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Chaos and Thermalization in Isolated Quantum Systems of Interacting Particles

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Onset of chaos and thermalization in isolated quantum systems of interacting particles

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"Quantum chaos" in deterministic systems

S.G.Casati, B.V.Chirikov, F.M.Izraelev, J.Ford, Stochastic Behavior of a Quantum Pendulum under a Periodic Perturbation, Lect. Notes in Phys. {\bf 93} (1979) 334.

- 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.

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."

Universality of chaos





Chaotic eigenstates

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AN EXAMPLE OF CHAOTIC EIGENSTATES IN A COMPLEX ATOM

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Received 7 January 1985

Statistically processing a group of excited states with the total angular momentum and parity $J^{*} = 1^{*}$ 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.

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]).

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.

E.Lansing, May 7, 2014

(problem of electron recombination)

Basic relations

$$H = H_0 + V$$

$$H|\alpha\rangle = E^{\alpha}|\alpha\rangle \qquad \qquad |\alpha\rangle = \sum_{n} C_{n}^{\alpha}|n\rangle$$

Strength function:

$$F_n(E) = \sum_{\alpha} \left| C_n^{\alpha} \right|^2 \delta(E - E^{\alpha})$$

Occupation numbers:

$$n_{s}^{\alpha} = \left\langle \alpha \left| \hat{n}_{s} \right| \alpha \right\rangle = \sum_{n} \left| C_{n}^{\alpha} \right|^{2} \left\langle n \left| \hat{n}_{s} \right| n \right\rangle$$

Thermalization in an isolated gold atom



FIG. 7. Orbital occupation numbers in Au²⁴⁺ 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.

Two-Body Interaction Model

$$H = \sum_{k}^{m} \varepsilon_{k} a_{k}^{\dagger} a_{k} + \frac{1}{2} \sum_{kqpr} V_{kqpr} a_{k}^{\dagger} a_{q}^{\dagger} a_{p} a_{r}$$

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



two-body matrix elements (random or dynamical)

 $H_0 = \sum_{k=0}^{M} \varepsilon_k a_k^{\dagger} a_k$

- *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

determines the basis in which the dynamics occurs

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.

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 meaning of temperature, entropy and heat capacity;
(d) the increase of temperature due to the interaction...."

Transition to "chaos": chaotic eigenstates



Fermi-Dirac distribution





Circles: analytical description versus numerical data, Diamonds: Fermi-Dirac with thermodynamical temperature

$$S_{\rm th} = \ln\rho(E) + {\rm const},$$
$$\frac{1}{T_{\rm th}} = \frac{dS_{\rm th}}{dE} = \frac{d\,\ln\rho}{dE}.$$

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 $\varepsilon_k = \frac{4\pi^2 k^2}{I^2}$

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

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

Experimental setup is proposed to observe this transition

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



 $m \equiv M$

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

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

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

 $\lambda_{cr} \approx 0.5$

 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

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

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

BW is characterized by half-width:

Gauss is characterized by its variance:

$$\Gamma_{n_0} \approx 2\pi \left| \overline{H_{n_0 m}} \right|^2 \rho_m$$
$$\sigma_{n_0}^2 = \sum_{m \neq n_0} \left| H_{n_0 m} \right|^2$$

Transition to chaos occurs when

 $\Gamma \approx \sigma \parallel$

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.

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).

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

Foundation of statistical mechanics

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

Thermodynamical limit N→∞;
 Exponential instability plus boundary in phase space (λ > 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 !

Summary

(a) Quantum chaos in terms of eigenstates

(b) Many-body chaos --- energy shell, form of strength function

(c) Origin of thermalization --- chaotic eigenstates

(d) Chaos in integrable systems

Thank you for your attention!