# Physics of level density and thermalization

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Work in progress

- Thermalization, Quantum Chaos, and Level Density
- Shell model and Moments method
- "Constant temperature" model

Many-body quantum system with no random elements, internally developed chaotic behavior

In physical terms, one may say that quantum thermalization occurs in the Hilbert space rather than phase space /T. Mori et al. J. Phys. B51, 112001 (2018)./

**General method – diagonalization of Hamiltonian matrix** 

"Eigenfunction thermalization hypothesis" – read Landau and Lifshits

# **Microscopic description of Nuclear Level Density**

### Shell model (the most successful)

- Restricted model space
   Dim(sd) ~ 10<sup>6</sup>
   Dim(fp) ~ 10<sup>10</sup>
- Need effective interaction
- Numerical diagonalization
- High accuracy:  $\delta E \sim \pm 200 \text{KeV}$

### How it works:

Many-body states in Shell Model: 
$$|\alpha\rangle = \sum_{k=1}^{Dim} C_k^{\alpha} |k\rangle$$
.

Schrödinger equation: 
$$\hat{H}|\alpha\rangle = E_{\alpha}|\alpha\rangle \Rightarrow \hat{H}\vec{C}_{\alpha} = E_{\alpha}\vec{C}_{\alpha}$$



# FAMILY OF ENTROPIES FOR A MESOSCOPIC SYSTEM

• THERMODYNAMIC (Boltzmann)

 $\rho(E) \propto \exp(S_{\rm th})$ 

- QUASIPARTICLE (Landau Fermi-liquid)
- $S_{\text{s.p.}}^{\alpha} = -\sum_{i} \{ n_{i}^{\alpha} \ln(n_{i}^{\alpha}) + (1 n_{i}^{\alpha}) \ln(1 n_{i}^{\alpha}) \}$
- INFORMATION (Shannon)

 $|\alpha\rangle = \sum_k C_k^{\alpha} |k\rangle, \quad S_{\inf}^{\alpha} = -\sum_k \{|C_k^{\alpha}|^2 \ln |C_k^{\alpha}|^2\}$ 

 $\langle n_i \rangle_E = [e^{(\epsilon_i - \mu)/T_{\text{s.p.}}} + 1]^{-1}$ 

Temperature T(E)

$$T_{\rm th} = \left(\frac{dS_{\rm th}}{dE}\right)^{-1}$$

$$T_{\rm inf} = \left(\frac{d\bar{S}_{\rm inf}}{dE}\right)^{-1}$$

T(s.p.) and T(inf) = for individual states !



### **EFFECTIVE TEMPERATURE of INDIVIDUAL STATES**

From occupation numbers in the shell model solution (dots) From thermodynamic entropy defined by level density (lines)



Occupation numbers in multicharged ions Au25+

(recombination as analog of neutron resonances in nuclei)

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

/G. Gribakin, A. Gribakina, V. Flambaum/

Average over individual states is equivalent to a thermal ensemble



d5/2, d3/2, s1/2

Single – particle occupation numbers Thermodynamic behavior identical in all symmetry classes FERMI-LIQUID PICTURE 28 Si



Artificially strong interaction (factor of 10) Single-particle thermometer cannot resolve spectral evolution





S. Karampagia, V.Z. Nucl. Phys. A962 (2017)

J = 0 - 7, positive parity level density



FIG. 3: Comparison of the level density of <sup>56</sup>Fe calculated in the pf model space (black line with circles) versus the one calculated in the  $pf + g_{9/2}$  model space (red line with triangles), using the  $E_{g.s.}$ =-197.100, which minimizes the difference of the low-lying level densities between the two model spaces.



No diagonalization required

$$\rho(E,\alpha) = \sum_{\kappa} D_{\alpha\kappa} \cdot G_{\alpha\kappa}(E)$$

[Wong]

$$G_{\alpha\kappa}(E) = G(E + E_{\text{g.s.}} - E_{\alpha\kappa}, \sigma_{\alpha\kappa})$$
$$G(x, \sigma) = C \cdot \begin{cases} \exp\left(-x^2/2\sigma^2\right) &, & |x| \le \eta \cdot \sigma \\ 0 &, & |x| > \eta \cdot \sigma \end{cases}$$

 $E_{\alpha\kappa} = \langle H \rangle_{\alpha\kappa},$ 

$$\alpha = \{n, J, T_z, \pi\}$$
Quantum numbers

$$\kappa = \{n_1, n_2, \dots, n_q\}$$

Exact quantum numbers

<u>Finite range</u> Gaussian



**Partitions** 

Many-body dimension

$$\operatorname{Tr}^{(J)}[\cdots] = \operatorname{Tr}^{(J_z)}[\cdots]_{J_z = J} - \operatorname{Tr}^{(J_z)}[\cdots]_{J_z = J+1}$$

 $\langle H \rangle_{\alpha\kappa} = \operatorname{Tr}^{(\alpha\kappa)}[H]/D_{\alpha\kappa}, \quad \underline{Centroids}$ 

 $\langle H^2 \rangle_{\alpha\kappa} = \mathrm{Tr}^{(\alpha\kappa)} [H^2] / D_{\alpha\kappa}$ 

 $\sigma_{\alpha\kappa} = \sqrt{\langle H^2 \rangle_{\alpha\kappa} - \langle H \rangle_{\alpha\kappa}^2}$ 

<u>Centroids – first moment</u>

Widths - second moment



Partition structure in the shell model

(a) All 3276 states ; (b) energy centroids



28

Si

(result of geometric chaoticity!) Also in multiconfigurational method (hybrid of shell model and density functional)

$$\sigma_k^2 = \langle k | (H - H_{kk})^2 | k \rangle = \sum_{l \neq k} H_{kl}^2 ,$$

Widths add in quadratures

### <sup>2°</sup>Si, parity=+1, some *J*, *sd*-shell

Shell Model (solid line) vs. Moments Method (dashed line).









Generic shape (Gaussian)

# Level density for different classes of states in 285i

Full agreement between <u>exact shell model</u> and <u>moments method</u>

Problems: truncated orbital space, only positive parity in sd-model, ...



R.Sen'kov, V.Z. PRC 93 (2016)

## MEAN FIELD COMBINATORICS

S. Goriely et al. Phys. Rev. C 78, 064307 (2008) C 79, 024612 (2009)

http://www.astro.ulb.ac.be/pmwiki/Brusslin/Level

Hartree – Fock – Bogoliubov plus Collective enhancement with certain phonons Monte Carlo Shell model – Y. Alhassid +...

S. Goriely, A.-C. Larsen, D. Muecher Comprehensive test of nuclear level density models Phys. Rev. C **106**, 044315 (2022) Constant temperature model









# **CONSTANT TEMPERATURE PHENOMENOLOGY**

LEVEL DENSITY (E) = (const) exp (E/T)

Ericson (1962), Gilbert and Cameron (1965) Moretto (1975) – pairing phase transition T – "effective constant temperature" 1/T – rate of increase of level density



# **CONSTANT TEMPERATURE PHENOMENOLOGY**

# Level density (const) exp(E/T)

$$T_{t-d} = \left(\frac{\partial S}{\partial E}\right)^{-1} = T\left(1 - e^{-E/T}\right)$$

Partition function = Trace{exp[-H/T(t-d)]} diverges at T > T(t-d)

Cumulative level number N(E) = exp(S),Entropy S(E)= In(N) Thermodynamic temperature T(t-d) = dS/dE = T[1 - exp(-E/T)]Parameter T is *limiting temperature* (Hagedorn temperature in particle physics) Pairing phase transition? (Moretto) - Chaotization

**1/T** – rate of increase of the level density









**Degenerate single-particle levels – smaller T (faster chaotization)** 



# **Eliminating pairing interaction**



k(1) < 0 "antipairing"



М2





4 valence neutrons

4 proton holes

Space – only T=2, Two-body interaction through T=1 channel

$$ho^{(0)}(E,J,0)=
ho(E,J,0)$$
 . Nhw classification

Pure Total (N=0)

$$\rho^{(0)}(E, J, 1) = \rho(E, J, 1) - \sum_{\substack{J' = |J-1| \\ \rho^{(0)}(E, J, N) = \rho(E, J, N) -}}^{J+1} \rho(E, J', 0) \quad (N=1)$$

- --

$$-\sum_{K=1}^{N}\sum_{J_K=J_{\min}}^{N,\text{step }2}\sum_{J'=|J-J_K|}^{J+J_K}\rho^{(0)}(E,J',(N-K)).$$

- -

**Recursive relation** 

Exclusion of c.m. states




/"collective enhancement"/



## Sensitivity to the fit interval

### What next?

- \* Tables for **pf-shell** and further?
- \* Comparison of phenomenological descriptions with "Constant temperature" model
- \* New methods Lanczos algorithm
  - hybrid methods
  - random interactions
- \* Mesoscopic applications (disordered solids)
- \* Can we analytically derive CTM?
- \* Computational progress
- \* Continuum effects, width distribution, overlapping resonances
- \* Application to reactions

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V. Z., B.A. Brown, N. Frazier and M. Horoi. The nuclear shell model as a testing ground for many-body quantum chaos. Phys. Reports 276 (1996) 315.

V. Z.. Quantum chaos and complexity in nuclei. Annu. Rev. Nucl. Part. Sci. 46 (1996) 237.

A.Volya and V. Z. Invariant correlational entropy as a signature of quantum phase transitions in nuclei. Phys. Lett. B 574 (2003) 27.

V. Z. and A. Volya. Nuclear structure, random interactions and mesoscopic physics. Phys. Rep. 391 (2004) 311.

F. Borgonovi, F.M. Izrailev, L.F. Santos, and V.Z. Quantum chaos and thermalization in isolated systems of interacting particles. Physics Reports 626 (2016) 1.

V.Z. and A. Volya. Chaotic features of nuclear structure and dynamics: Selected topics. Physica Scripta 91 (2016) 033006.

V.Z. and M. Horoi. *Nuclear level density, thermalization, chaos and collectivity.* Progress in Particle and Nuclear Physics, **105**, **180** (2019). M. Horoi, J. Kaiser, and V. Z. *Spin- and parity-dependent nuclear level densities and the exponential convergence method.* Phys. Rev. C **67** (2003) 054309.

M. Horoi, M. Ghita, and V. Z. *Fixed spin and parity nuclear level density for restricted shell model configurations*. Phys. Rev. C **69** (2004) 041307(R).

M. Horoi and V. Z. *Exact removal of the center-of-mass spurious states from level densities*. Phys. Rev. Lett. **98** (2007) 262503.

R.A. Sen'kov, M. Horoi, and V.Z. *High-performance algorithm for calculating non-spurious spin- and paritydependent nuclear level densities.* Phys. Lett. B **702** (2011) 413.

R.A. Sen'kov, M. Horoi, and V.Z. *A high-performance Fortran code to calculate spin- and paritydependent nuclear level densities*. Computer Physics Communications **184** (2013) 215. R.A. Sen'kov and V. Z. *Nuclear level density: Shell-model approach.* Phys. Rev. C **93** (2016) 064304. S. Karampagia and V. Z. *Nuclear shape transitions, level density, and underlying interactions.* Phys. Rev. C **94** (2016) 014321.

S. Karampagia, A. Renzaglia, and V.Z. *Quantum phase transitions and collective enhancement of level density in odd-A and odd-odd nuclei*. Nucl. Phys. A962 (2017) 46.

S. Karampagia, R.A. Sen'kov, and V.Z. *Level density in the sd-nuclei - statistical shell model predictions*. ADNDT, 120, 1-120 (2018).

V.Z. and S. Karampagia. *Nuclear level density and related physics*.

EPJ Web of Conferences, 194, 01001 (2028).

V. Z., S. Karampagia, and A. Berlaga. *Constant temperature model for nuclear level density*. Phys. Lett. B 783 (2018) 428.

S. Karampagia and V.Z. Nuclear shell model and level density.

Int. J. Mod. Phys. E 29 (2020) 2030005.

V. Z. and S. Karampagia. *Physics of thermalization and level density in an isolated system of strongly interacting particles*. Eur. Phys. J. Spec. Top. 230 (2021) 755.

#### **MANY-BODY QUANTUM CHAOS AS AN INSTRUMENT**

**SPECTRAL STATISTICS** – signature of chaos

- missing levels
- purity of quantum numbers
- level density without full diagonalization
- presence of time-reversal invariance

**EXPERIMENTAL TOOL** – unresolved fine structure

- width distribution (more work required)
- damping of collective modes
- **NEW PHYSICS** statistical enhancement of weak perturbations (parity violation in neutron scattering and fission)
  - mass fluctuations
  - chaos on the border with continuum

#### THEORETICAL CHALLENGES

- order out of chaos
- chaos and thermalization
- development of computational tools
- new approximations in many-body problem

# **INSIDE CHAOS**

I. Percival, J. Phys. B6 (1973) L229

- $\bullet$  DISORDERED wave functions
- Any *SIMPLE* operator has matrix elements of the same order of magnitude between any two of these eigenfunctions
- All typical wave functions of roughly the same energy LOOK ROUGHLY THE SAME being spread over the large region of configuration space

Random matrix canonical ensembles – only as mathematical limit

# Chaotic motion in mesoscopic systems

- \* Mean field (one-body chaos) classical features
- \* Strong interaction (many-body chaos)
- \* High level density
- \* Mixing of simple configurations
- \* Destruction of quantum numbers,
  - (in nuclei: conserved only energy; J,M; T,T3; parity)
- \* Local spectral statistics Gaussian Orthogonal Ensemble
- \* Correlations between classes of states
- \* Coexistence with (damped) collective motion
- \* Thermal equilibrium without heat bath
- \* Continuum effects open system

## CLOSED MESOSCOPIC SYSTEM

## at high level density

Two languages: individual stationary wave functions thermal excitation

- \* Mutually exclusive ?
- \* Complementary ?
- \* Equivalent ?

Answer depends on thermometer

#### CHAOS versus THERMALIZATION

- L. BOLTZMANN Stosszahlansatz = MOLECULAR CHAOS
- **N. BOHR** Compound nucleus = MANY-BODY CHAOS
- N. S. KRYLOV Foundations of statistical mechanics
- L. Van HOVE Quantum ergodicity
- L. D. LANDAU and E. M. LIFSHITZ "Statistical Physics"

Average over the equilibrium ensemble should coincide with the expectation value in a generic individual eigenstate of the same energy – the results of measurements in a closed system do not depend on exact microscopic conditions or phase relationships if the eigenstates at the same energy have similar macroscopic properties

#### **Eigenstate Thermalization Hypothesis**

## **TOOL: MANY-BODY QUANTUM CHAOS**



LEVEL DYNAMICS WAY to CHAOS: MULTIPLE AVOIDED CROSSINGS as a function of interaction strength

(shell model of 24Mg as a typical example)

Fraction (%) of realistic strength

*From turbulent to laminar level dynamics* Chaos due to particle interactions at high level density

#### MEASURING COMPLEXITY

Eigenstate  $|\alpha\rangle$  in a shell model basis  $|k\rangle$   $|\alpha\rangle = \sum_k C_k^{\alpha} |k\rangle$ Information entropy  $S^{\alpha} = -\sum_k |C_k^{\alpha}|^2 \ln |C_k^{\alpha}|^2$ No mixing:  $S^{\alpha} \to 0$ "Microcanonical" mixing:  $S^{\alpha} \to \ln N$ GOE:  $\overline{S^{\alpha}} = \ln(0.48N)$ 

Shannon entropy

Information entropy is basis-dependent
- special role of mean field



28 Si Shell Model (artificially weak interaction)



### **INFORMATION ENTROPY of EIGENSTATES**

(a) function of energy; (b) function of ordinal number

ORDERING of EIGENSTATES of GIVEN SYMMETRY

SHANNON ENTROPY AS THERMODYNAMIC VARIABLE



## 9 INDIVIDUAL STATES

AVERAGE OVER

10, 100, 400 STATES

**STRENGTH FUNCTION**  $F_k(E) = \sum_{\alpha} (C_k^{\alpha})^2 \delta(E - E_{\alpha})$  Local density of states in condensed matter physics





#### **GROUND STATE ENERGY OF RANDOM MATRICES**

#### EXPONENTIAL CONVERGENCE

## SPECIFIC PROPERTY of RANDOM MATRICES ?

/The proof based on the Lanczos algorithm/



REALISTIC SHELL MODEL

48 Cr

Excited state J=2, T=0

<u>EXPONENTIAL</u> <u>CONVERGENCE</u> !

E(n) = E + exp(-an) $n \sim 4/N$ 



REALISTIC SHELL MODEL

## EXCITED STATES 51Sc

1/2-, 3/2-

Faster convergence: E(n) = E + exp(-an) $a \sim 6/N$ 





Exact shell model:stair-dashed (with CM) and stair-solid (no CM)Method of moments:straight-dashed (with CM) and straight-solid (no CM)Dotted line:spurious states



"THE BEAUTY OF THIS IS THAT IT IS ONLY OF THEORETICAL IMPORTANCE, AND THERE IS NO WAY IT CAN BE OF ANY PRACTICAL USE WHATSDEVER." Analytical results for tridiagonal matrices

$$H = \begin{pmatrix} \epsilon_1 & V_2 & 0 & 0 & 0 & 0 \\ V_2 & \epsilon_2 & V_3 & 0 & 0 & 0 \\ 0 & V_3 & \epsilon_3 & V_4 & 0 & 0 \\ 0 & 0 & \dots & \dots & 0 \\ 0 & 0 & 0 & \dots & \dots & V_n \\ 0 & 0 & 0 & 0 & V_n & \epsilon_n \end{pmatrix}$$

Recurrence relation for determinants

 $D_n(E) = (\epsilon_n - E)D_{n-1}(E) - V_n^2 D_{n-2}(E)$ 

New method for shell-model level density /B.A. Brown, 2018/

Convergence is determined by

$$\lambda_n^2 = V_n^2 / (\epsilon_n \epsilon_{n-1})$$

Assume existence of the limit

 $\lambda_n \Rightarrow \lambda$ at $n \Rightarrow \infty$ 









Level density (0+) on two sides of deformation shape transition

/"collective enhancement"/



States J=0

#### PAIR CORRELATOR

(b) Only pairing

(d) Non-pairing interactions

(f) All interactions

$$\mathcal{H}_P = \sum_{t=0,\pm 1} P_t^{\dagger} P_t$$

$$P_t = \frac{1}{\sqrt{2}} \sum_{j} [a_j a_j]_{J=0,T=1,T_3=1}$$



PAIR CORRELATOR as a THERMODYNAMIC FUNCTION





V(1) = matrix elements of the two-body interaction
with change of orbital momentum of one particle
by 2 units (the same parity) – way to deformation





## Number of 0+ levels up to energy 10 MeV



J=0 – 10 for 26 Al, 28 Al, 30 P (up to 10 MeV)

J=1/2 – 21/2 for 27 Al (up to 10 MeV)

J=0 – 10 for 50 Mn (up to 60 MeV)


#### Removal of the center-of-mass spurious states

#### Harmonic oscillator:

$$\mathcal{N}_{spur}(K\hbar\omega)\sim\sum_{K'=1}^{K}\mathcal{N}_{pure}((K-K')\hbar\omega),$$



where K' presents how many times we act with  $A_{cm}^{\dagger}$ 

P. Van Isacker, Phys. Rev. Lett. 89, 262502 (2002)



#### Nuclear level density. Recursive method:

$$\rho_{\textit{pure}}(E, J, K) = \rho(E, J, K) - \sum_{K'=1}^{K} \sum_{J_{K'}=J_{\min}}^{K, \textit{step 2}} \sum_{J'=|J-J_{K'}|}^{J+J_{K'}} \rho_{\textit{pure}}(E, J', K-K')$$

M. Horoi and V. Zelevinsky, Phys. Rev. Lett. 98, 262503 (2007)



TABLE III: Cumulative Number of Levels (NoL) of J = 0 up to energy 10 MeV for different  $(k_1, k_2)$  combinations for <sup>28</sup>Si, <sup>24</sup>Mg and <sup>52</sup>Fe found with the moments method. The column NoL corresponds to the calculation of the moments method, while the column Renorm corresponds to the renormalized level density (NoL up to 0.4).

shape	case	nucleus	$R_{4/2}$	NoL	Renorm
deformed	$k_1 = 1.0, k_2 = 0.4$	<sup>28</sup> Si	3.31	22	60
deformed	$k_1 = 1.0, k_2 = 0.5$	<sup>28</sup> Si	3.33	17	54
deformed	$k_1 = 1.0, k_2 = 0.6$	<sup>28</sup> Si	3.21	13	49
spherical	$k_2 = 1.0, k_1 = 0.9$	<sup>28</sup> Si	2.12	5	34
deformed	$k_1 = 1.0, k_2 = 0.5$	$^{24}Mg$	3.20	10	24
deformed	$k_1 = 1.0, k_2 = 0.6$	$^{24}Mg$	3.21	8	21
spherical	$k_2 = 1.0, k_1 = 0.3$	$^{24}Mg$	2.03	6	18
deformed	$k_1 = 1.0, k_2 = 0.4$	<sup>52</sup> Fe	3.07	236	6516
spherical	$k_2 = 1.0, k_1 = 0.0$	$^{52}$ Fe	2.25	30	2617

H = k(1)V(1) + k(2)V(2)

V(1) – matrix elements of

single-particle transfer

### Statistical approach to Nuclear Level Density (cont.)

$$\rho(\boldsymbol{E},\beta) = \sum_{\kappa} \boldsymbol{D}_{\beta\kappa} \cdot \boldsymbol{G}(\boldsymbol{E} - \boldsymbol{E}_{\beta\kappa}, \sigma_{\beta\kappa})$$

 $G(x, \sigma)$  - Gaussian distribution

- $\beta = \{n, J, T_z, \pi\}$  quantum numbers
- $\kappa$  configurations



 $D_{\beta\kappa}$  - number of many-body states with given  $\beta$  that can be built for a given configuration  $\kappa$ 

Moments of *H* for each configuration  $\kappa$ :

$$E_{\beta\kappa} = \operatorname{Tr}^{(\beta\kappa)}[H]/D_{\beta\kappa}$$

$$\sigma_{\beta\kappa}^{2} = \mathrm{Tr}^{(\beta\kappa)}[H^{2}]/D_{\beta\kappa} - \left(\mathrm{Tr}^{(\beta\kappa)}[H]/D_{\beta\kappa}\right)^{2}$$

M. Horoi, M. Ghita, and V. Zelevinsky, PRC 69 (2004) 041307(R)

## No diagonalization required







Effective temperature for the level density at low energy (up to 6 – 8 Mev) **Even-odd** staggering **Clear minima in** the vicinity of N=Z



# $H = h + \lambda U_1 + U_2.$

U(1) = matrix elements of the two-body interaction with change of orbital momentum of one particle by 2 units (the same parity) – way to deformation

N = 10

N = 11

N = 12N = 13

N = 14 N = 15 N = 16 N = 17N = 18

