Dynamics of incomplete relaxation and memory of the initial conditions in an isolated quantum cold-atom system. Properties of a one-dimensional gas of spin-$1/2$ atoms in an axial potential.

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Collaboration:
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Outline

Part I

Memory of the initial conditions in incompletely-chaotic quantum systems with no selection rules

Concrete examples:

— two zero-range-interacting ultracold atoms in a circular harmonic waveguide

— two zero-range-interacting ultracold atoms in an anisotropic harmonic trap

— rough billiards — systems with random-matrix interactions

Dynamics of relaxation:

— relaxation time

— fluctuations

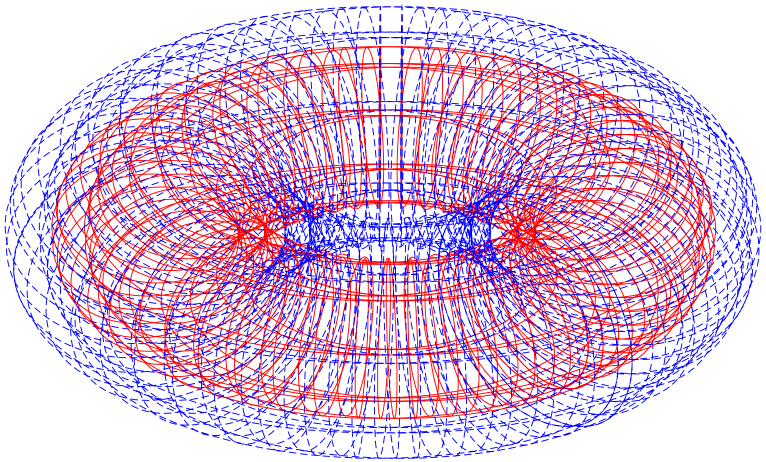
$$\hbar = 1$$

Part II

A one-dimensional gas of spin-1/2 atoms in an axial potential
Eigenstates — irreducible representations of the symmetric group
Energy spectra.
Perspectives for non-equilibrium dynamics

HAMILTONIAN CHAOS IN CLASSICAL MECHANICS

Integrable system:
A complete set of integrals of motion:
N degrees of freedom —
N functionally-independent regular integrals of motion in involution.
Regular motion:
phase-space trajectories lie on invariant tori.



Predictable evolution

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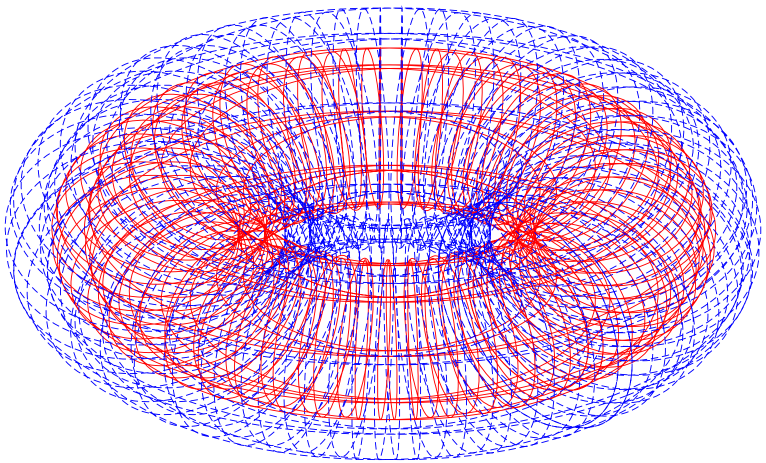


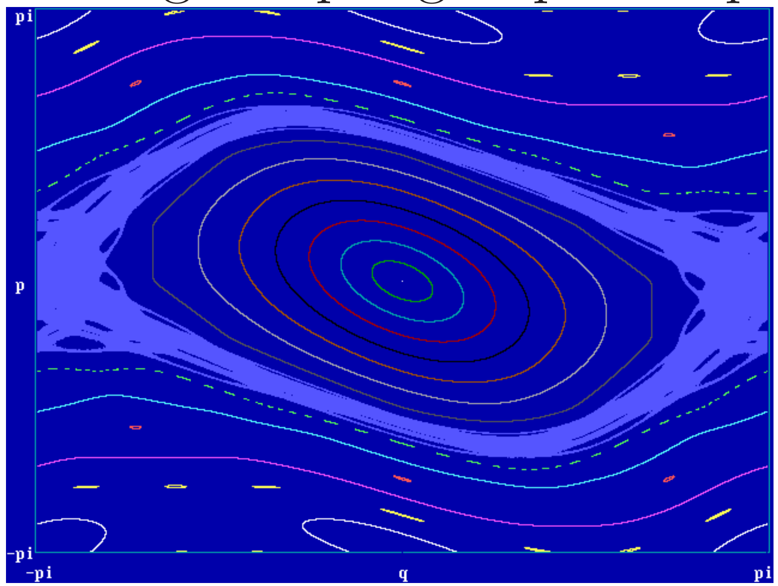
Predictable evolution

Non-integrable systems:

An incomplete set of integrals of motion

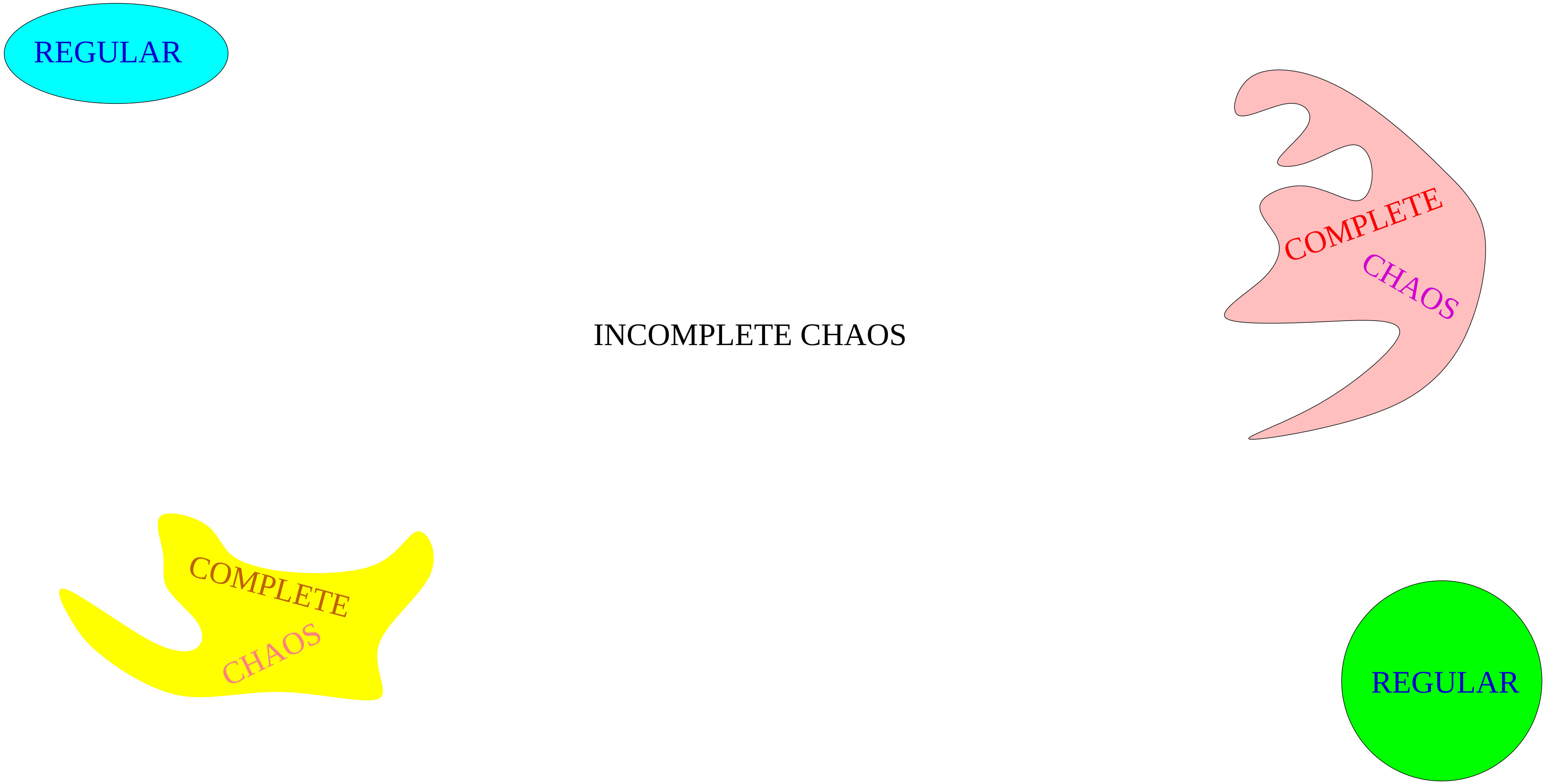
Irregular motion:

Mixing sampling of phase-space regions.



Complete chaos — ergodic sampling of all available phase space.

Statistical behavior, thermalization


REGULAR
COMPLETE
CHAOS
INCOMPLETE CHAOS
COMPLETE
CHAOS
REGULAR

WAVEFUNCTION COMPOSITION

INTEGRABLE SYSTEM

$$\hat{H}_0|\vec{n}\rangle = E_{\vec{n}}|\vec{n}\rangle$$

NON-INTEGRABLE SYSTEM

$$[\hat{H}_0 + \hat{V}]|\alpha\rangle = E_\alpha|\alpha\rangle$$

WAVEFUNCTION COMPOSITION

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$$[\hat{H}_0 + \hat{V}]|\alpha\rangle = E_\alpha|\alpha\rangle$$

$\eta_\alpha = \sum_{\vec{n}} |\langle\alpha|\vec{n}\rangle|^4$ — Inverse Participation Ratio

— the inverse of the number of the principal components:

$$|\langle\alpha|\vec{n}_i\rangle| = \frac{1}{\sqrt{N}} \quad (1 \geq i \geq N) \qquad \Rightarrow \qquad \eta_\alpha = \frac{1}{N}$$

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Integrable system — $\eta_\alpha = 1$ ($|\alpha\rangle \equiv |\vec{n}_0\rangle$)
Completely-chaotic system $\eta_\alpha \ll 1$ for any set $|\vec{n}\rangle$
(Eigenstate α consists of many eigenstates of each integrable system)

Incomplete chaos: $\eta \lesssim 1$

RELAXATION OF AN ISOLATED QUANTUM SYSTEM

Non-equilibrium initial state $\hat{\rho}_{\rm in} \equiv \hat{\rho}(t=0)$
The quantum-mechanical mean of any observable $\hat{A}$:

$$\langle \hat{A}(t) \rangle = \sum_{\alpha,\alpha'} \langle \alpha | \hat{A} | \alpha' \rangle \langle \alpha' | \hat{\rho}_{\rm in} | \alpha \rangle \exp\left(i(E_{\alpha'} - E_\alpha)t \right)$$

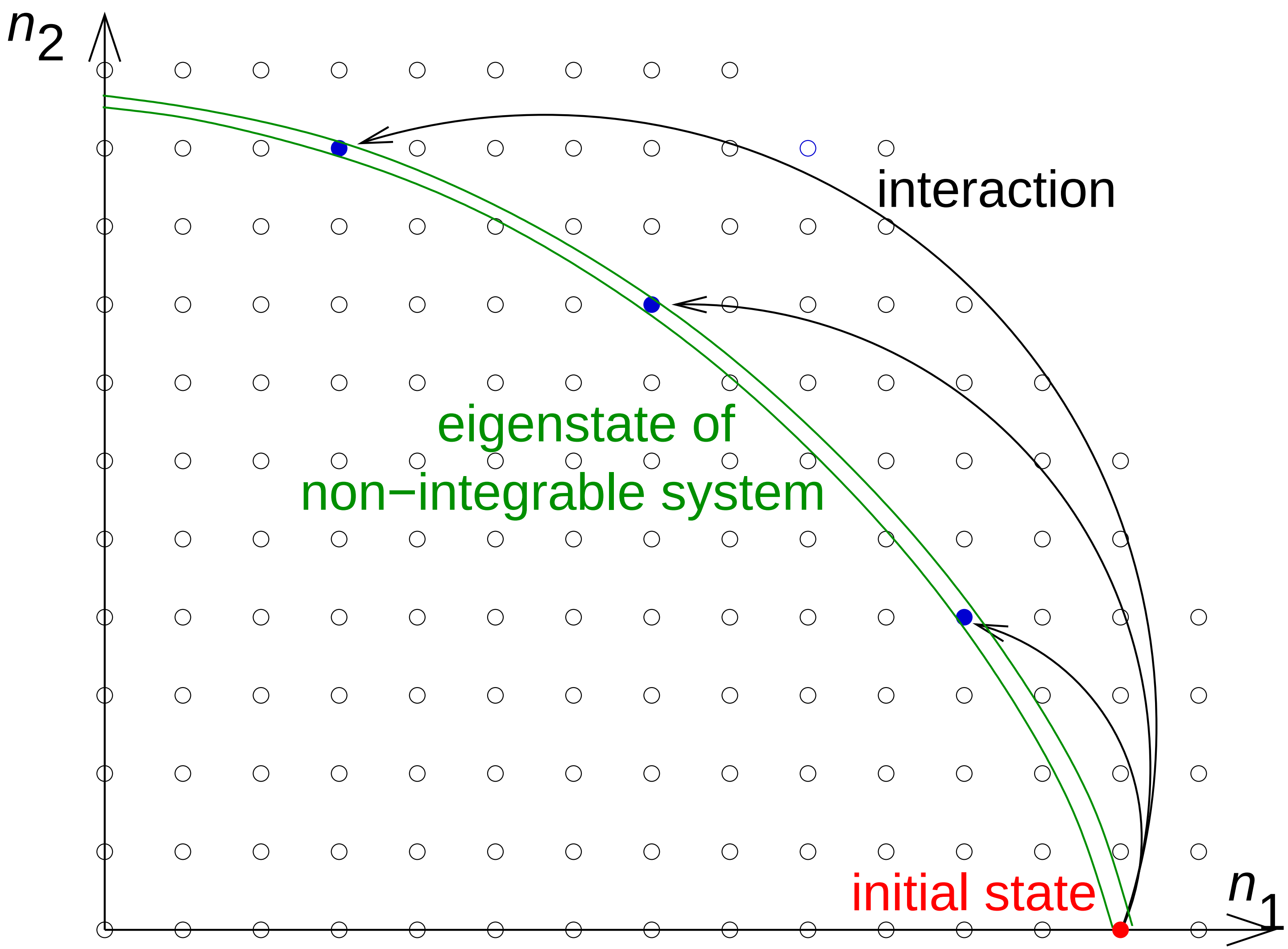
Relaxes to the infinite time average

$$A_{\rm rel} \equiv \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \langle \hat{A}(t) \rangle = \sum_\alpha \langle \alpha | \hat{\rho}_{\rm in} | \alpha \rangle \langle \alpha | \hat{A} | \alpha \rangle.$$

The observable $\hat{A}$ — integral of motion, $\langle \vec{n} | \hat{A} | \vec{n}' \rangle = A_{\vec{n}} \delta_{\vec{n}\vec{n}'}$
The initial state $\hat{\rho}_{\rm in}$ — diagonal, $\langle \vec{n} | \hat{\rho}_{\rm in} | \vec{n}' \rangle = \rho^{\rm in}_{\vec{n}} \delta_{\vec{n}\vec{n}'}$

$$A_{\rm rel} = \sum_{\vec{n},\vec{n}',\alpha} A_{\vec{n}} |\langle \vec{n} | \alpha \rangle \langle \alpha | \vec{n}' \rangle|^2 \rho^{\rm in}_{\vec{n}'}$$

$$A_{\rm rel} = \sum_{\vec{n},\vec{n}',\alpha} A_{\vec{n}} \left|\langle\vec{n}|\alpha\rangle\langle\alpha|\vec{n}'\rangle\right|^2 \rho^{\rm in}_{\vec{n}'} \qquad (|\langle\vec{n}|\hat{V}|\vec{n}'\rangle| \approx \text{const— no selection rules})$$



$|\alpha\rangle$ contributes $\bar{\eta}^{-1} = 4$ states $|\vec{n}\rangle$ into the equilibrium state

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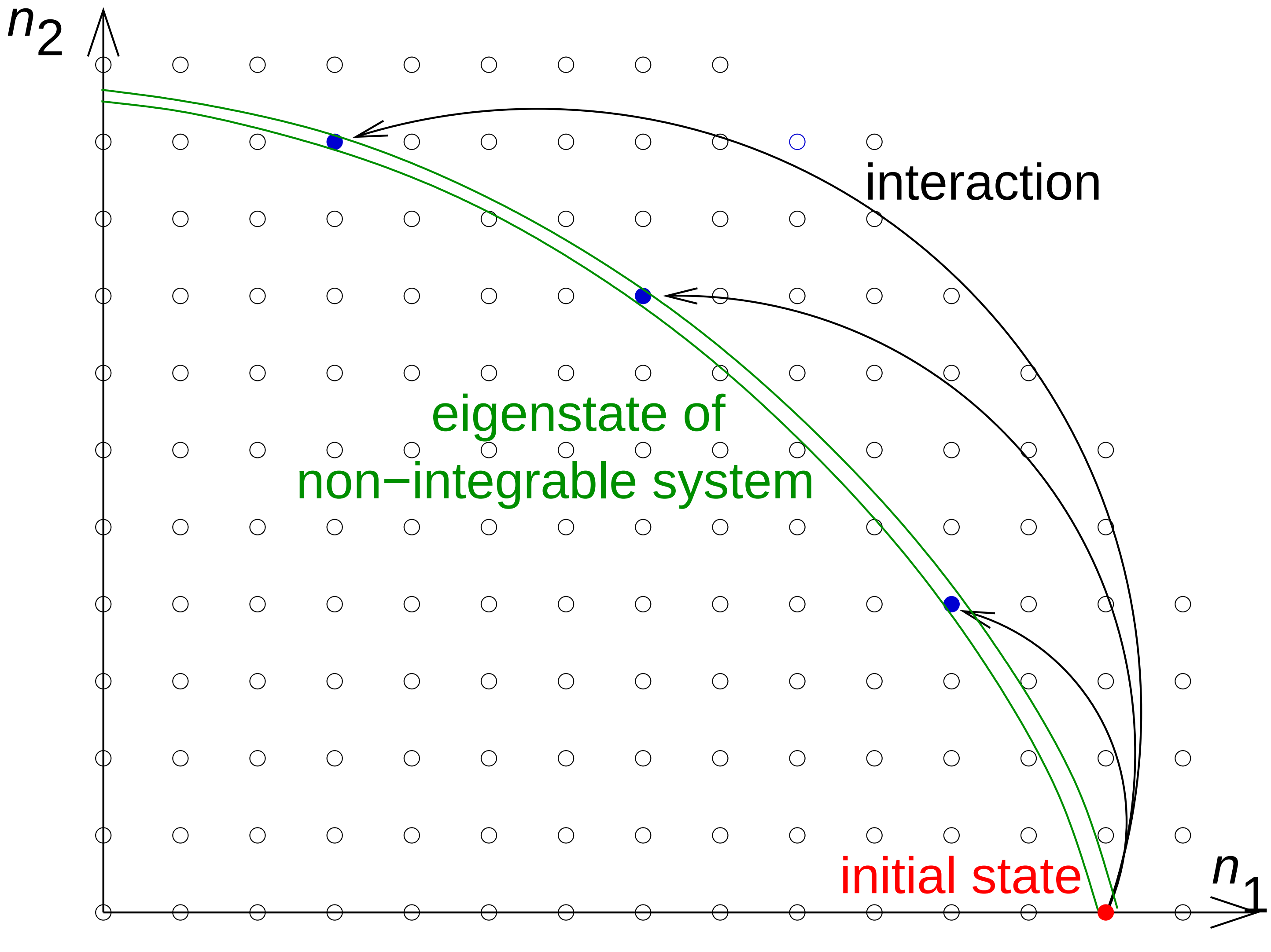

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One $|\vec{n}'\rangle$ taken from the initial state is retained in the equilibrium state with the weight $1/4 = \bar{\eta}$

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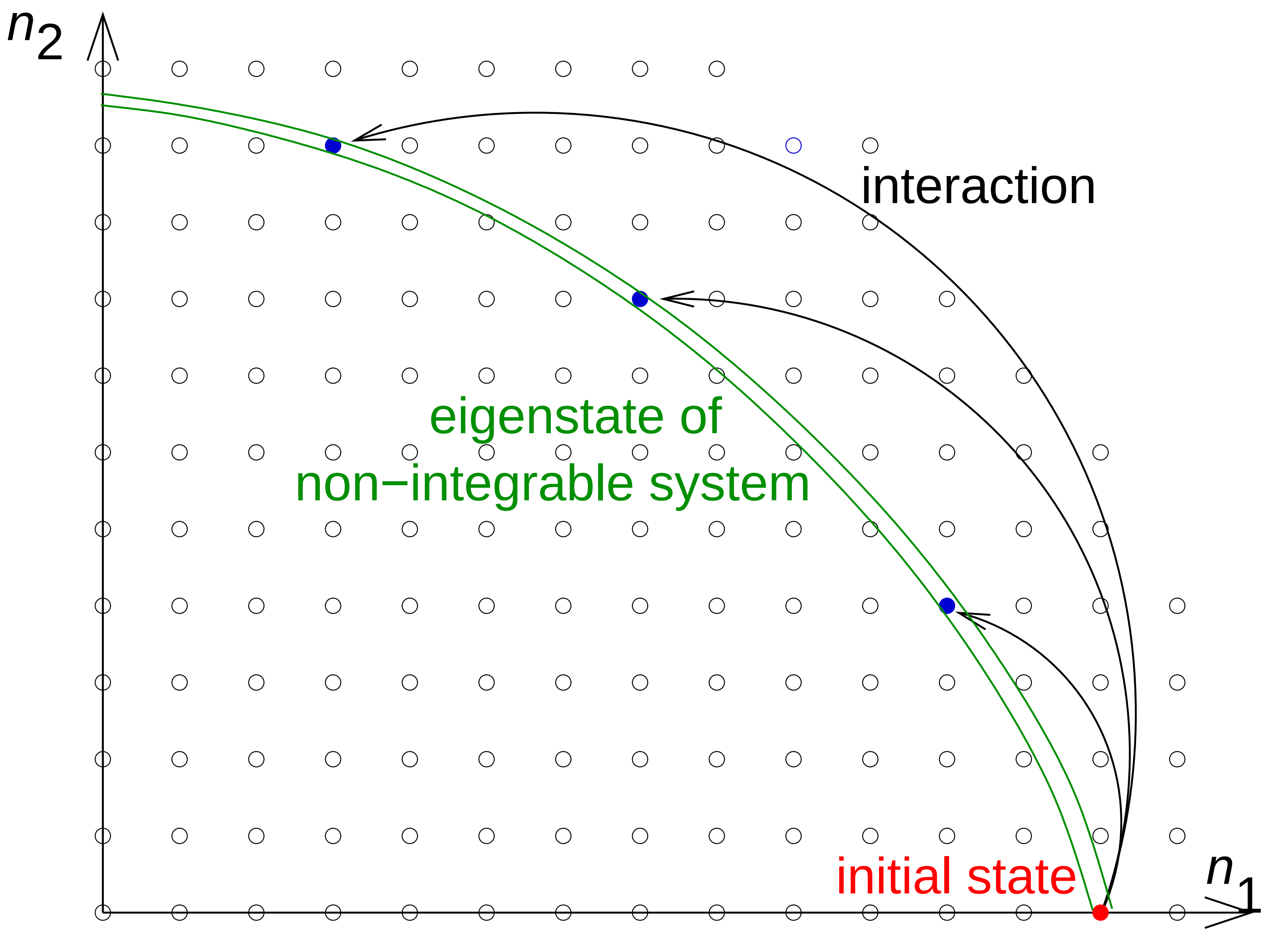

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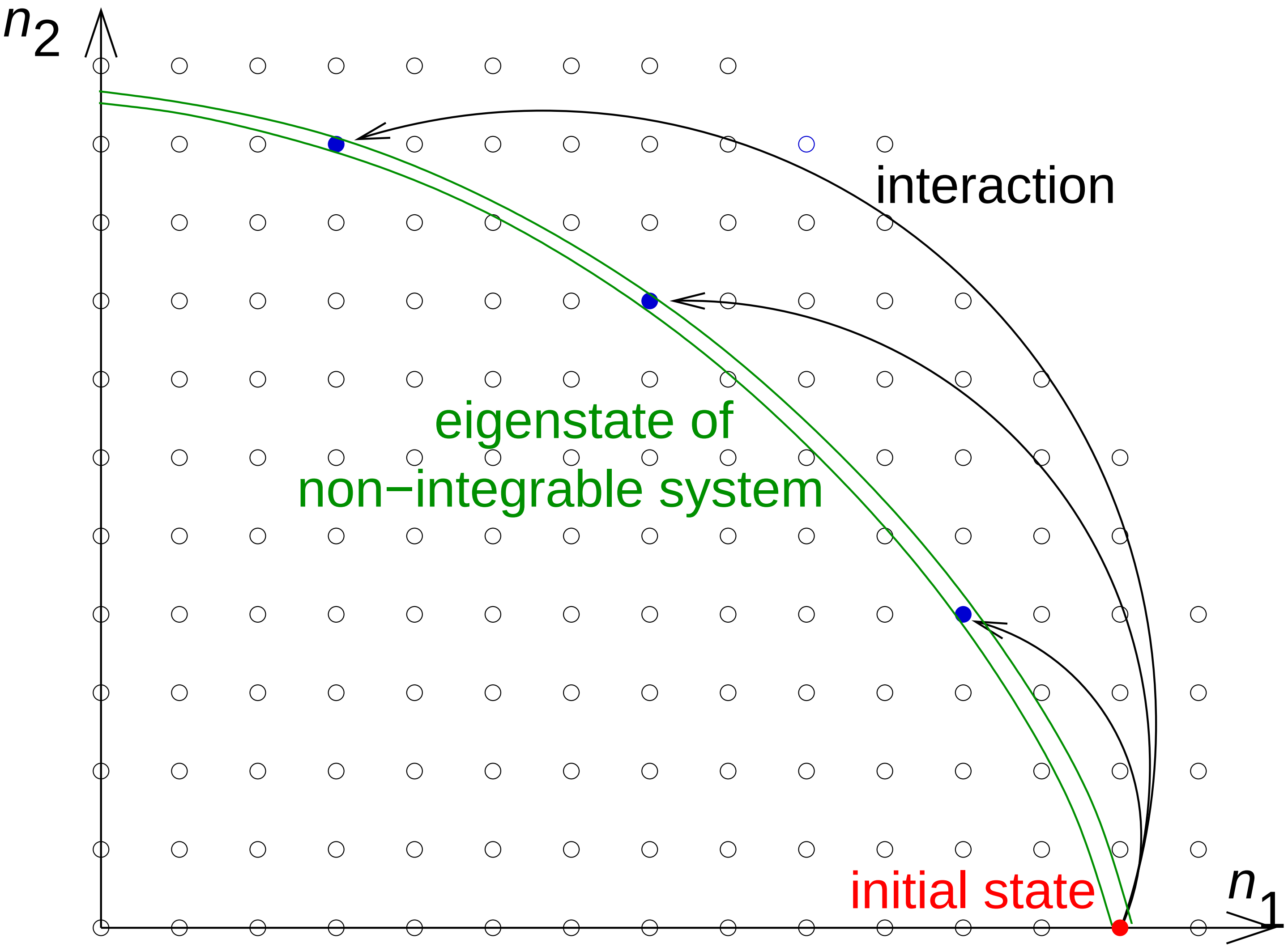
Three $|\vec{n}\rangle$ states

— drawn indiscriminately

— thermal contribution

— weight $3/4 = 1 - \bar{\eta}$

$$A_{\rm rel} = \sum_{\vec n, \vec n', \alpha} A_{\vec n} \left| \langle \vec n | \alpha \rangle \langle \alpha | \vec n' \rangle \right|^2 \rho^{\rm in}_{\vec n'} \qquad (|\langle \vec n | \hat V | \vec n' \rangle| \approx \text{const— no selection rules})$$



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$$A_{\rm rel} \approx \bar{\eta} A_{\rm in} + (1-\bar{\eta}) A_{\rm therm}$$

$A_{\rm in} = \sum_{\vec{n}} A_{\vec{n}} \rho_{\vec{n}}^{\rm in}$ — the initial expectation value (the infinite-time average for the integrable system)

$A_{\rm therm} = \sum_{\vec{n}} A_{\rm MC}(E_{\vec{n}}) \rho_{\vec{n}}^{\rm in}$ — microcanonical expectation value averaged over the initial state

$\bar{\eta}$ — averaged IPR — a universal parameter (it is the same for all observables and insensitive to the shape of the initial state)

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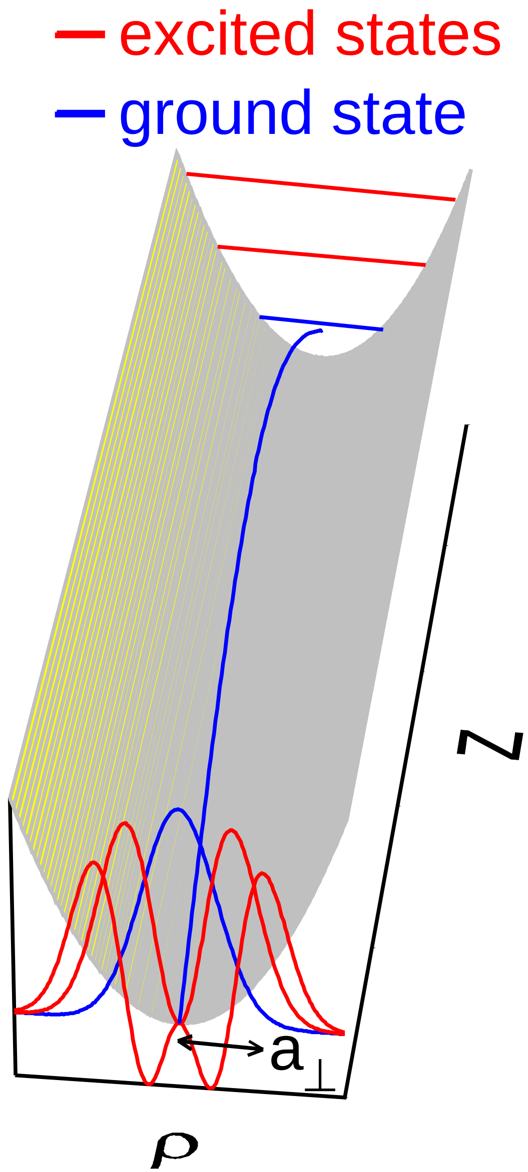
Integrable system: $\bar{\eta} = 1$, $A_{\mathrm{rel}} = A_{\mathrm{in}}$

Complete chaos: $\bar{\eta} \ll 1$, $A_{\mathrm{rel}} \approx A_{\mathrm{therm}}$ — relaxation to the thermal equilibrium

Derivation: [VY & Olshanii PRL **106**,025303 (2011); Olshanii, Jacobs, Rigol, Dunjko, Kennard & VY, Nature Communications 3, 641 (2012)]

TWO ULTRACOLD ATOMS IN A CYRCULAR WAVEGUIDE



[VY & Olshanii, PRA **81**,043641 (2010)]

Harmonic waveguide — center-of-mass can be separated

$$\hat{H}_0 = -\frac{1}{2\mu}\left[\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho}\right] + \frac{\mu}{2}\omega_\perp^2 \rho^2 \quad (\textbf{relative})$$

$$\hat{V} = \frac{2\pi}{\mu} a_s \delta(\mathbf{r}) \frac{\partial}{\partial r}[r.] \quad \text{—Fermi-Huang}$$

a_s — s-wave scattering length.

Circular waveguide

— L-periodic boundary conditions along z

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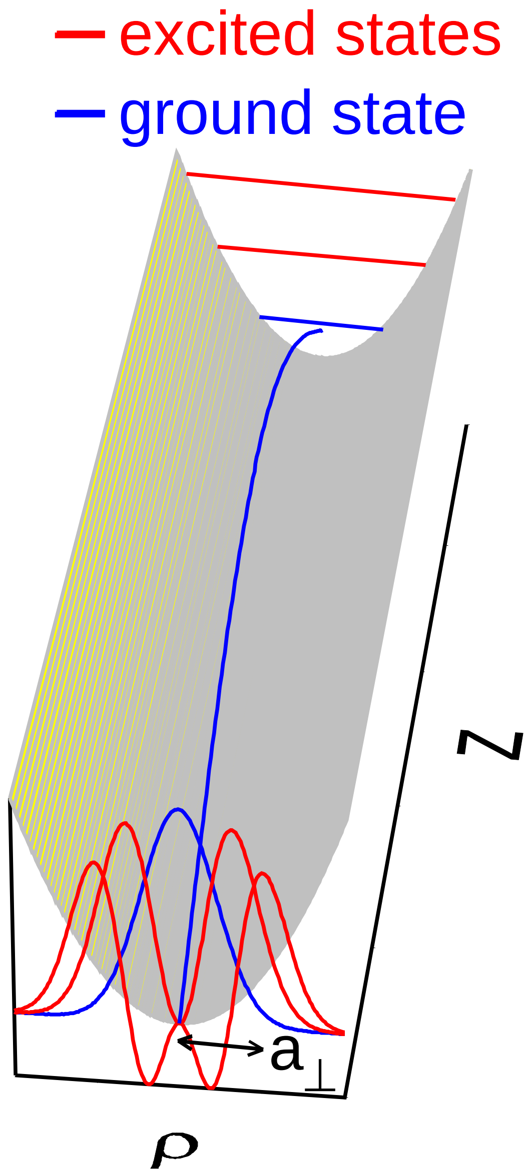

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Circular waveguide

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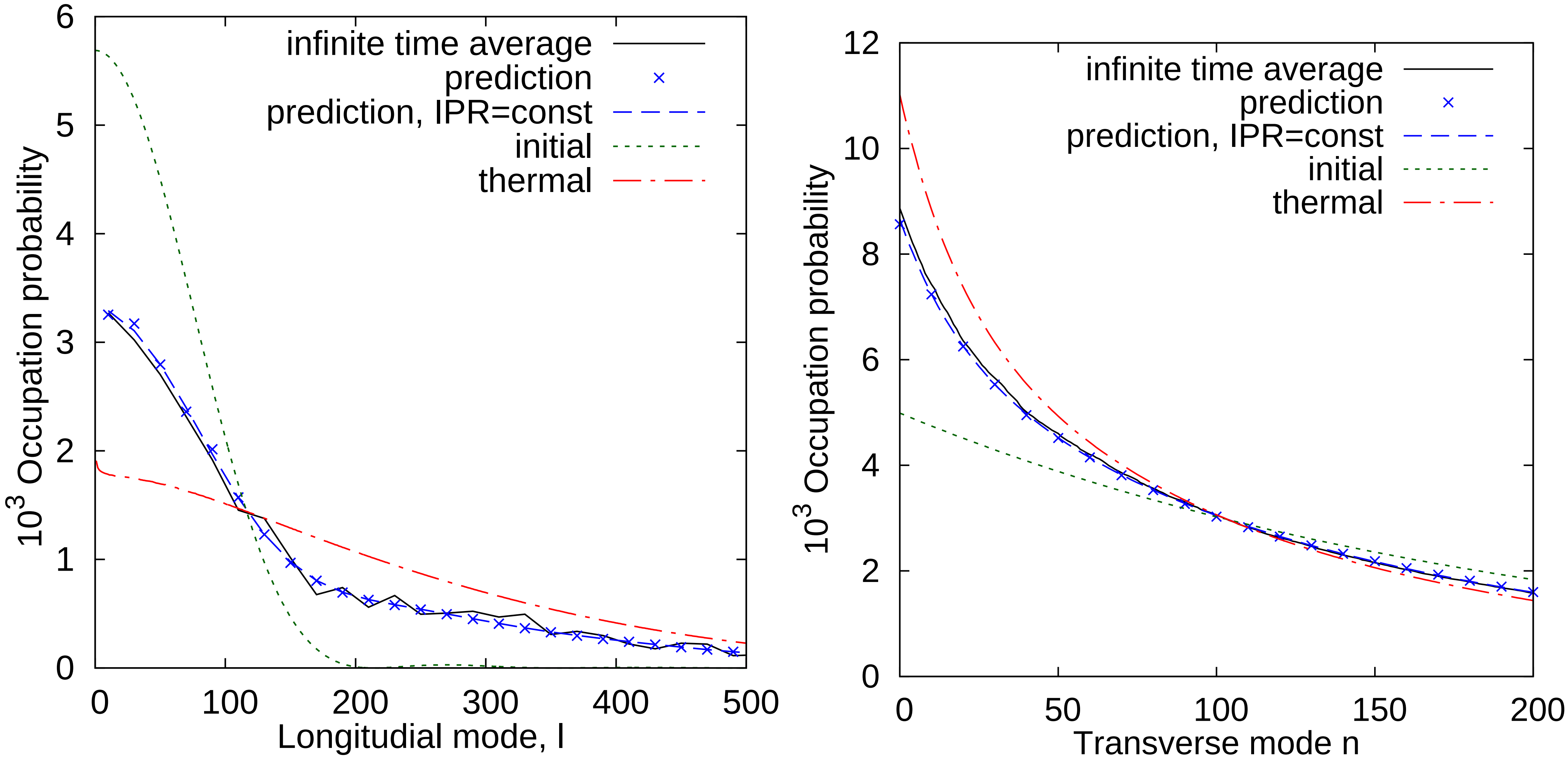
Similar models:

Šeba (1990)— Šeba billiard (2D billiard + zero-range scatterer); Idziaszek & Calarco (2005) — (3D HO + zero-range interaction)

Analytical solution (infinite series)

Transcendent equation for eigenenergies



infinite time average
prediction
prediction, IPR=const
initial
thermal
10^3 Occupation probability
0
1
2
3
4
5
6
0
100
200
300
400
500
Longitudial mode, l
infinite time average
prediction
prediction, IPR=const
initial
thermal
10^3 Occupation probability
0
2
4
6
8
10
12
0
50
100
150
200
Transverse mode n

NON-DIAGONAL INITIAL STATE

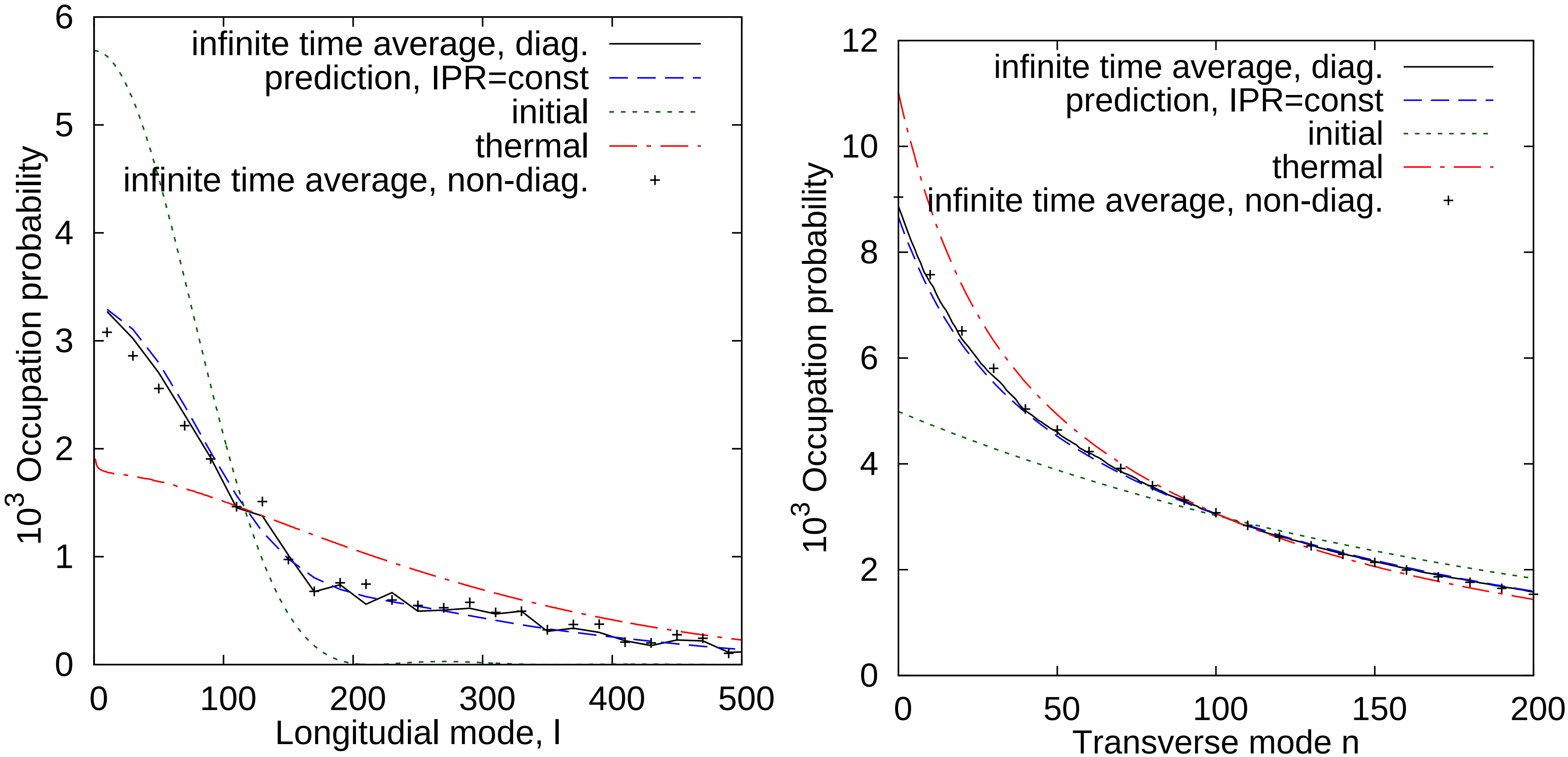
$\langle\vec{n}|\hat{\rho}_{\rm in}|\vec{n}'\rangle \neq 0$, $\vec{n} \neq \vec{n}'$

Leading correction:

$$A_{\rm rel} \approx \bar{\eta} A_{\rm in} + (1-\bar{\eta}) A_{\rm therm} - \sum_{\vec{n}\neq\vec{n}'} A_{\vec{n}} \langle\vec{n}'|\hat{\eta}_2(E_{\vec{n}})|\vec{n}\rangle \frac{\langle\vec{n}|\hat{\rho}_{\rm in}|\vec{n}'\rangle}{(E_{\vec{n}} - E_{\vec{n}'})^2}$$

Small correction:
—the non-diagonal matrix elements of $\hat{\rho}_{\rm in}$ have arbitrary phase;
— no energy-neighboring modes $\vec{n}$ and $\vec{n}'$
(uniform occupation of all modes = the thermal equilibrium).

The worst case — $\langle\vec{n}|\hat{\rho}_{\rm in}|\vec{n}'\rangle = \langle\vec{n}|\psi_{\rm in}\rangle\langle\psi_{\rm in}|\vec{n}'\rangle$
— non-diagonal terms are comparable to the diagonal ones;
— overlaps $\langle nl|\psi_{\rm in}\rangle$ are positive



infinite time average, diag.
prediction, IPR=const
initial
thermal
infinite time average, non-diag.
10^3 Occupation probability
Longitudial mode, l
0
1
2
3
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100
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10^3 Occupation probability
Transverse mode n
0
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NON-DIAGONAL OBSERVABLE

$\langle \vec{n}|\hat{A}|\vec{n}'\rangle \neq 0$, $\vec{n} \neq \vec{n}'$

$A_{\rm in} = \sum_{\vec{n}} A_{\vec{n}} \rho^{\rm in}_{\vec{n}}$
is the infinite-time average for evolution of the integrable system.
(not the actual initial expectation value)

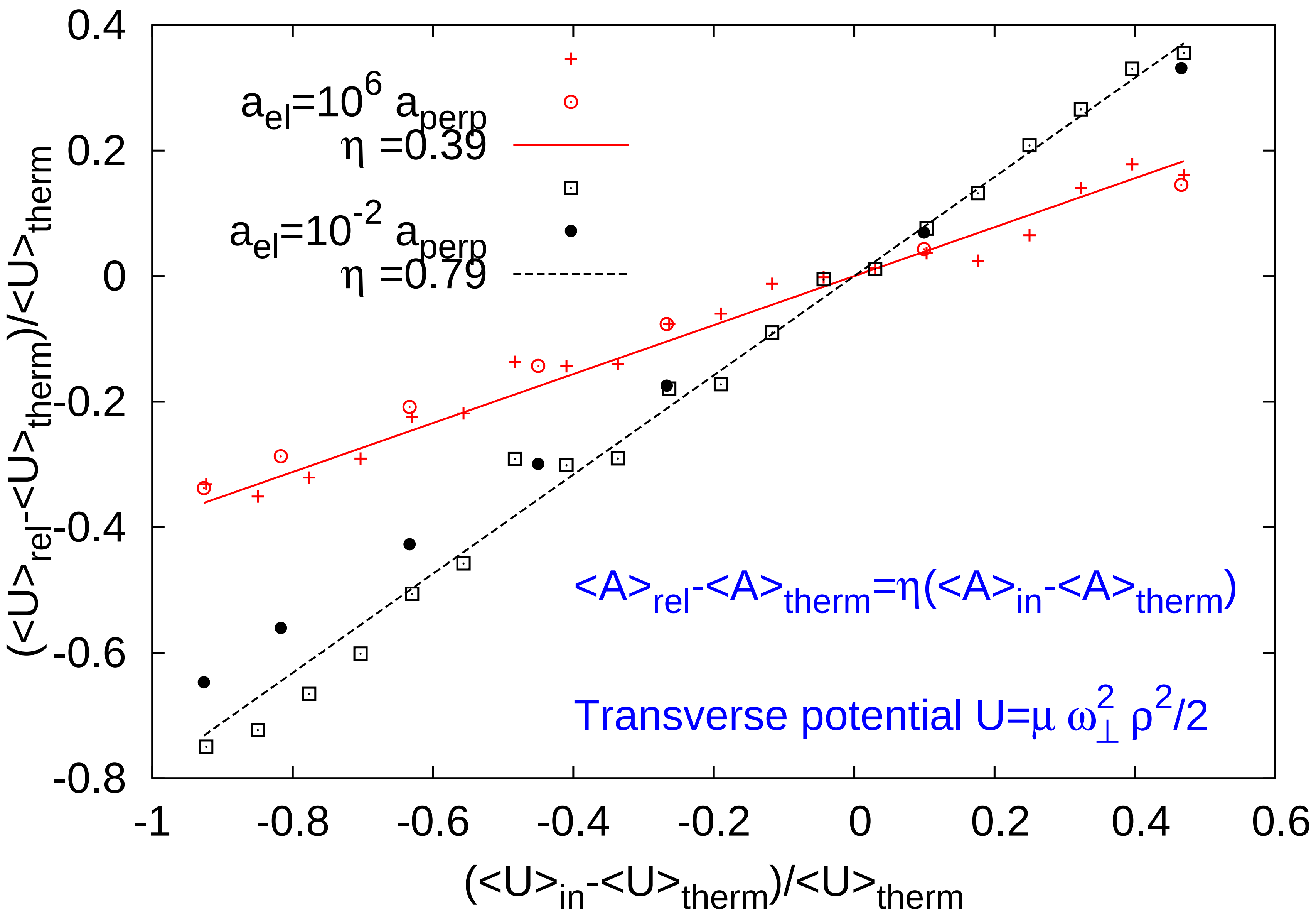
Leading correction:

$$A_{\rm rel} \approx \bar{\eta} A_{\rm in} + (1-\bar{\eta}) A_{\rm therm}$$

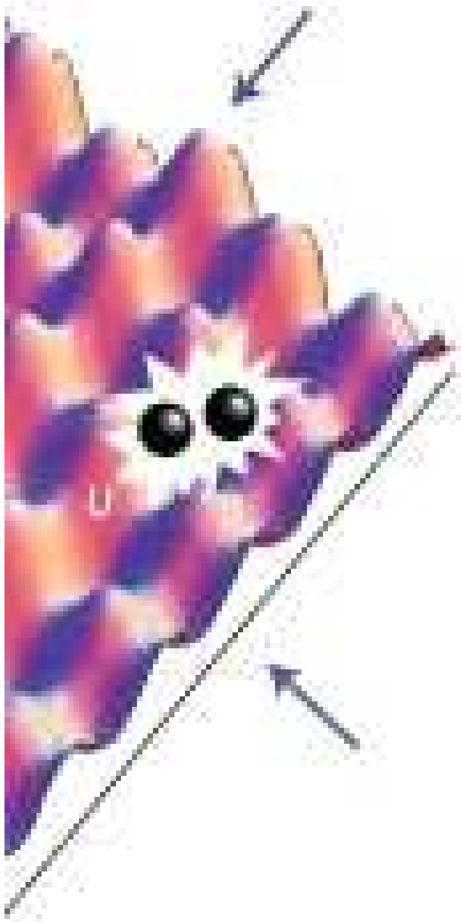
$$-\sum_{\vec{n}\neq\vec{n}'} \frac{\langle \vec{n}|\hat{A}|\vec{n}'\rangle}{(E_{\vec{n}} - E_{\vec{n}'})^2} \Big[\langle \vec{n}'|\hat{\eta}_2(E_{\vec{n}})|\vec{n}\rangle \langle \vec{n}|\hat{\rho}_{\rm in}|\vec{n}\rangle - \langle \vec{n}|\hat{\eta}_2(E_{\vec{n}}) + \hat{\eta}_2(E_{\vec{n}'})|\vec{n}\rangle \langle \vec{n}'|\hat{\rho}_{\rm in}|\vec{n}\rangle \Big]$$

Small correction:
$\hat{A}$ does not couple energy-neighboring states of the integrable system
(do not act on some degrees of freedom).

NON-DIAGONAL OBSERVABLE



TWO ULTRACOLD ATOMS IN A HARMONIC TRAP



Trap potential:

$$U = \frac{m}{2}\left(\omega_{\|}^2 z^2 + \omega_{\perp}^2 \rho^2\right)$$

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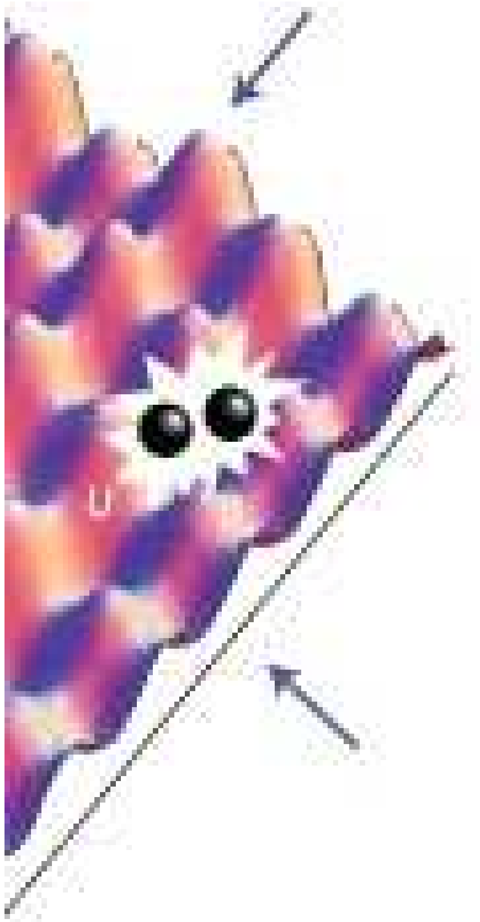
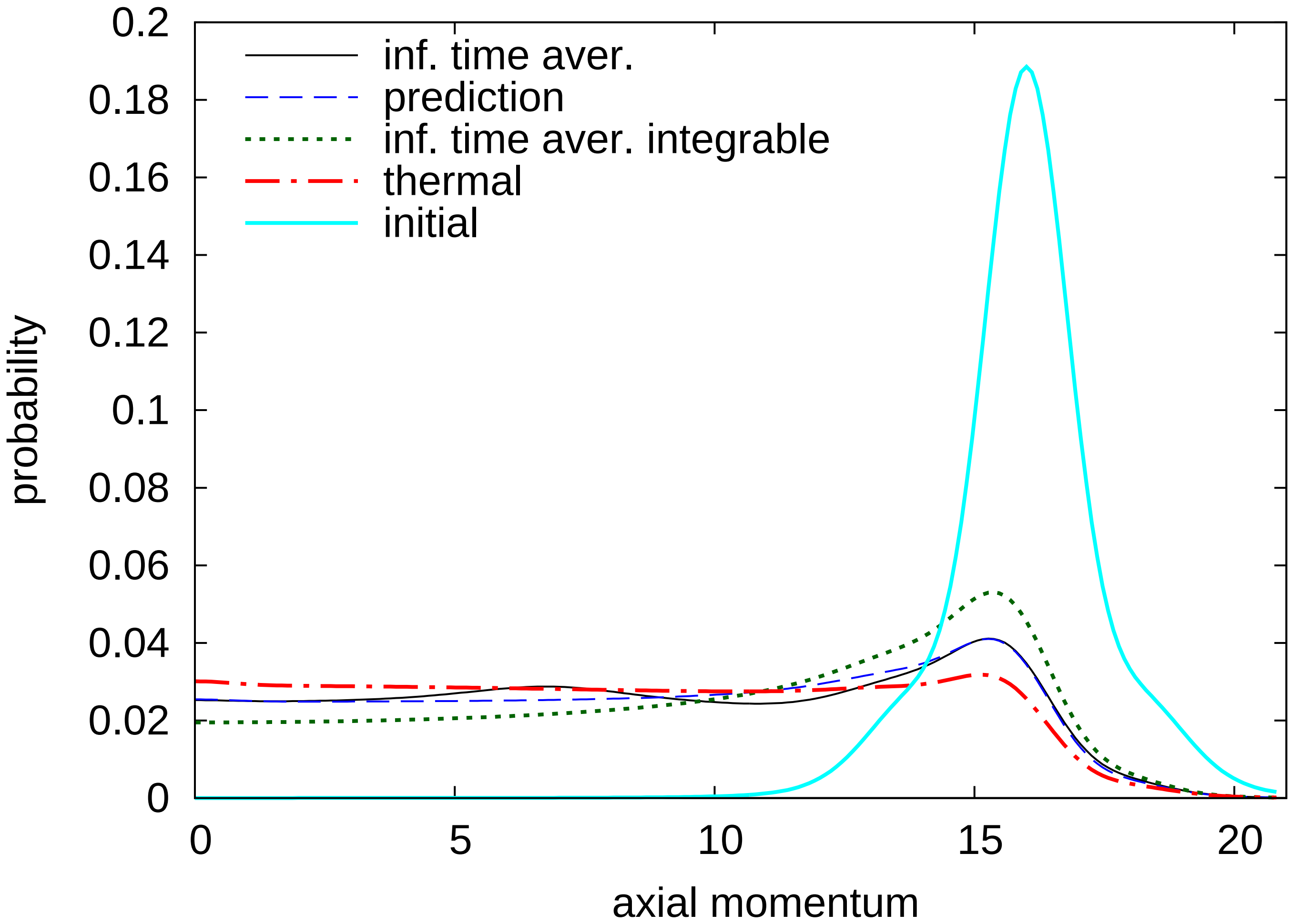


Solution — Idziaszek & Calarco (2005)
Harmonic trap — center-of-mass can be separated.
Axial momentum — a non-diagonal observable.



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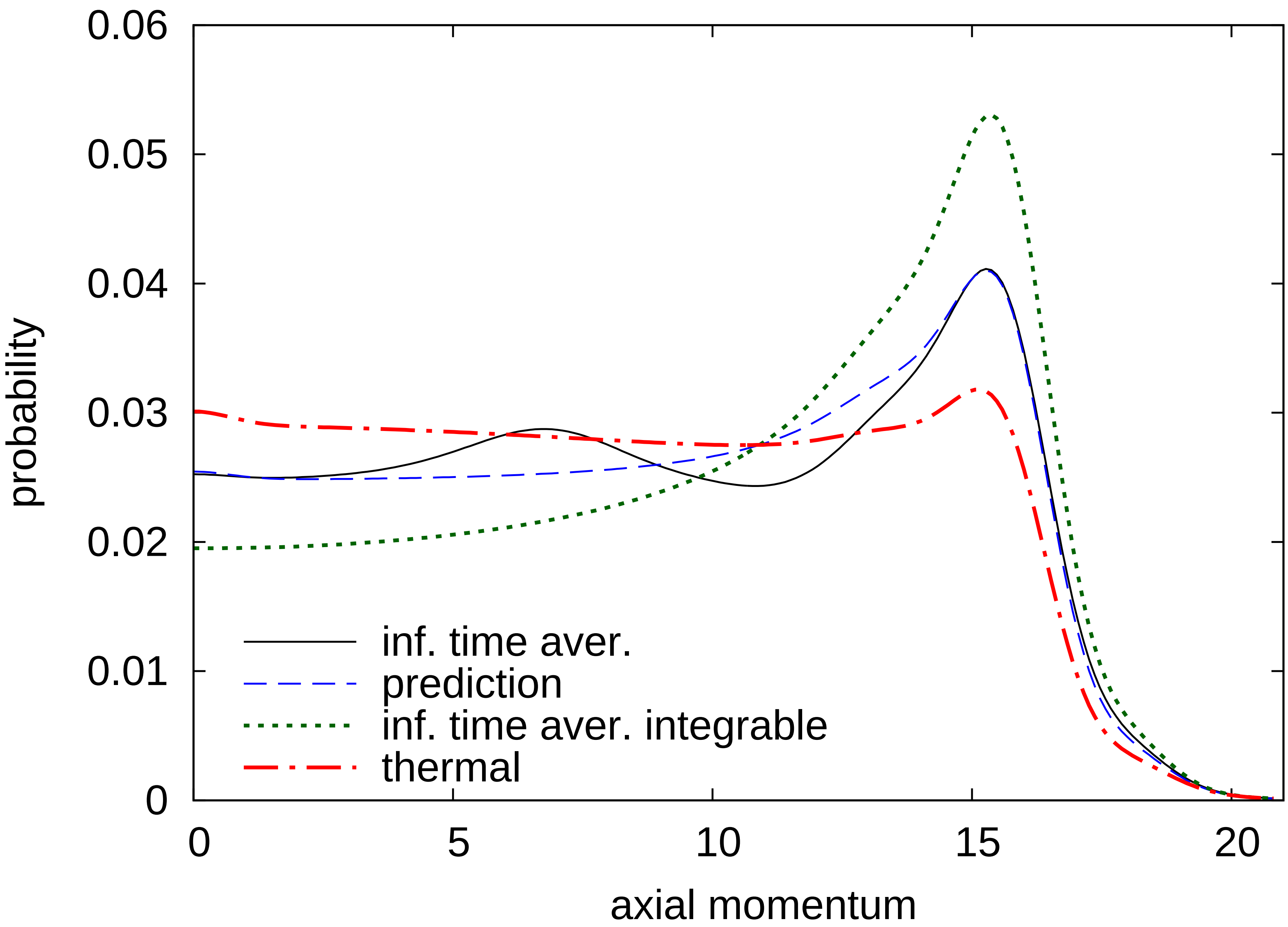
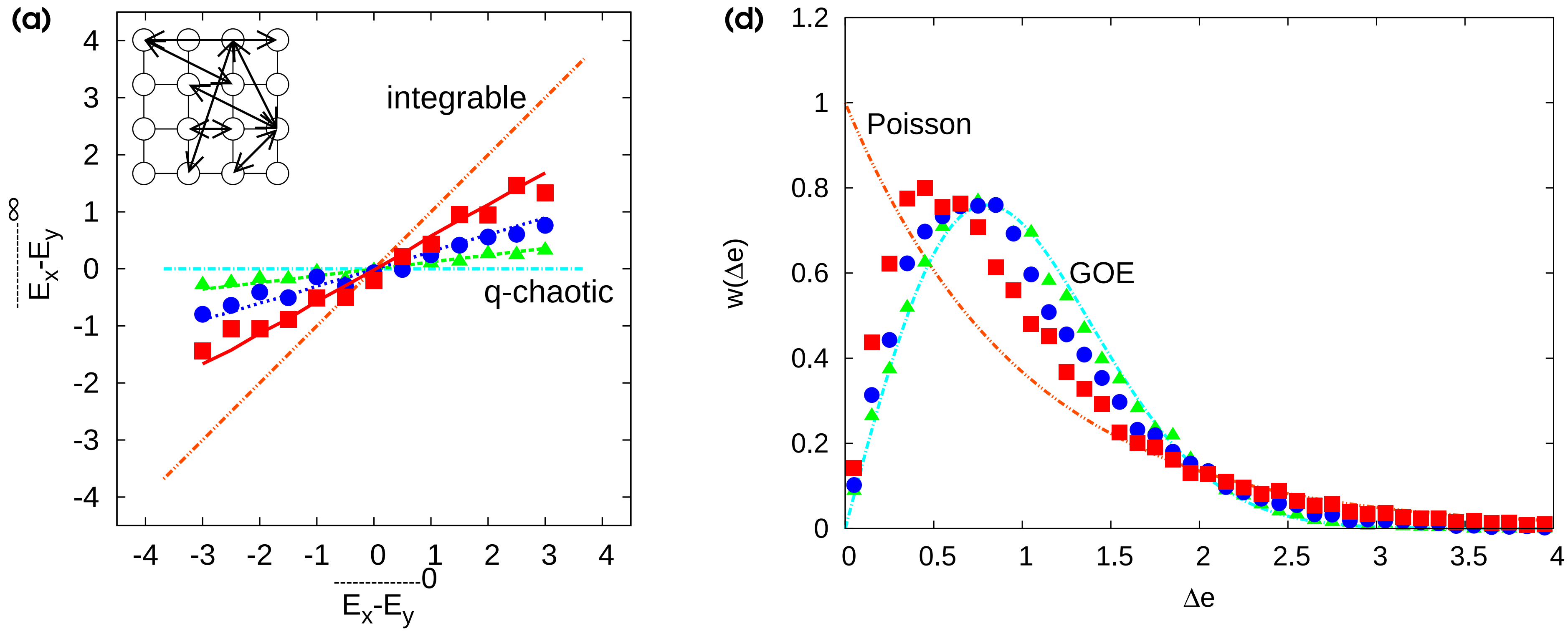


0.06
0.05
0.04
0.03
0.02
0.01
0
0
5
10
15
20
probability
axial momentum
inf. time aver.
prediction
inf. time aver. integrable
thermal

ROUGH QUANTUM BILLIARDS

An atom in a 33×33-site two-dimensional lattice with a periodic boundary conditions threaded by AharonovBohm fluxes.
The integrability-breaking perturbation — a Gaussian random matrix.



[Olshanii, Jacobs, Rigol, Dunjko, Kennard & VY, Nature Communications 3, 641 (2012)]

DYNAMICS OF RELAXATION AND FLUCTUATIONS

[VY, Ben-Reuven & Olshanii, J. Phys. Chem. B **115**, 5340 (2011)]
The quantum-mechanical mean of any observable $\hat{A}$:

$$\langle \hat{A}(t) \rangle = \sum_{\alpha,\alpha'} \langle \alpha | \hat{A} | \alpha' \rangle \langle \alpha' | \hat{\rho}_{\text{in}} | \alpha \rangle \exp\left(i(E_{\alpha'} - E_{\alpha})t \right)$$

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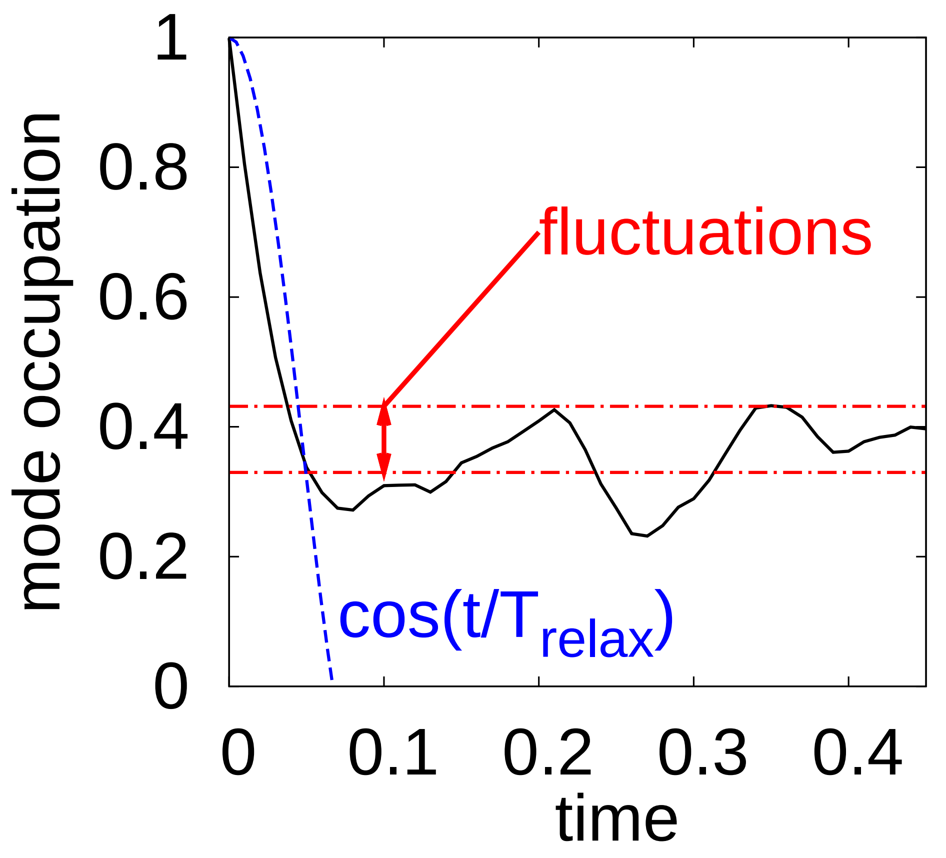
Relaxation time (the longest period)

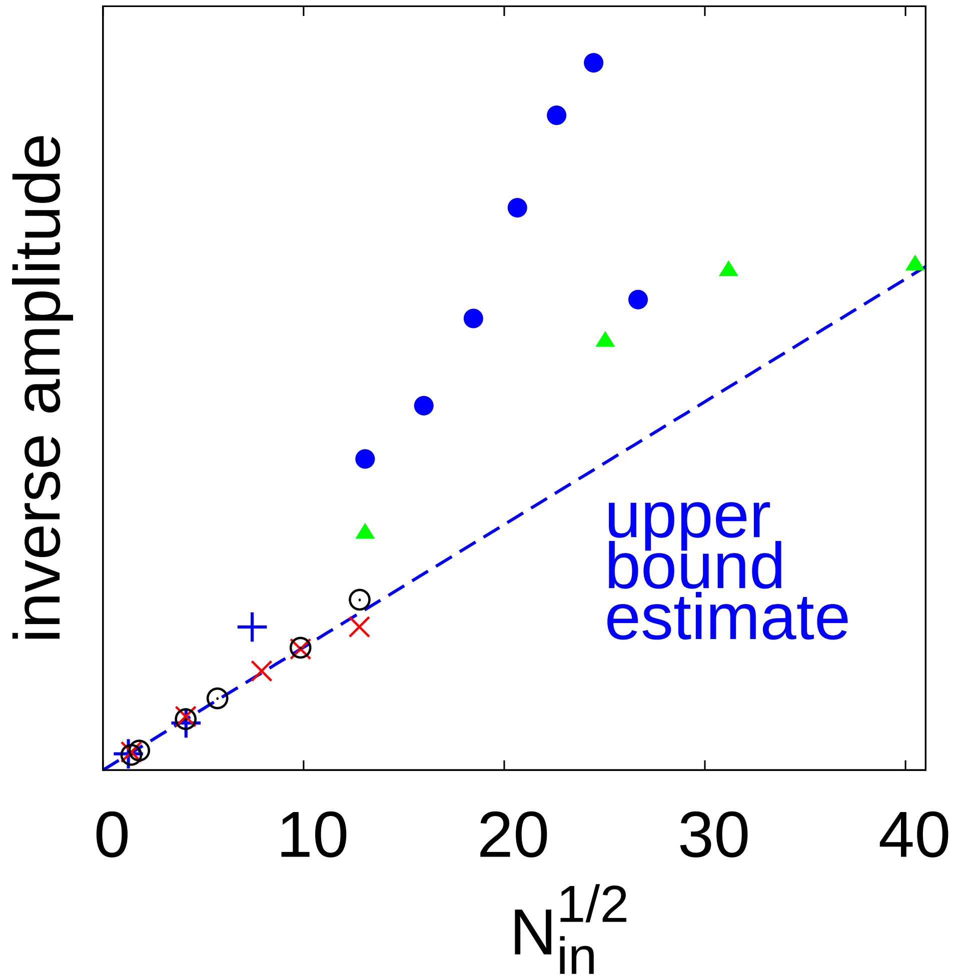
$$T_{\text{relax}} \approx \frac{1}{\min |E_\alpha - E_{\alpha'}|} \approx \frac{2\sqrt{2}\pi\omega_\perp}{L\sqrt{\mu E}}$$

Root-mean-square fluctuations

$$A_{\text{fluc}}^2 = \sum_{\alpha \neq \alpha'} \left| \langle \alpha | \hat{\rho}_{\text{in}} | \alpha' \rangle \langle \alpha | \hat{A} | \alpha' \rangle \right|^2$$



FLUCTUATION AMPLITUDE



$$N_{\rm in} = \left(\sum_{\vec{n}} \langle \vec{n} | \hat{\rho}_{\rm in} | \vec{n} \rangle^2 \right)^{-1}$$

— number of modes in the initial state

An estimate for the upper bound of the fluctuation amplitude of mode occupations

$$(P_{\rm fluc}^{(n)})^2 \lesssim \bar{\eta}_8 / N_{\rm in}$$

$$\bar{\eta}_8 = \left(\sum_{\alpha} |\langle \alpha | \vec{n} \rangle|^4 \right)^2 - \sum_{\alpha} |\langle \alpha | \vec{n} \rangle|^8$$

— a universal parameter

Conclusions

The memory of the initial state in non-integrable systems with no selection rules is controlled by the inverse participation ratio.

This prediction is in a good agreement with the exact results on the relaxation in cold-atomic systems.

Scaling lows for the relaxation time and fluctuation amplitude are obtained.

Part II

Properties of a one-dimensional gas of spin-$1/2$ atoms in an axial potential.

Eigenstates — irreducible representations of the symmetric group
Energy spectra.
Perspectives for non-equilibrium dynamics

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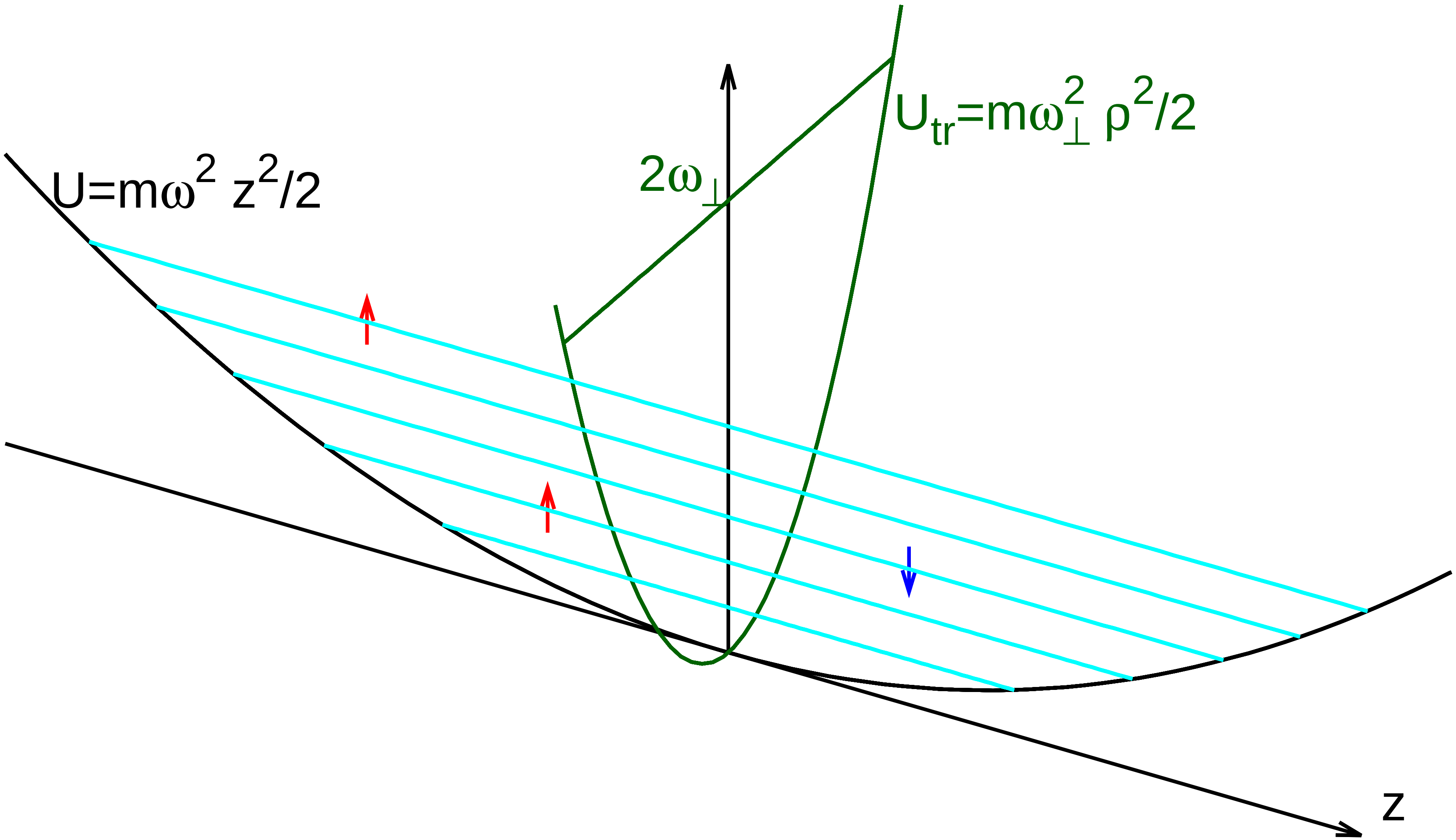
Other properties:
Correlation functions
Effects of spin-dependent interactions

1D SPIN-1/2 BOSE AND FERMI GASES

— non-degenerate gas of Bose or Fermi atoms
— two internal states $|\uparrow\rangle$ and $|\downarrow\rangle$
— prolongated trap, only the ground transverse state is occupied



THE SYMMETRIC GROUP IRREDUCIBLE REPRESENTATIONS

The wavefunction transformation on a permutation $\mathcal{P}$ of particles

$$\mathcal{P}\Phi_{Str} = \sum_{t'} D^{[\lambda]}_{t't}(\mathcal{P})\Phi_{St'r}$$

S — the total spin

f_S representations, labeled by the Young tableaux r

f_S functions, labeled by the Young tableaux t, in each representation

$[\lambda] = [N/2 + S, N/2 - S]$ — the Young diagram

$D^{[\lambda]}_{t't}(\mathcal{P})$ — Young orthogonal matrices

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$[\lambda] = [N/2 + S, N/2 - S]$ — the Young diagram
$D^{[\lambda]}_{t't}(\mathcal{P})$ — Young orthogonal matrices

Only **one-dimensional** ($f_S = 1$) representations ($D^{[\lambda]}_{t't}(\mathcal{P}) = \pm 1$) are allowed for the total wavefunction (the Pauli principle).

SPATIAL AND SPIN FUNCTIONS

$$\Psi_{Sr} = f_S^{-1/2} \sum_t \Xi_{St} \Phi_{Str}.$$

Multidimensional representations for spatial Φ_{Str} and spin Ξ_{St} functions

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$$\Phi_{Str} = \left(\frac{f_S}{N!} \right)^{1/2} \sum_{\mathcal{P}} D_{tr}^{[\lambda]}(\mathcal{P}) \prod_{j=1}^{N} \varphi_{n_j}(\mathcal{P}j)$$

($n_j \neq n'_j$, N atoms occupy N states) [Wigner, Z. Phys., 1926]

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Spin wavefunction — N atoms occupy 2 states

SPATIAL AND SPIN FUNCTIONS

$$\Psi_{Sr} = f_S^{-1/2} \sum_t \Xi_{St} \Phi_{Str}.$$

Multidimensional representations for spatial Φ_{Str} and spin Ξ_{St} functions

$$\Phi_{Str} = \left(\frac{f_S}{N!}\right)^{1/2} \sum_{\mathcal{P}} D_{tr}^{[\lambda]}(\mathcal{P}) \prod_{j=1}^{N} \varphi_{n_j}(\mathcal{P}j)$$

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Spin wavefunction — N atoms occupy 2 states

$$\Xi_{SS_zt} = C_{SS_z} \sum_{\mathcal{P}} D_{t[0]}^{[\lambda]} \prod_{i=1}^{N/2+S_z} |\uparrow(\mathcal{P}i)\rangle \prod_{i=N/2+S_z+1}^{N} |\downarrow(\mathcal{P}i)\rangle$$

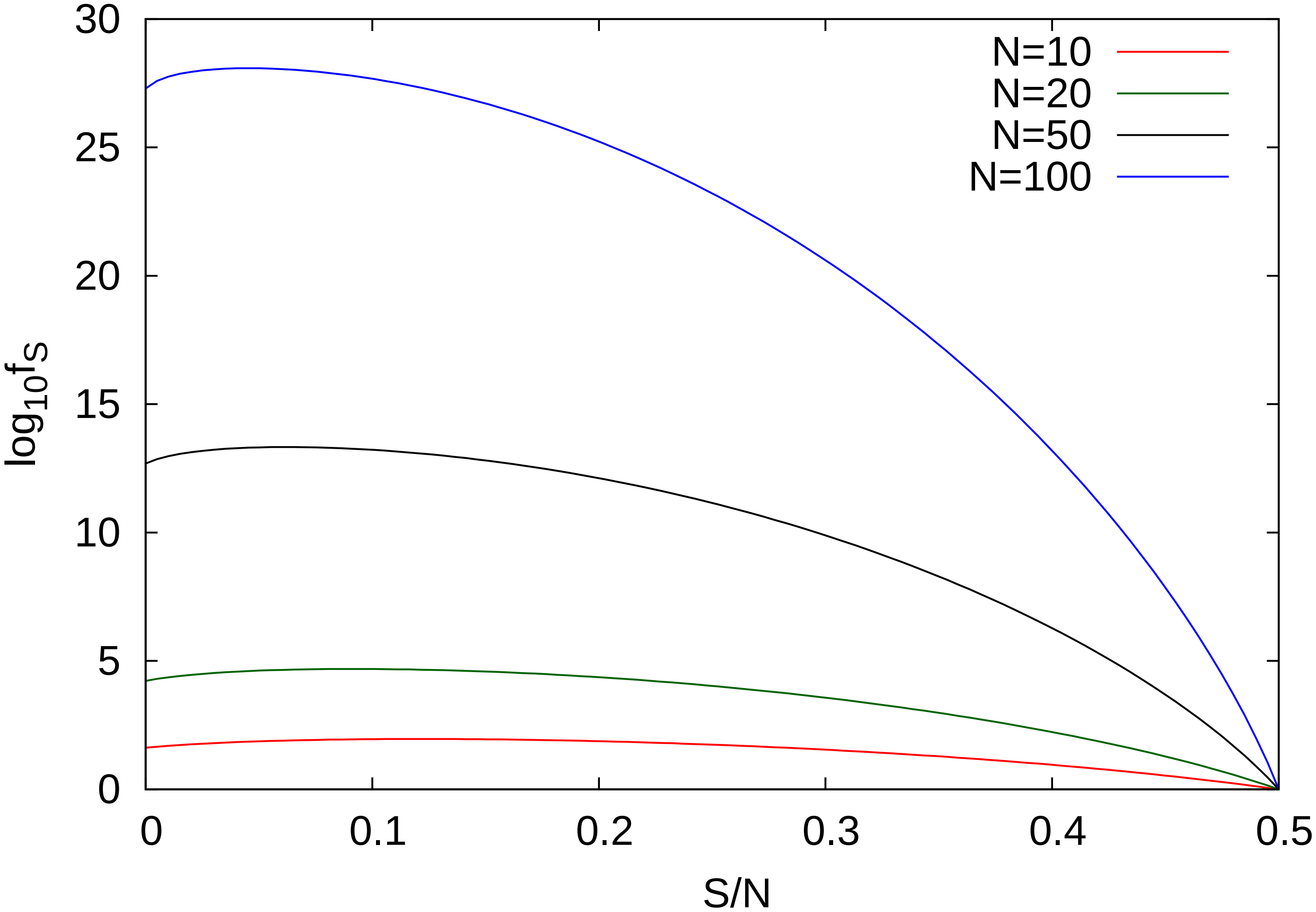
$$C_{SS_z} = \frac{1}{(N/2+S_z)!(N/2-S)!} \sqrt{\frac{(2S+1)(S+S_z)!}{(N/2+S+1)(2S)!(S-S_z)!}}$$

[VY, Int. J. Quant. Chem., 2012, in press]

NUMBER OF STATES

$$\Psi_{Sr} = f_S^{-1/2} \sum_t \Xi_{St} \Phi_{Str}.$$

— f_S states for the given spin and the set of spatial quantum numbers $\{n\}$.



SELECTION RULES

$$\hat{H} = \sum_{i=1}^{N} \left[\left(-\frac{1}{2m}\frac{d^2}{dz_i^2} + U(z_i) \right) + \sum_{i'<i} V_{1D}\delta(z_i - z_i') \right]$$

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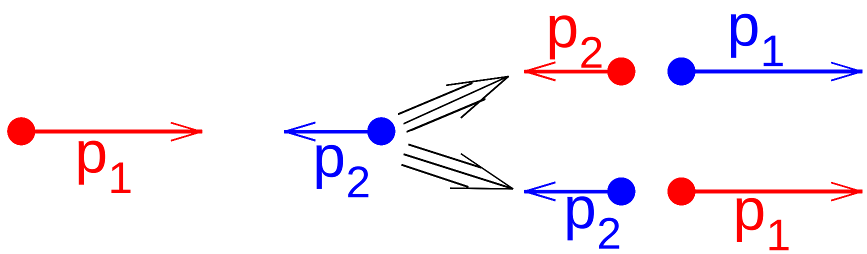
U =const — the Yang-Gaudin model

Energy and momentum conservation



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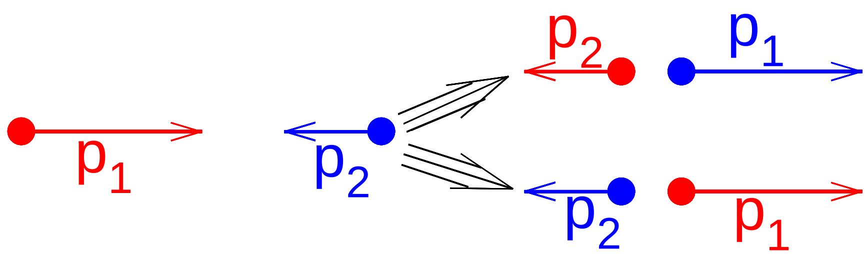
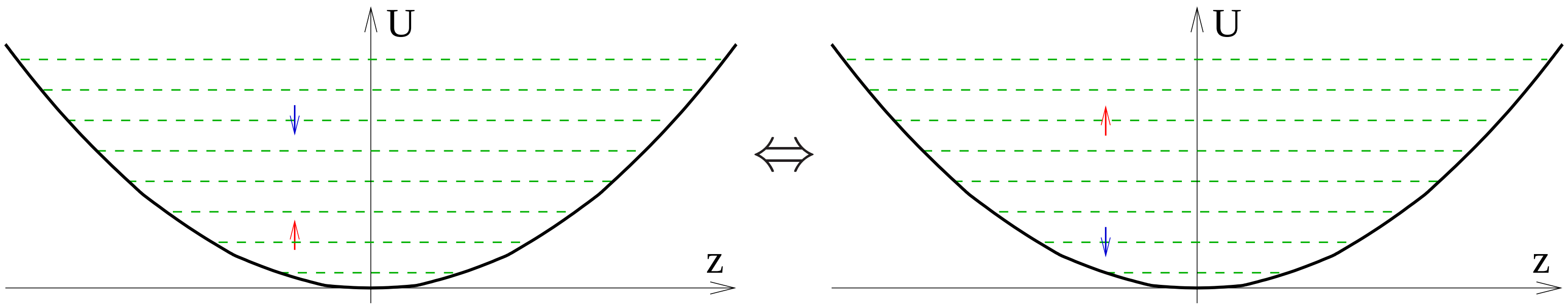


U $\neq$const — Approximate selection rules



Different sets of spatial quantum numbers $\{n\}$ are uncoupled

ENERGY SPECTRA

First order in V_{1D}

f_S degenerate unperturbed states — a diagonalization of a $f_s \times f_s$ matrix.

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First order in V_{1D}

f_S degenerate unperturbed states — a diagonalization of a $f_s \times f_s$ matrix.

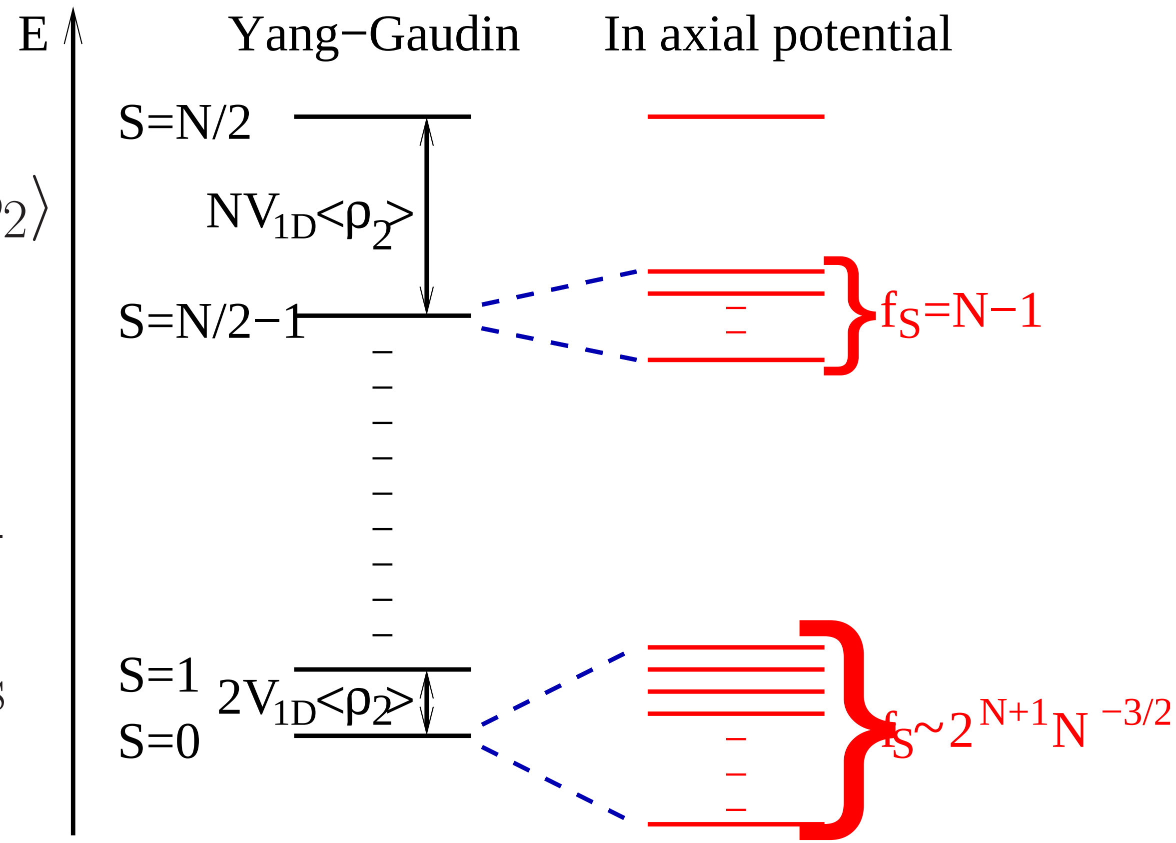
Average multiplet energy

$$\bar{E}_S = \frac{N(N-1)}{2} V_{1D}[1 \pm \chi_S(\{2\})] \langle \rho_2 \rangle$$

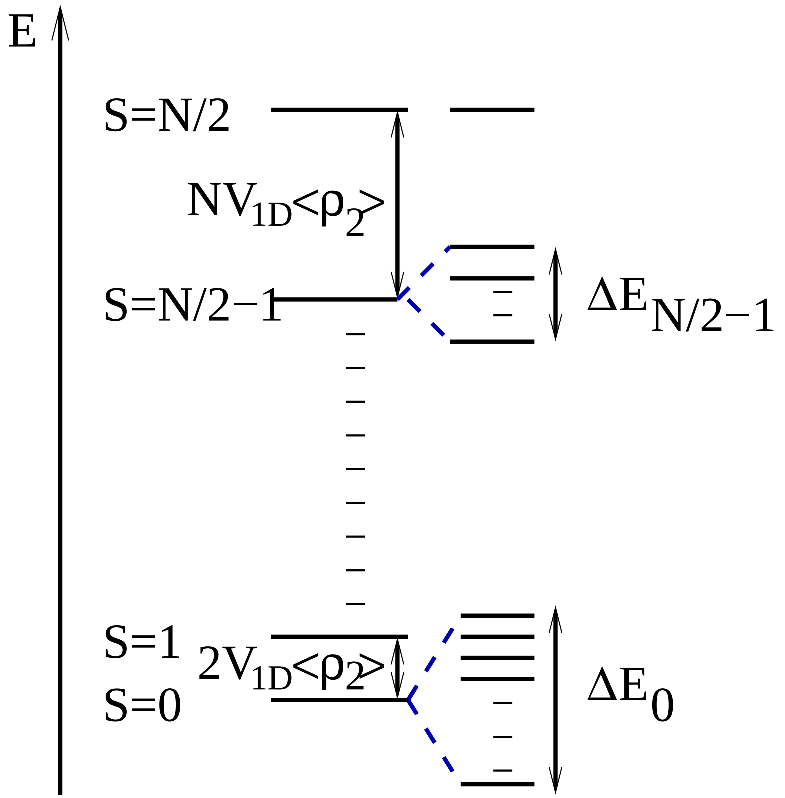
$$\chi_S(\{2\}) = \frac{4S^2 + N^2 + 4S - 4N}{2N(N-1)}$$

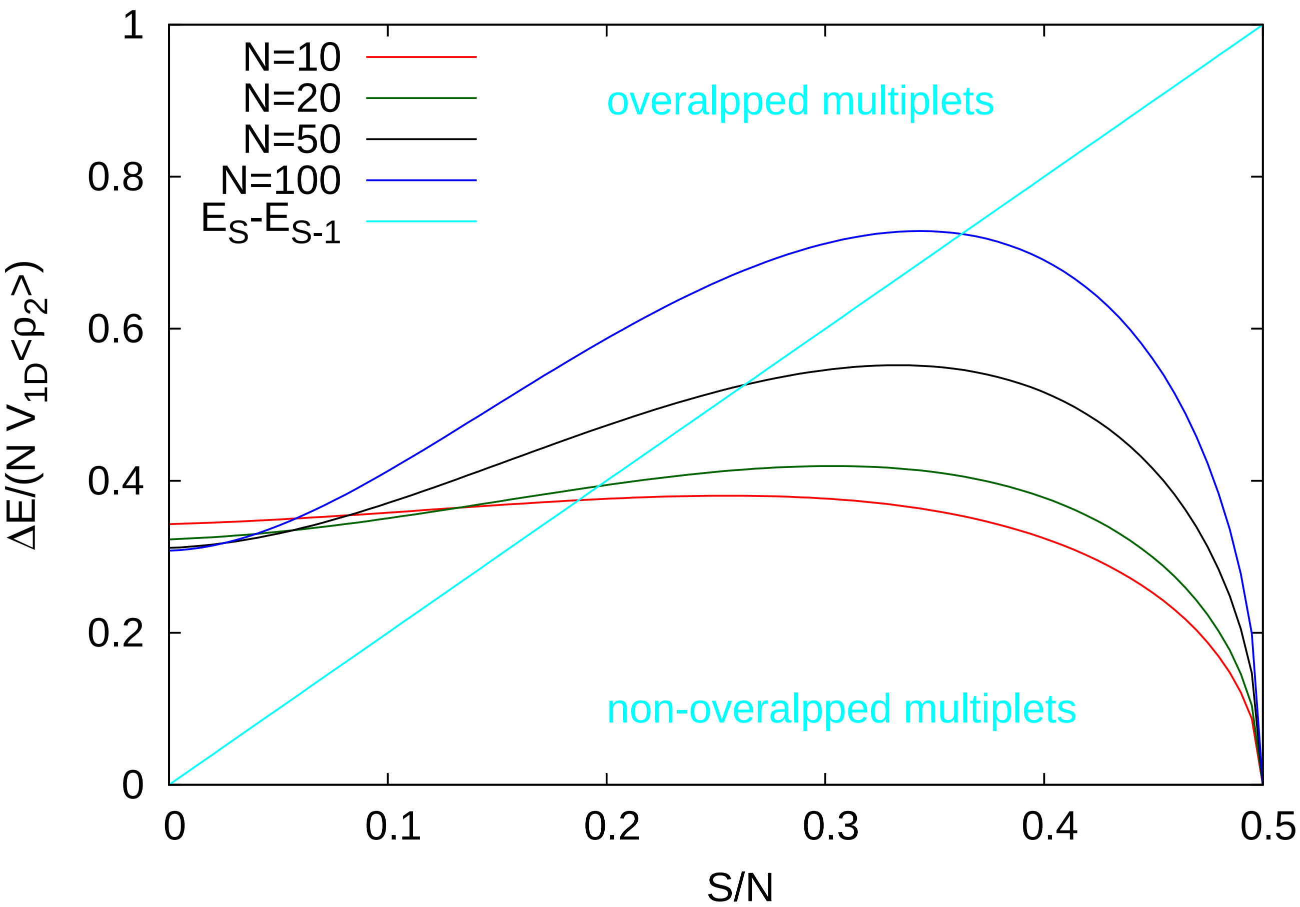
— irreducible representation characters

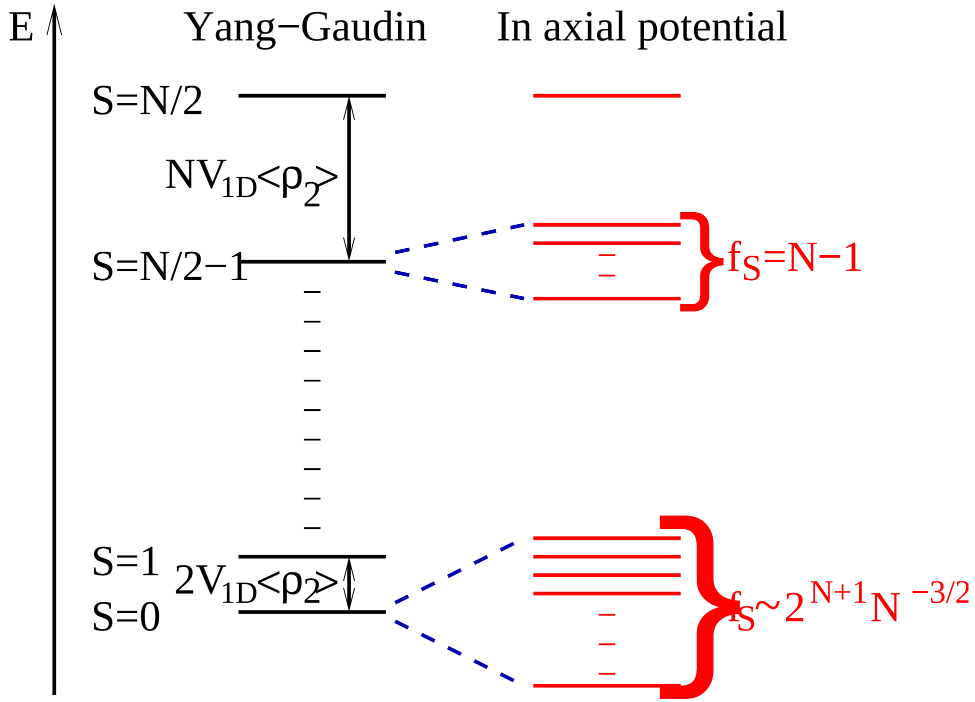
Agrees to the general relations [Haitrler, 1927]

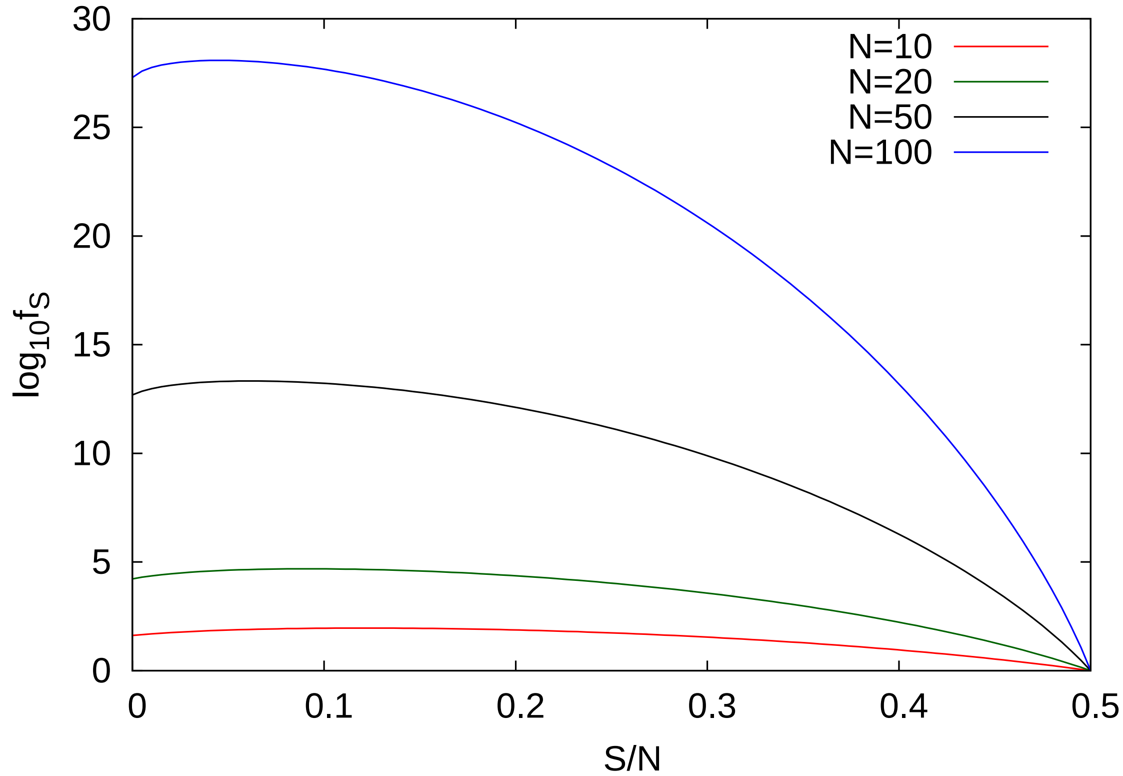


MULTIPLET ENERGY WIDTH









A multi-level system with a strong irregular coupling:

$$\langle \Psi_{Sr}|\hat{V}|\Psi_{Sr'}\rangle = \sum_{j<j'} \left[\delta_{rr'} + D^{[\lambda]}_{rr'}(\mathcal{P}_{jj'})\right] V_{1D} \int dz \varphi^2_{n_j}(z)\varphi^2_{n_{j'}}(z)$$

Change N and S — change the number of levels f_S.

Quantum chaos? Relaxation? Thermalization?

DERIVATION DETAILS

$$A_{\text{rel}} = \sum_{\vec{n},\vec{n}',\alpha} A_{\vec{n}} |\langle\vec{n}|\alpha\rangle\langle\alpha|\vec{n}'\rangle|^2 \rho^{\text{in}}_{\vec{n}'} = \sum_{\vec{n},\vec{n}',\alpha} A_{\vec{n}} \left| \frac{\langle\vec{n}|\hat{V}|\alpha\rangle\langle\alpha|\hat{V}|\vec{n}'\rangle}{(E_\alpha - E_{\vec{n}})(E_\alpha - E_{\vec{n}'})} \right|^2 \rho^{\text{in}}_{\vec{n}'}$$

$\vec{n} = \vec{n}'$: $\eta_4(E_{\vec{n}}) = \sum_\alpha |\langle\vec{n}|\alpha\rangle|^4$ — inverse participation ratio

$$\left(\overline{\eta} \equiv \sum_{\vec{n}} \eta_4(E_{\vec{n}}) \rho^{\text{in}}_{\vec{n}} = \overline{\eta_\alpha} \right)$$

$\vec{n} \neq \vec{n}'$: rational function decomposition

$$\frac{1}{(E_\alpha - E_{\vec{n}})^2 (E_\alpha - E_{\vec{n}'})^2} = \frac{1}{(E_{\vec{n}} - E_{\vec{n}'})^2} \left[\frac{1}{(E_\alpha - E_{\vec{n}})^2} + \frac{1}{(E_\alpha - E_{\vec{n}'})^2} \right] + \frac{2}{(E_{\vec{n}} - E_{\vec{n}'})^3} \left[\frac{1}{(E_\alpha - E_{\vec{n}})} - \frac{1}{(E_\alpha - E_{\vec{n}'})} \right]$$

$$A_{\text{rel}} = \sum_{\vec{n}} A_{\vec{n}} \eta_4(E_{\vec{n}}) \rho^{\text{in}}_{\vec{n}} + \sum_{\vec{n} \neq \vec{n}'} A_{\vec{n}} \underbrace{\left[\frac{\eta_2(E_{\vec{n}}) + \eta_2(E_{\vec{n}'})}{(E_{\vec{n}} - E_{\vec{n}'})} \right]^2} \rho^{\text{in}}_{\vec{n}'}$$

In **average** ($A_{\vec{n}}$ involves many $|\vec{n}\rangle$, $\rho^{\text{in}}_{\vec{n}'}$ involves many $|\vec{n}'\rangle$)

- no selection rules — $\eta_2(E_{\vec{n}})$ does not correlate to quantum numbers $\vec{n}$
- several degrees of freedom, incommensurable frequencies — quantum numbers of highly-excited energy-neighboring states are uncorrelated
- $A_{\vec{n}}$ depends on quantum numbers only

$$A_{\vec{n}} \Leftarrow A_{\text{MC}}(E_{\vec{n}'}) = \langle A_{\vec{n}} \rangle_{E_{\vec{n}} \approx E_{\vec{n}'}}$$

$|\alpha\rangle$ form an orthogonal and complete basis set

$$\sum_{\vec{n}' \neq \vec{n}} \overbrace{\sum_{\alpha} |\langle \vec{n}|\alpha\rangle \langle \alpha|\vec{n}'\rangle|^2} = 1 - \eta_4(E_{\vec{n}'})$$