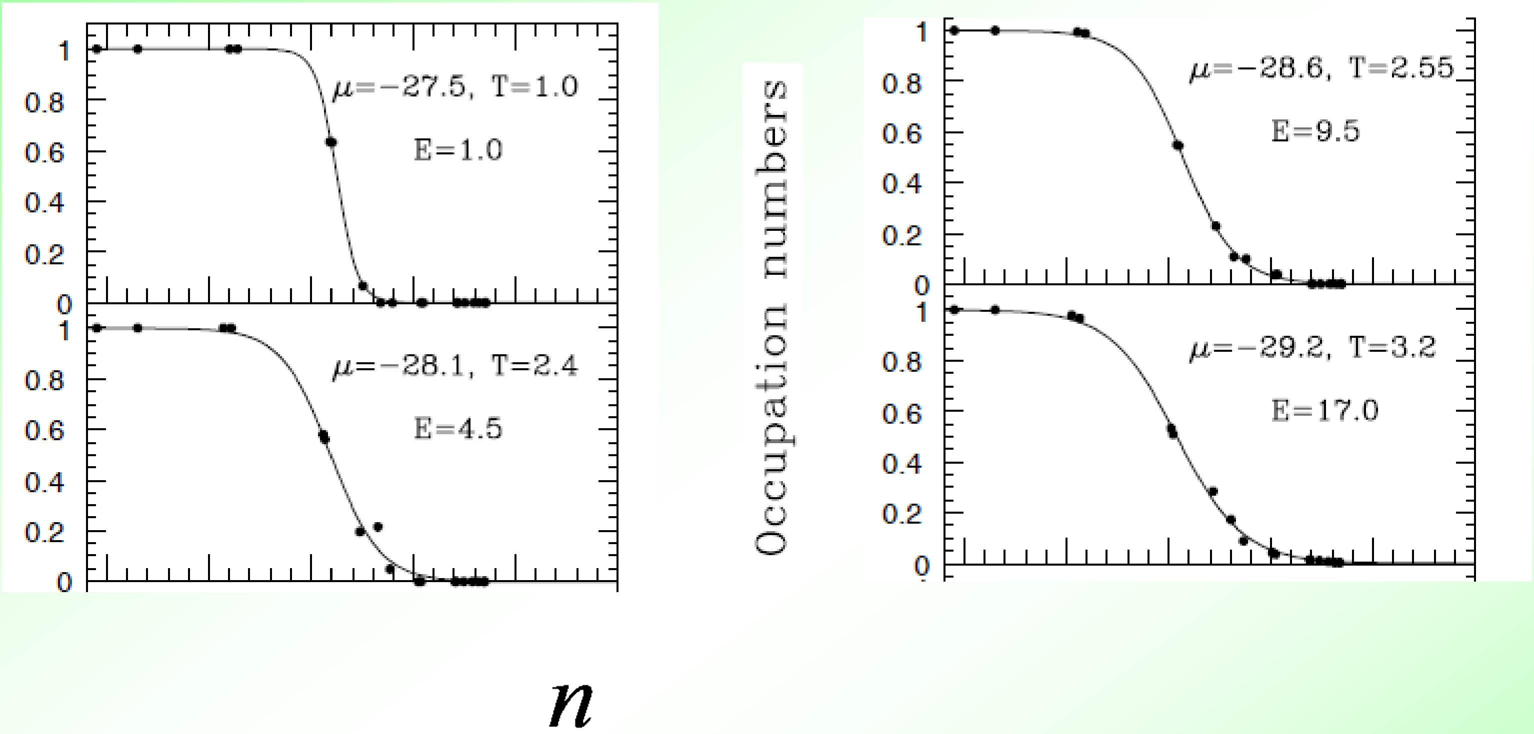


FIG. 7. Orbital occupation numbers in Au^{24+} calculated numerically from Eq. (7) at excitation energies $E = 1$, 4.5, 9.5, 17 and 27.5 a.u. (solid circles), and the Fermi-Dirac distributions (solid line) with temperature T and chemical potential μ chosen to give best fits of the numerical data.

Daejon, Sept. 3, 2018

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

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

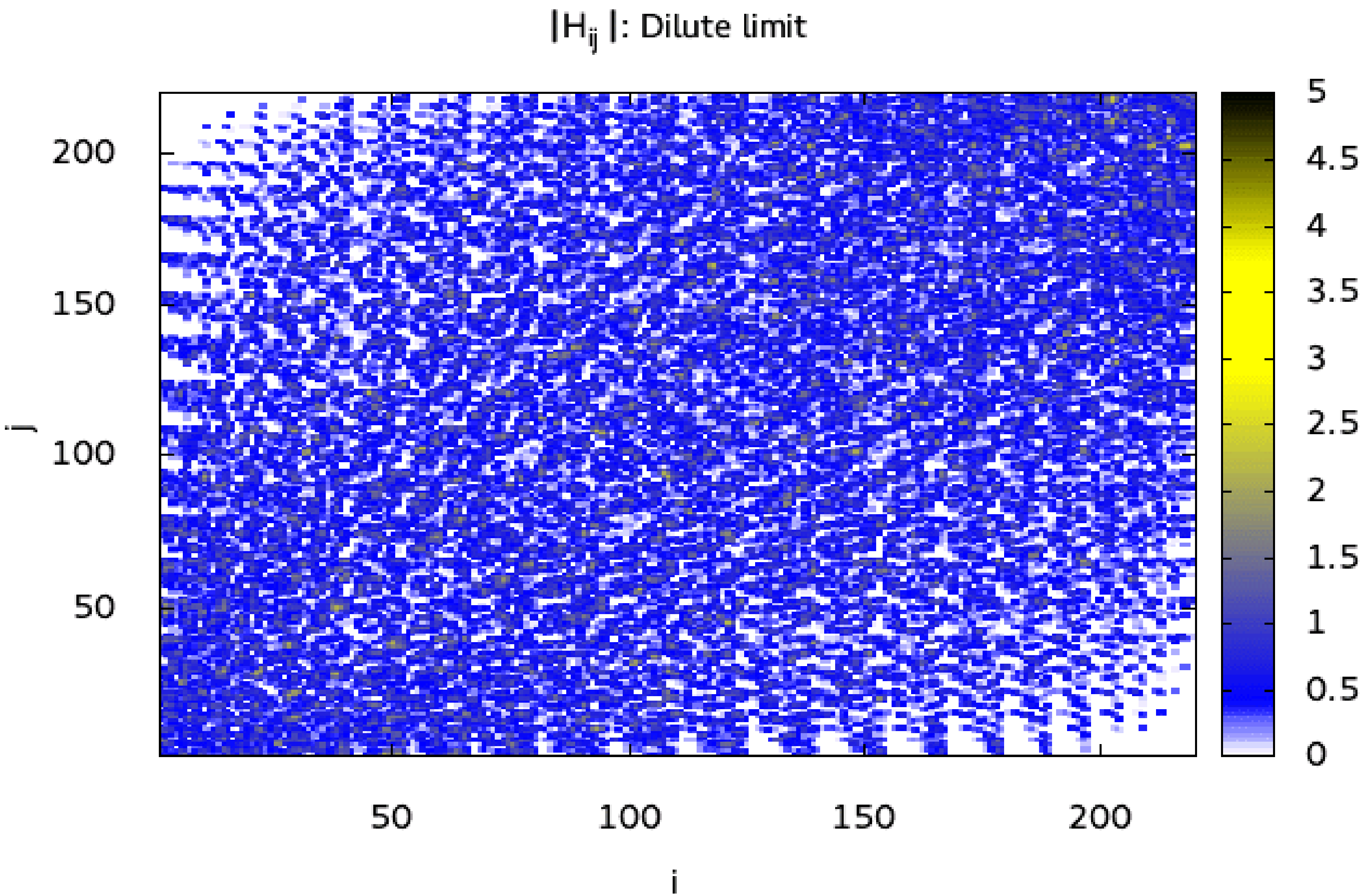
n number of particles ("quaisi-particles")

ε_k energy of single-particle states

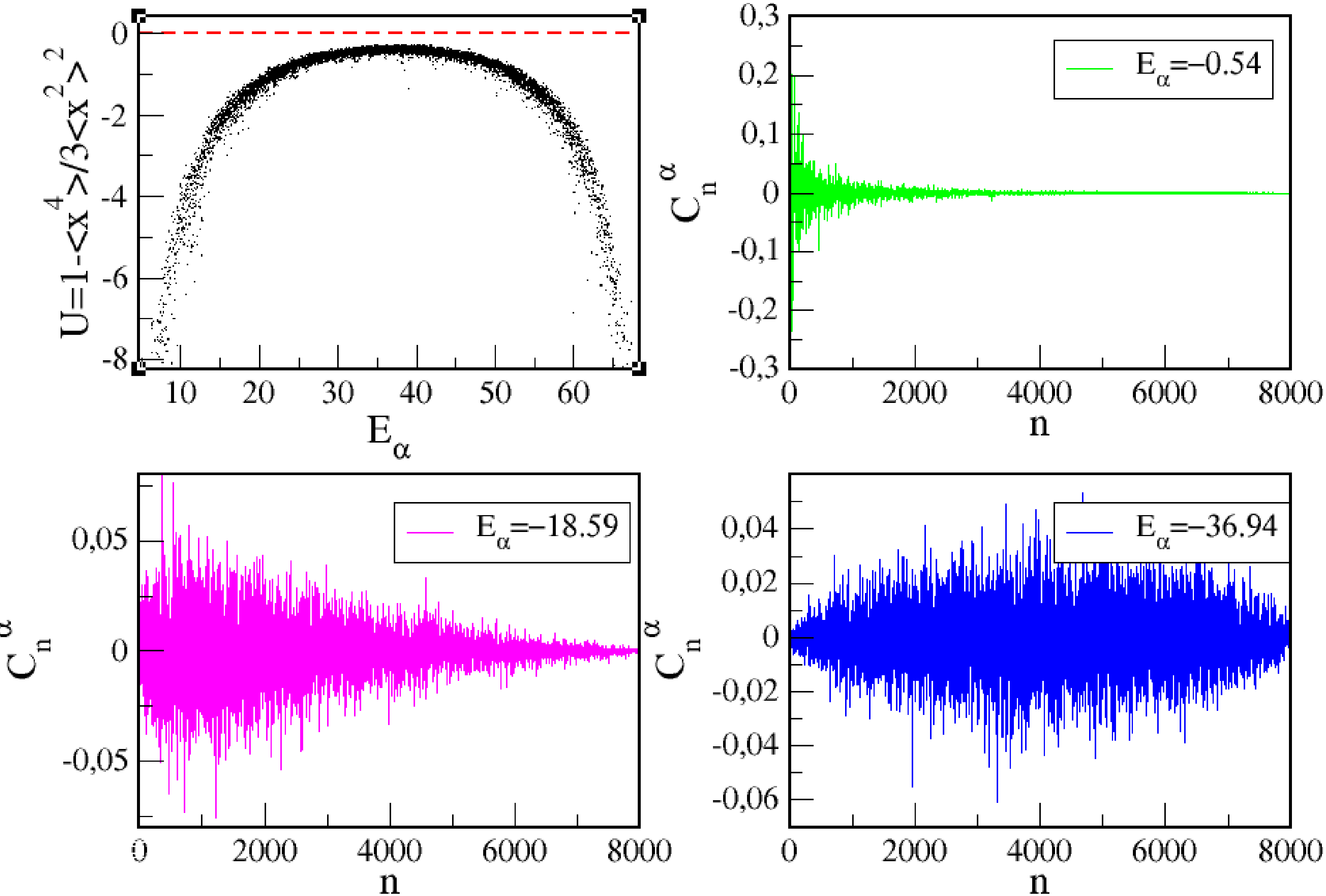
H is considered in the many-particle basis of

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

H_0 determines the basis in which the dynamics occurs


|H_ij |: Dilute limit
j
200
150
100
50
i
50
100
150
200
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0

TBRI, Δ=1, V=0.4, N=6, M=11



Daejon, Sept. 3, 2018

Model 1 : Interacting fully-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 : Interacting fully chaotic

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

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

Main result:

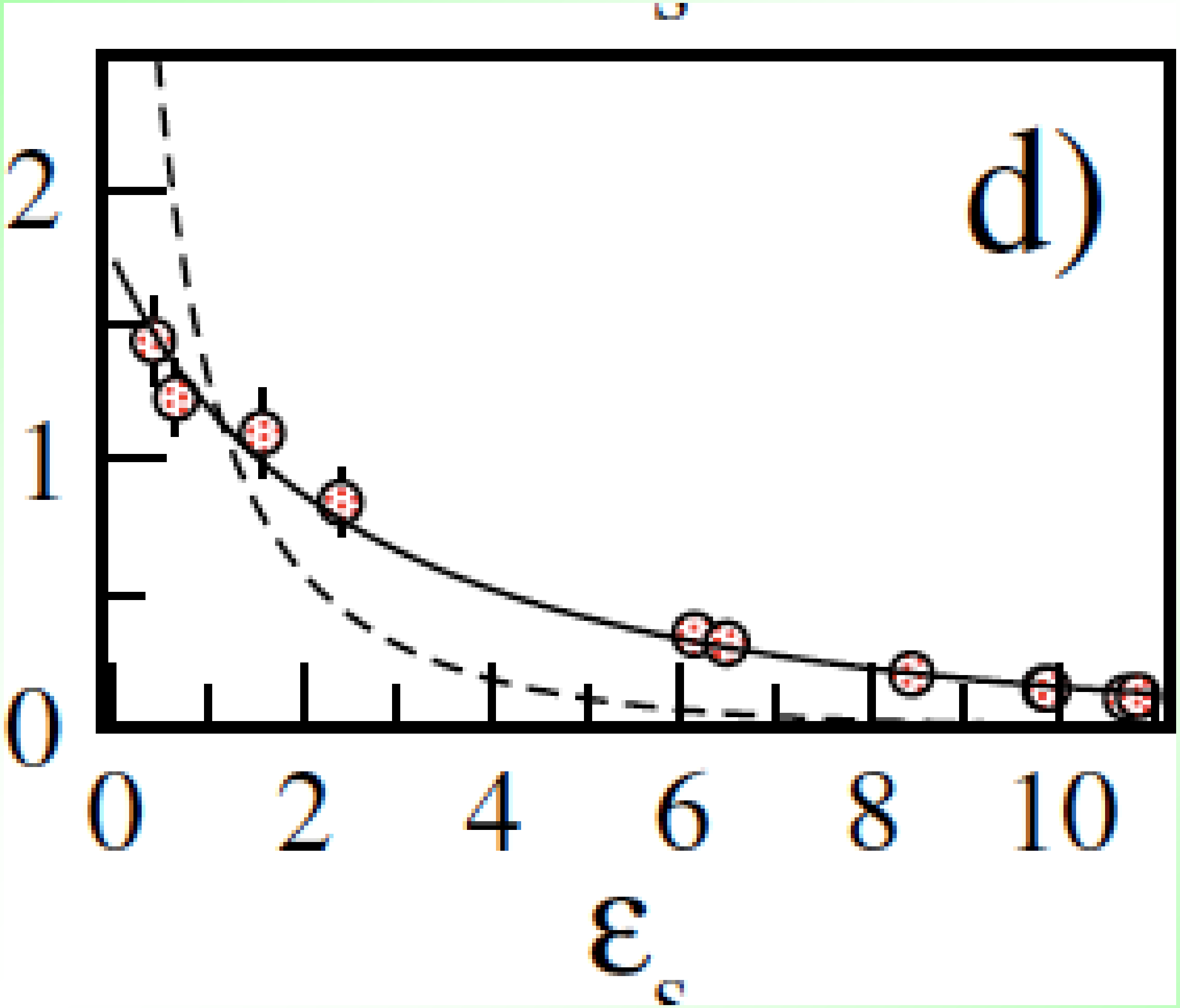
To take into account the inter-particle interaction we use the approach suggested in Refs [3, 4]. Specifically, we substitute the energy $E = E^{\alpha}$ in (10) with the "dressed" energy,

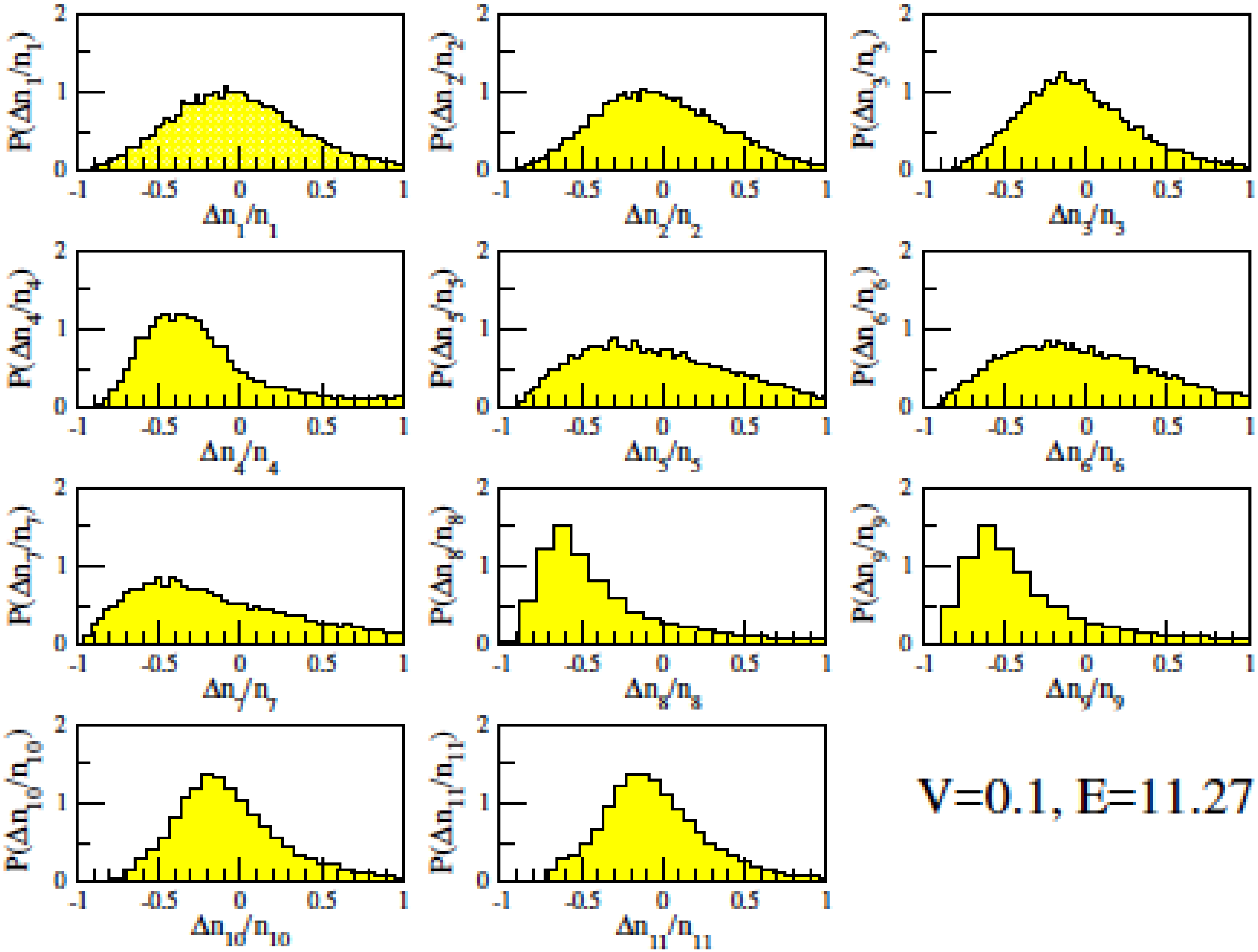
$$E^{dres} = \langle\alpha|H_0|\alpha\rangle \equiv E^{\alpha} + \Delta_{\alpha}. \qquad (12)$$

$$\sum_s n_s = N \qquad \sum_s \varepsilon_s n_s = E^{\alpha} + \Delta_{\alpha}$$

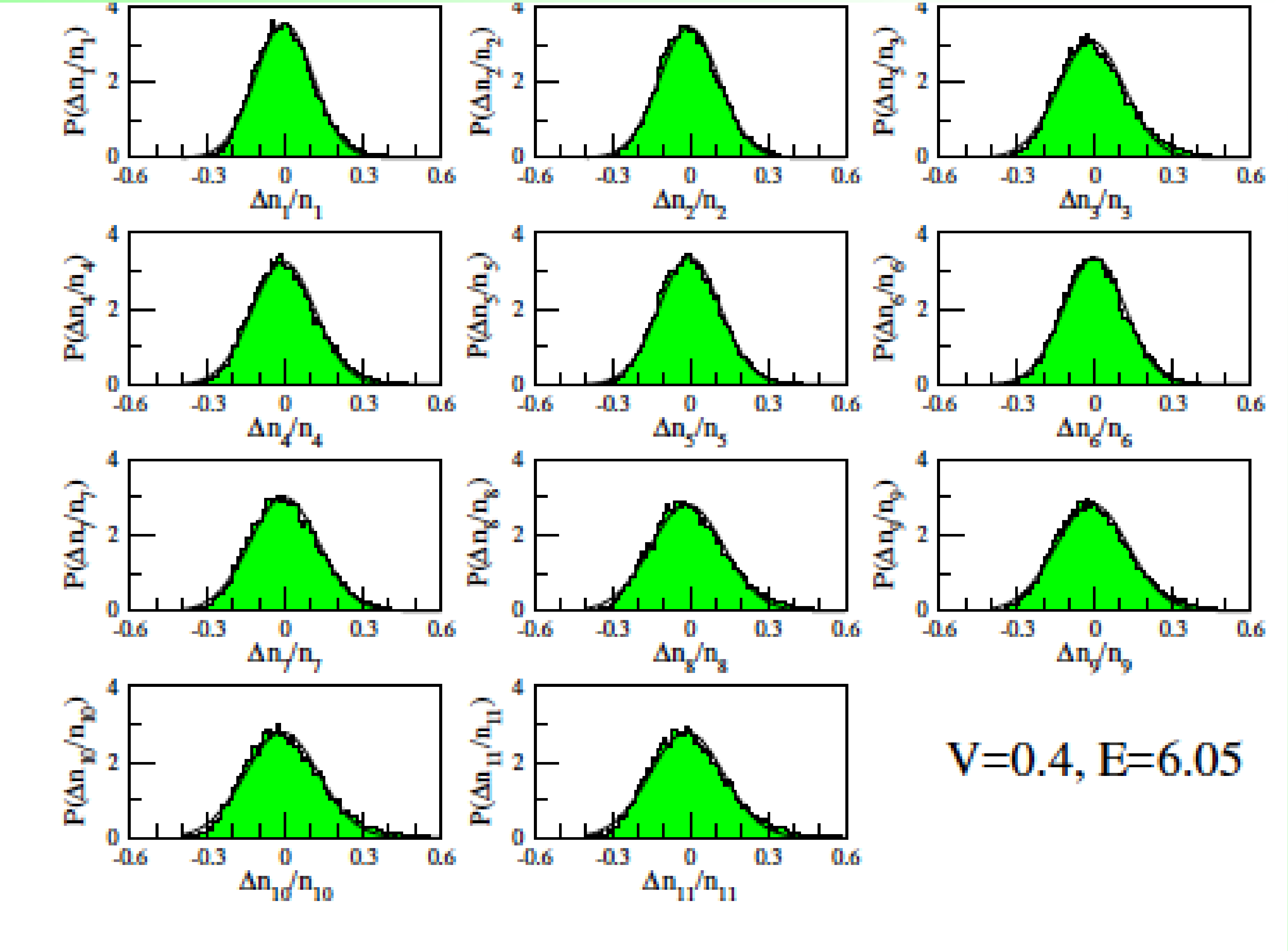
$$\Delta_{\alpha} = \frac{\overline{(\Delta E)^2}}{\overline{(\Delta E)^2} + \sigma_0^2}\left(E_c - E^{\alpha}\right)$$

$$\frac{\Delta T}{T} = \frac{\overline{(\Delta E)^2}}{\sigma_0^2}.$$


d)
0
1
2
0
2
4
6
8
10
ε_s



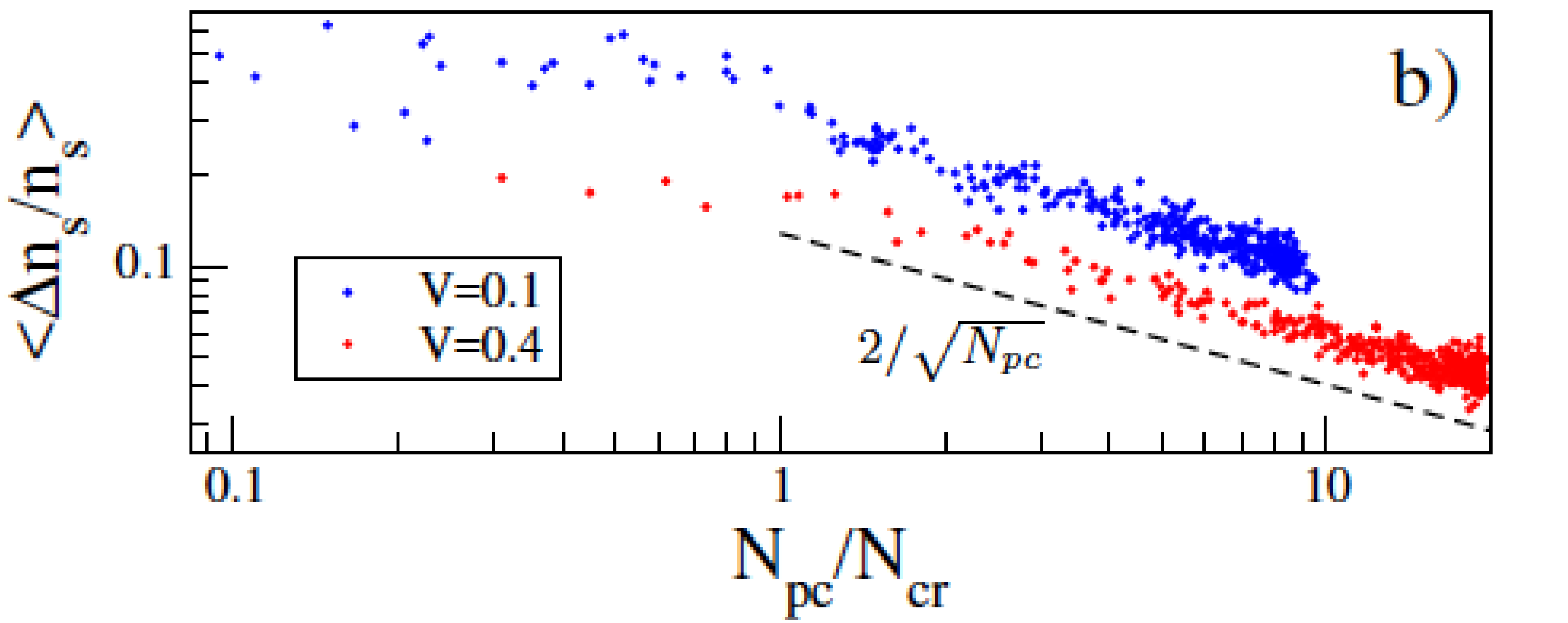
P(Δn_1/n_1)
Δn_1/n_1
P(Δn_2/n_2)
Δn_2/n_2
P(Δn_3/n_3)
Δn_3/n_3
P(Δn_4/n_4)
Δn_4/n_4
P(Δn_5/n_5)
Δn_5/n_5
P(Δn_6/n_6)
Δn_6/n_6
P(Δn_7/n_7)
Δn_7/n_7
P(Δn_8/n_8)
Δn_8/n_8
P(Δn_9/n_9)
Δn_9/n_9
P(Δn_10/n_10)
Δn_10/n_10
P(Δn_11/n_11)
Δn_11/n_11
V=0.1, E=11.27

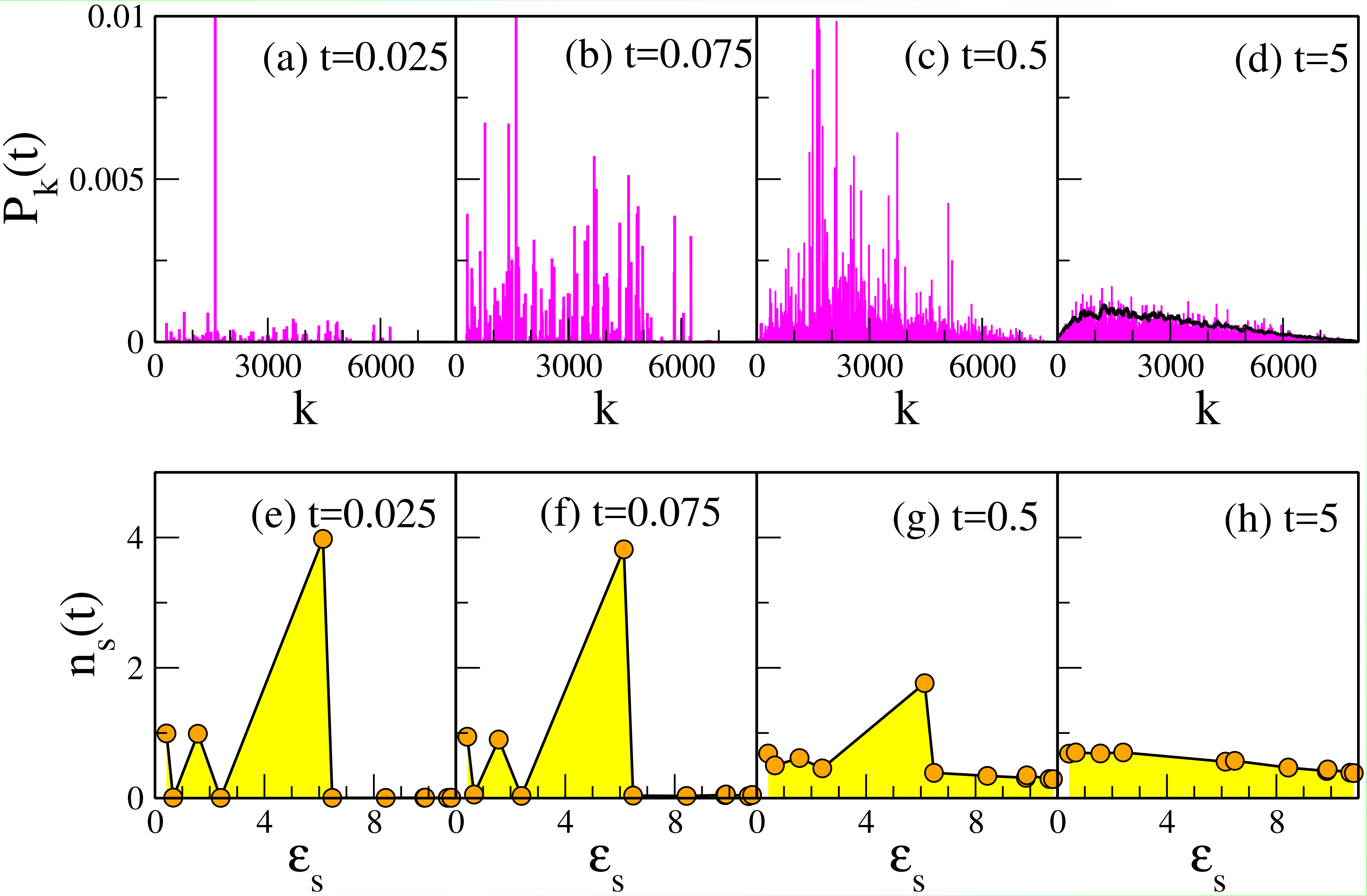


V=0.4, E=6.05

$$\frac{\Delta n_s}{n_s} \equiv \frac{n_s - \langle n_s \rangle}{\langle n_s \rangle}$$

$$N_{pc} = 1/\sum_k |C_k^\alpha|^4.$$





(a) t=0.025
(b) t=0.075
(c) t=0.5
(d) t=5
$P_k(t)$
0.01
0.005
0
0
3000
6000
k
(e) t=0.025
(f) t=0.075
(g) t=0.5
(h) t=5
$n_s(t)$
4
2
0
0
4
8
ε_s

$$\frac{dW_0}{dt} = -\Gamma(W_0 - \overline{W_0^\infty}),$$
$$\frac{dW_1}{dt} = -\Gamma(W_1 - \overline{W_1^\infty}) + \Gamma(W_0 - \overline{W_0^\infty}), \tag{8}$$

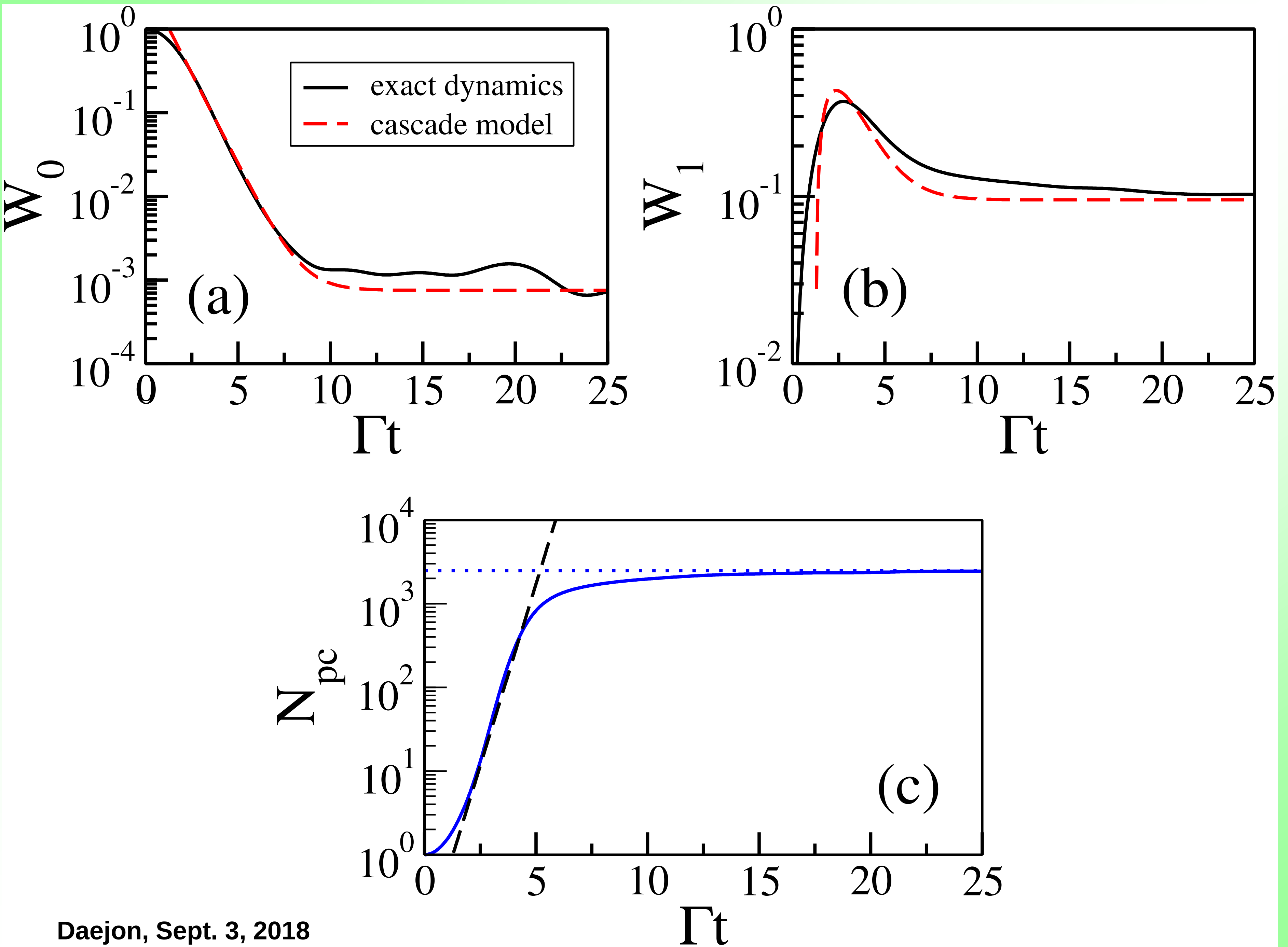
where the infinite time averages are $\overline{W_0^\infty} = \sum_\alpha |C_{k_0}^\alpha|^4$ and $\overline{W_1^\infty} = \sum_{k\in\mathcal{M}_1} \sum_\alpha |C_{k_0}^\alpha|^2 |C_k^\alpha|^2$.

$$W_0(t) = e^{-\Gamma t}(1 - \overline{W_0^\infty}) + \overline{W_0^\infty},$$
$$W_1(t) = \Gamma t e^{-\Gamma t}(1 - \overline{W_0^\infty}) + \overline{W_1^\infty}(1 - e^{-\Gamma t}). \tag{9}$$

With the expressions (9) one can derive the time dependence for $N_{pc}(t)$,

$$N_{pc}(t) \simeq \left[\sum_n W_n^2/\mathcal{N}_n\right]^{-1} \simeq \left[W_0^2 + W_1^2/\mathcal{N}_1\right]^{-1} \sim e^{2\Gamma t}, \tag{10}$$

where $\mathcal{N}_n$ is the number of states contained in the n-th class. This result shows that the number of basis



exact dynamics
cascade model
(a)
W_0
Γt
(b)
W_1
Γt
(c)
N_{pc}
Γt

states (see details in SM [35]). For $M \sim 2N$ and for $M, N \gg 1$ one gets the estimate

$$t_S \sim N/\Gamma = N t_\Gamma. \tag{13}$$

This is the time scale for the complete thermalization in quantum MBS. As one can see from Eq. (13), when the number of particles is very large, the two time scales are very different. Notice that t_S increases linearly with N due to the exponential growth with N of the Fock space and not because of the Gaussian shape of the density levels [35].

Inspired by the above studies, our results for the exponential growth of N_{pc} can be treated in terms of the phase-space volume $\mathcal{V}_E$ occupied by the wave packet, $\mathcal{V}_E(t) \sim N_{pc}(t)/\rho(E)$, where $\rho(E)$ is the total density of states. We can write

$$\mathcal{V}_E(t) = \mathcal{V}_E(0)e^{2\Gamma t} \sim \mathcal{V}_E(0)e^{h_{KS}t}. \quad (14)$$

Here, we associate 2Γ with the Kolmogorov-Sinai entropy [41], h_{KS}, which gives the exponential growth rate of phase-space volumes for classically chaotic MBS [41].

Occupation number distribution in time

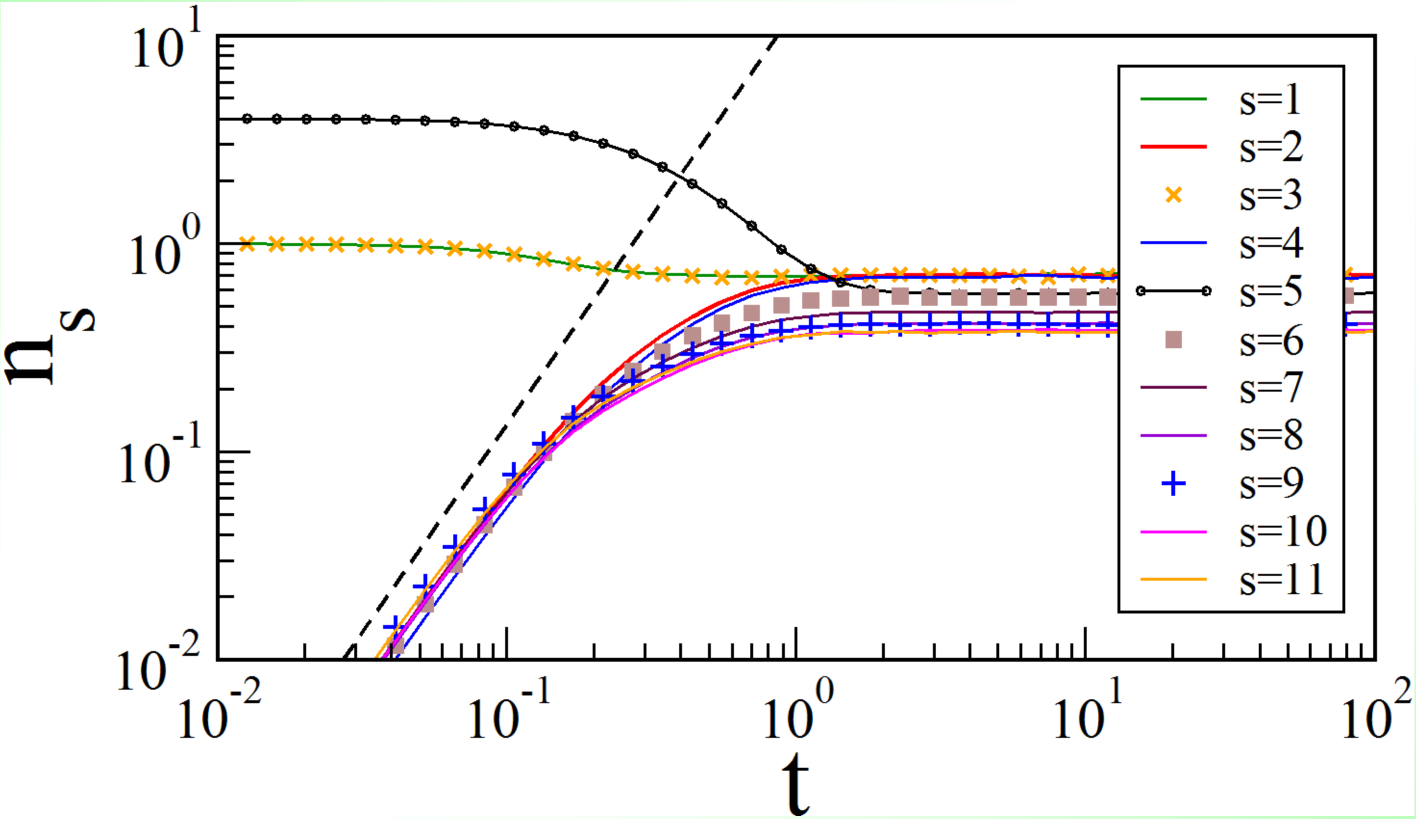
$$n_s(t) = \langle \psi(t) \,|\, \hat{n}_s \,|\psi(t)\, \rangle = \sum_k n_s^k |\langle k|\psi(t)\rangle|^2.$$

Expanding e^{-iHt} at second order one gets the time dependence for $n_s(t)$ at small times,

$$|\langle k|e^{-iHt}|k_0\rangle|^2 \simeq \delta_{k,k_0} + t^2 \left[H^2_{k,k_0} - \delta_{k_0,k_0}(H^2)_{k,k_0}\right] + o(t^4) \quad (6)$$

which results in the following estimate,

$$n_s(t) \simeq n_s^{k_0} + t^2 \sum_{k \neq k_0} (n_s^{k_0} - n_s^k) H^2_{k,k_0} + o(t^4) \quad (7)$$



10^1
10^0
10^{-1}
10^{-2}
n_s
10^{-2}
10^{-1}
10^0
10^1
10^2
t
s=1
s=2
s=3
s=4
s=5
s=6
s=7
s=8
s=9
s=10
s=11

First, we start with the two-point correlation function $C_{s,s+1}(t)$ between neighboring occupation numbers,

$$C_{s,s+1}(t) = \langle k_0 | [\hat{n}_s(t) - \hat{n}_s][\hat{n}_{s+1}(t) - \hat{n}_{s+1}] | k_0 \rangle. \quad (9)$$

els. Performing an expansion on a small time scale it is possible to show that

$$\mathcal{C}^{(2)}(t) \simeq t^2 | \sum_{s=1}^{M-1} \sum_{r=s+1}^{M} \sum_{k} H^2_{k,k_0} W^{sr}_{k,k_0} | + o(t^4) \quad (11)$$

with $W^{sr}_{k,k_0} = [n^k_s n^k_r + n^{k_0}_s n^{k_0}_r - n^{k_0}_s n^k_r - n^k_s n^{k_0}_r]$. As one can see, Eq. (11) does not contain both eigenvalues and eigenfunctions. This means that in order to get the initial spread of the correlator, there is no need to diagonalize the Hamiltonian. Concerning the saturation value, it can

As for the saturation values $\overline{n_s}$ after the relaxation time t_s, they can be also obtained analytically,

$$\overline{n_s} = \sum_k n_s^k \overline{|\langle k|\psi(t)\rangle|^2} = \sum_k n_s^k \sum_\alpha |C_{k_0}^\alpha|^2 |C_k^\alpha|^2. \quad (8)$$

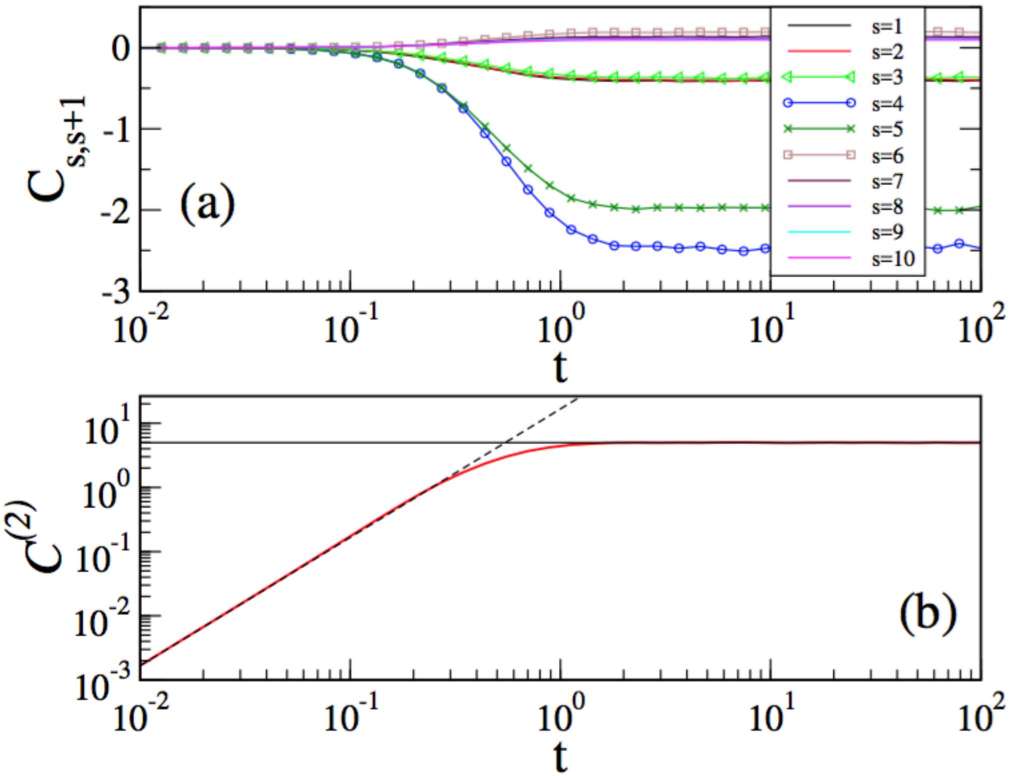


FIG. 3: (a) Correlation function $C_{s,s+1}(t)$ for all $s = 1, ..., M-1$. (b) Time evolution of the global two-point correlation function $\mathcal{C}^{(2)}(t)$. Dashed line is due to Eq.11. Horizontal line corresponds to Eq.12. The initial state and parameters are the same as in Fig.(2). The average over 10 random realizations of the potential V was used.

Thanks for your attention!

Assuming a Gaussian shape for both the density of states and the LDOS [33], we show that the maximal value of $\overline{N_{pc}^{\infty}}$ is

$$N_{pc}^{max} = \eta\sqrt{1-\eta^2}\mathcal{D} \tag{12}$$

where $\eta = \Gamma/\sigma\sqrt{2}$ and σ is the width of the density of states (see details in SM [33]). For $M \sim 2N$ and for $M, N \gg 1$ one gets the estimate

$$t_S \sim N/\Gamma = N t_\Gamma. \tag{13}$$

Comments to FPU

1. We do not need ergodicity for thermalization
2. Onset of chaos – dependence on N, and strength of interaction !
3. Dependence on initial conditions !!
4. Two different situations: finite N and thermodynamic limit $N \to \infty$
5. Thermalization as the relaxation to a steady-state distribution of energy

Comments to TBRI model

1. Condition for the onset of chaos
2. Analytical expression to find a temperature
3. Gaussian fluctuations around the mean occupation numbers
4. The control parameter is not the number of particles, but the number of principal components in chaotic eigenstates
5. Statistical (from the BE-distributions) equal to the thermodynamical temperature

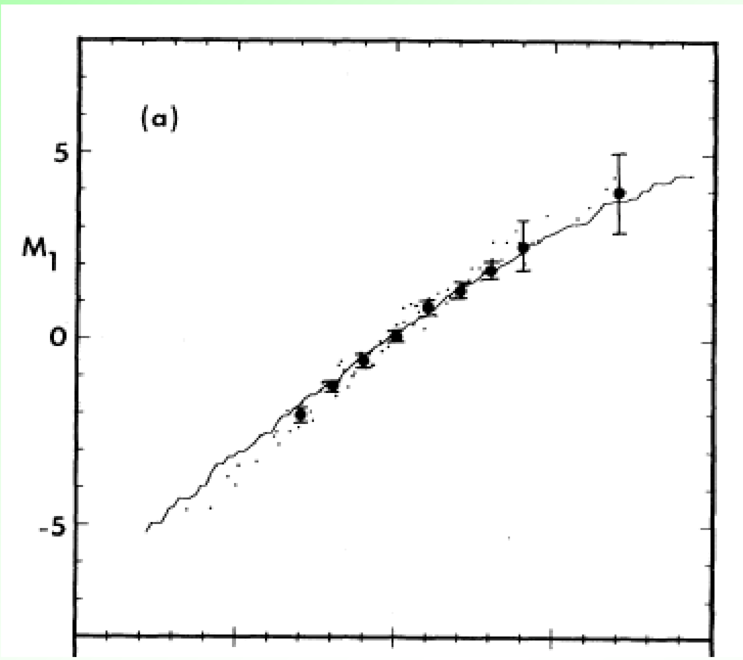
Fundamental principle of statistical physics

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)

R.V. Jensen and R. Shankar, "Statistical Behavior in Deterministic Quantum Systems with Few Degrees of Freedon", Phys. Rev. Lett. 54 (1985) 1879.



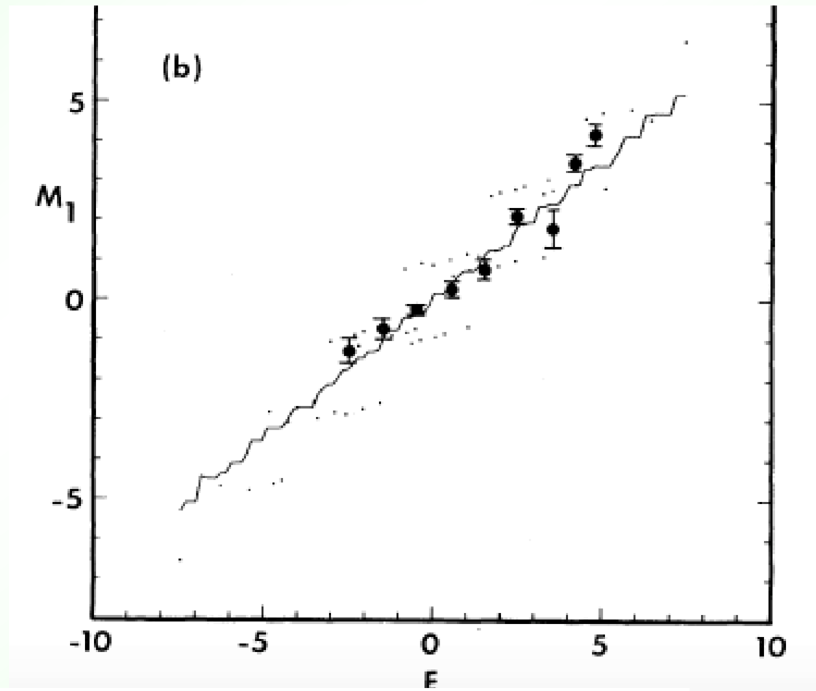


FIG. 2. The magnetization, M_1, plotted against energy for each of energy eigenstates (small dots) for (a) a nonintegrable Hamiltonian and (b) an integrable Hamiltonian; the solid curves represent the microcanonical average of the magnetization as functions of energy, and the large dots show the equilibrium values approached in numerical experiments performed with a variety of initial states. The associated error bars represent an estimate of the typical fluctuations from equilibrium.

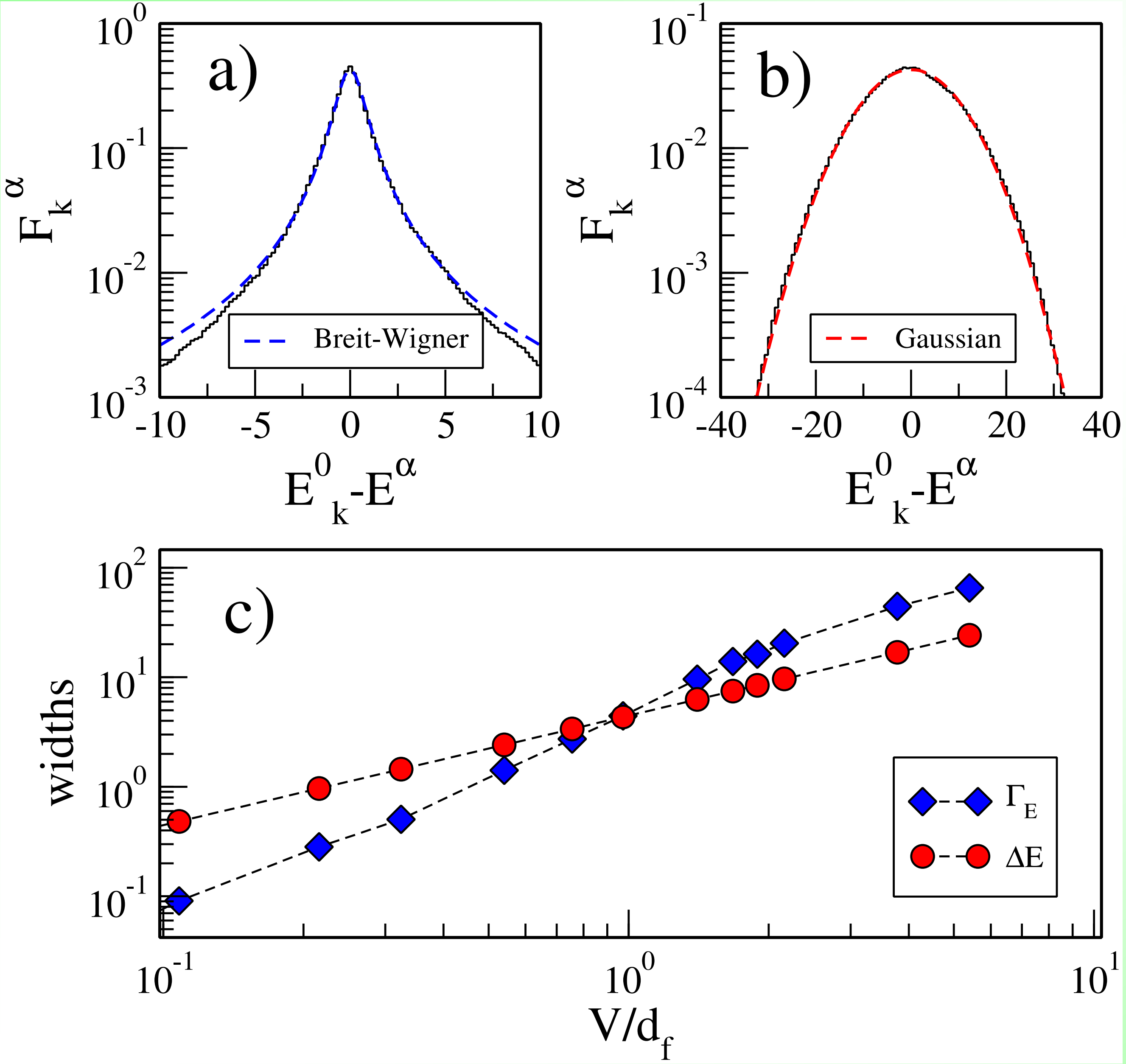
Strength function: from Breit-Wigner to Gauss
Onset of strong chaos

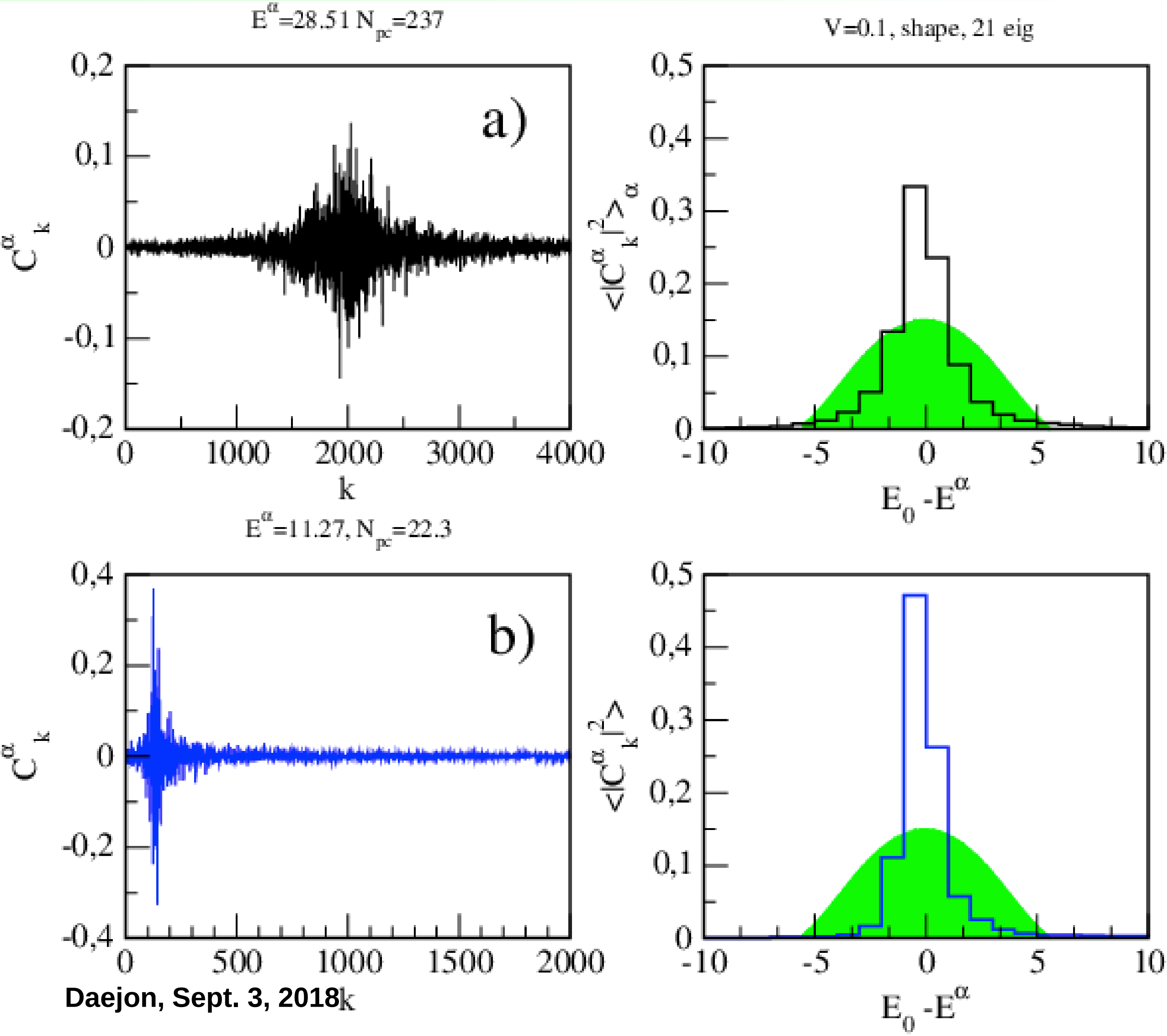
BW is characterized by half-width: $$\Gamma_{n_0} \approx 2\pi \overline{\left| H_{n_0 m} \right|}^2 \rho_m$$

Gauss is characterized by its variance: $$(\Delta E)^2_{n_0} = \sum_{m \neq n_0} \left| H_{n_0 m} \right|^2$$

Crossover to chaos occurs when

$$\Gamma \approx \Delta E$$ **!!**


a)
b)
c)
Breit-Wigner
Gaussian
F_k^α
$E^0_k - E^\alpha$
widths
V/d_f
Γ_E
ΔE



E^{α}=28.51 N_{pc}=237
V=0.1, shape, 21 eig
a)
C^{α}_{k}
k
$<|C^{\alpha}_{k}|^2>_{\alpha}$
E_0 -E^{α}
E^{α}=11.27, N_{pc}=22.3
b)
C^{α}_{k}
k
$<|C^{\alpha}_{k}|^2>$
E_0 -E^{α}

F..Borgonovi, F.Mattiotti and F.M.Izrailev,
"Temperature of a single chaotic eigenstate",
Phys. Rev. E., 95 (2017) 042135.

F..Borgonovi, F.M.Izrailev, L.F.Santos, V.G.Zelevinsky,
"Quantum Chaos and Thermalization in Isolated Systems of Interacting Particles", Phys. Rep. 625 (2016) 1-58.

Thank you for your attention!

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 .

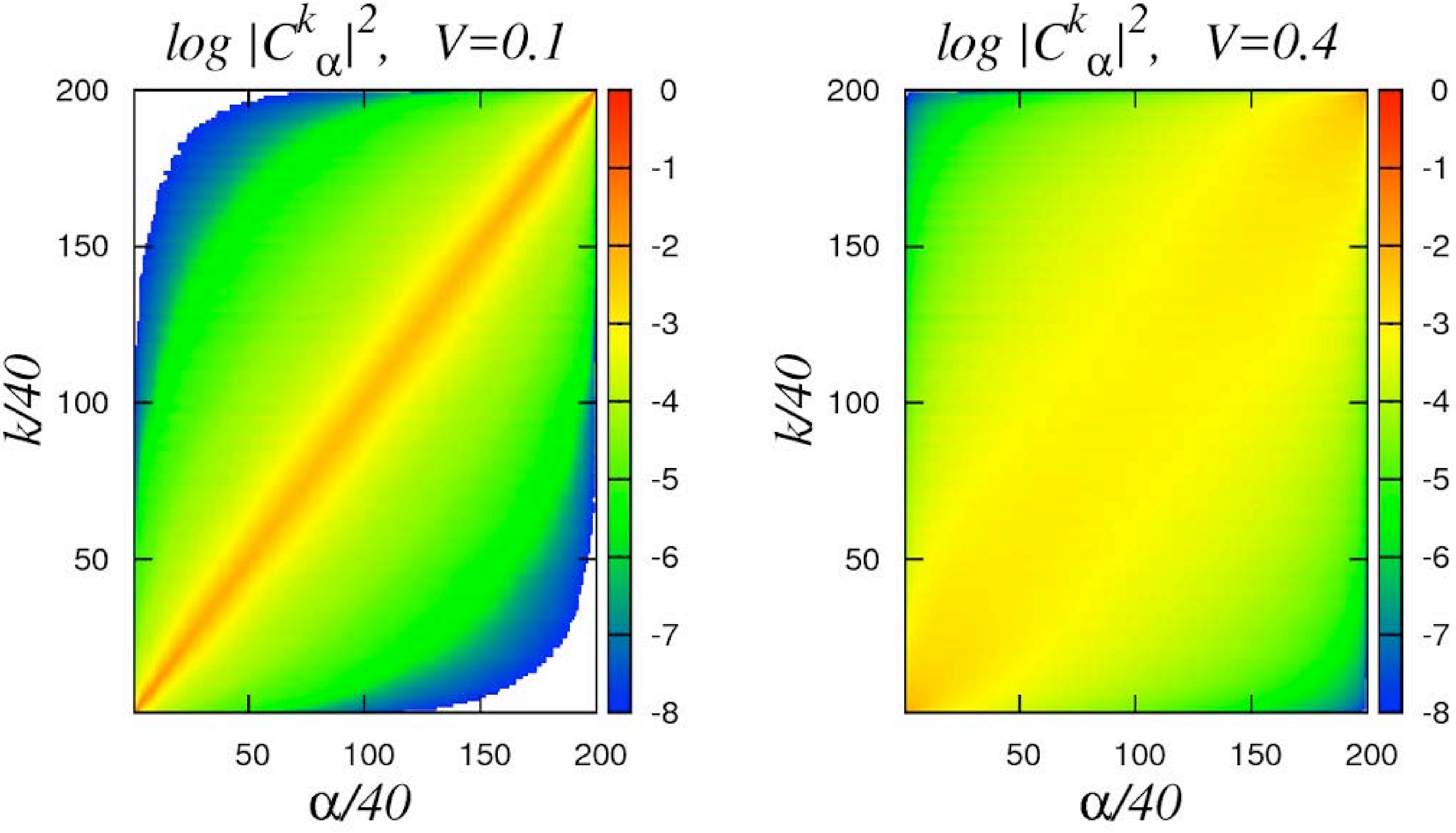
"Quantum chaos" in deterministic systems

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.


log |C^k_α|^2, V=0.1
log |C^k_α|^2, V=0.4
k/40
α/40
200
150
100
50
0
-1
-2
-3
-4
-5
-6
-7
-8

Emergence of chaotic states

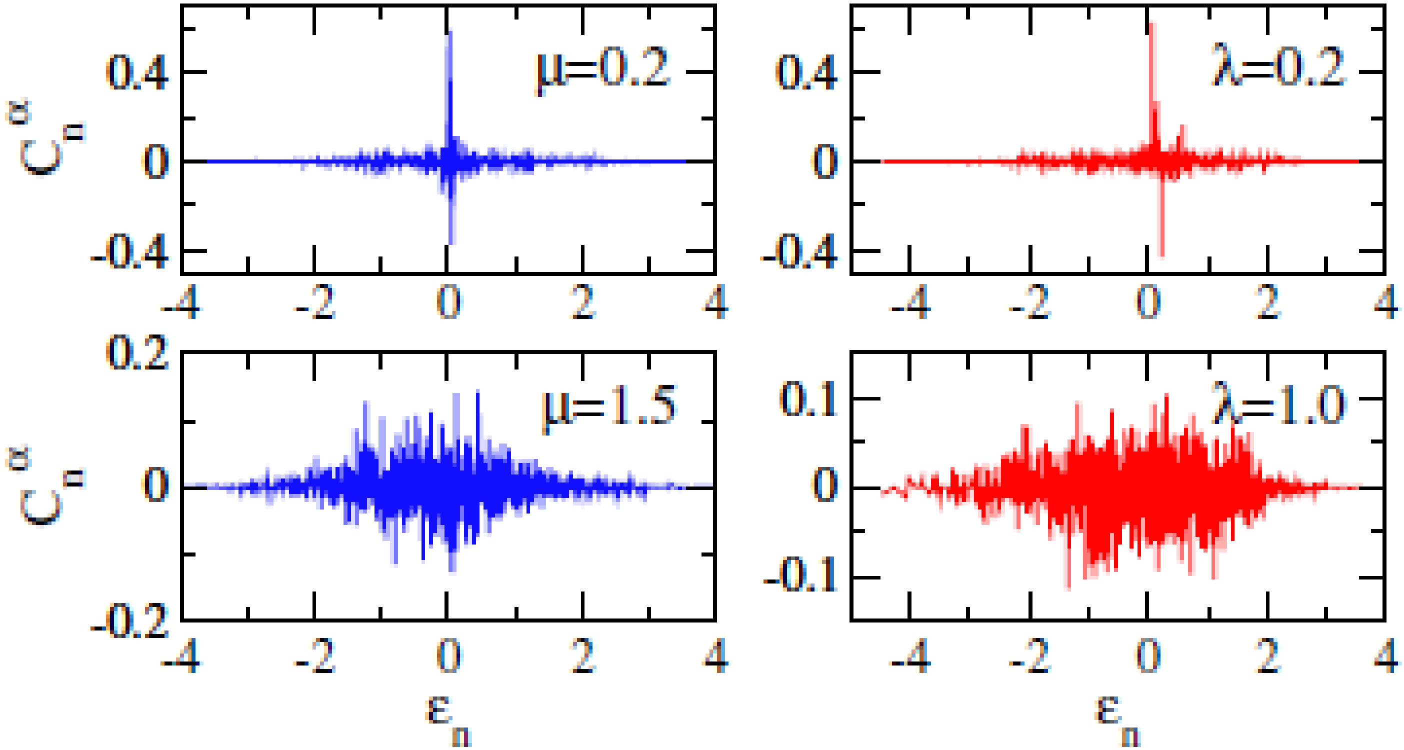


FIG. 2 (color online). Typical localized (top) and extended (bottom) eigenstates for model 1 (left) and model 2 (right).

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

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.

Delocalization in energy shell

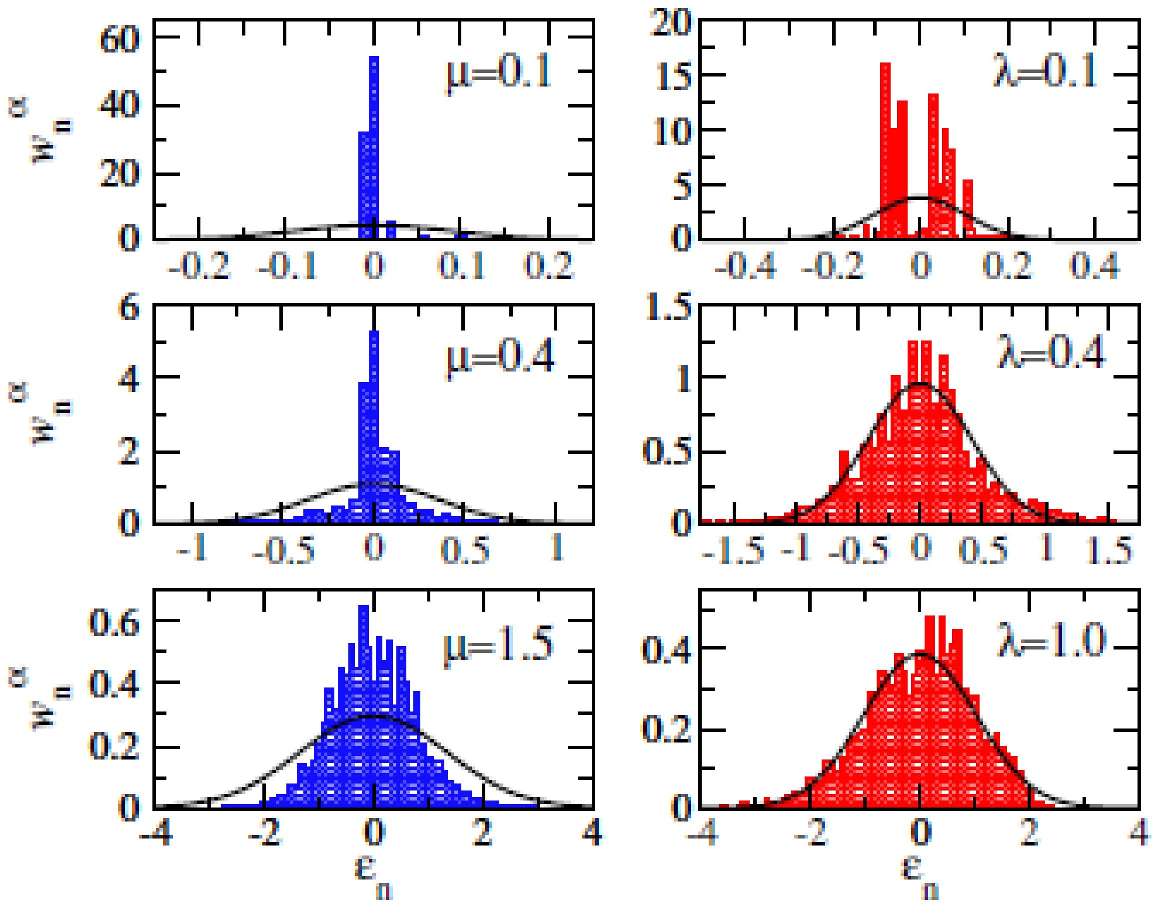


FIG. 4 (color online). Structure of eigenstates in the energy shells for model 1 (left) and model 2 (right) obtained by averaging over 5 states in the middle of the energy band. Solid curves correspond to the Gaussian form of the energy shell.

Strength functions (LDOS)

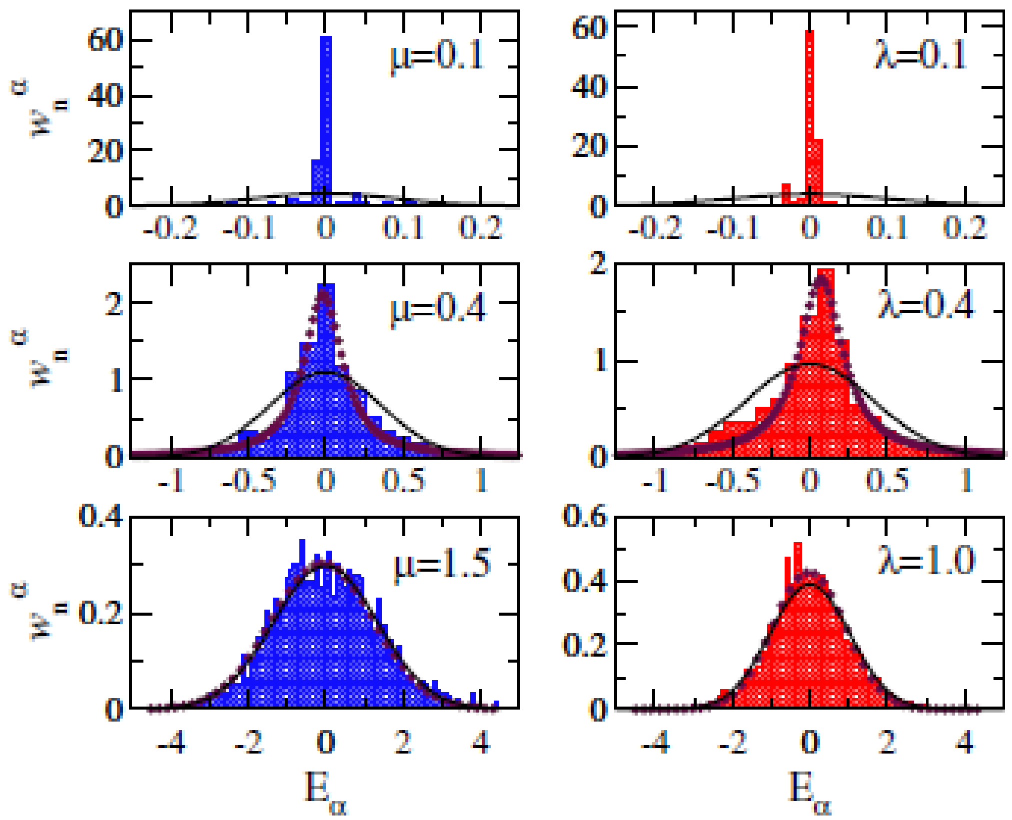


FIG. 3 (color online). Strength functions for model 1 (left) and model 2 (right) obtained by averaging over 5 close states in the middle of the spectrum. Middle panels: circles give a Breit-Wigner fit. Lower panels: circles stand for a Gaussian fit. In all panels, solid curves correspond to the Gaussian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

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…."