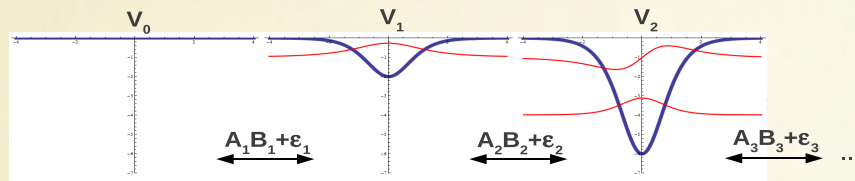


**GEOMETRY OF QUANTUM
OBSERVABLES, INTEGRABILITY-
THERMALIZABILITY TRANSITION,
AND EXTENDED THERMODYNAMICS
OF INTEGRABLE AND/OR
MESOSCOPIC SYSTEMS**



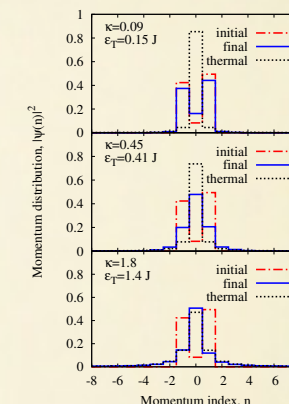
**MAXIM OLSHANII (OLCHANYI)
UNIVERSITY OF MASSACHUSETTS
BOSTON**

QM SUSY <--> GPE/sine-Gordon



PRE 84, 066601 (2011)

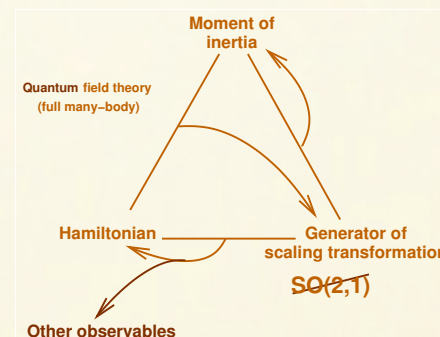
Thermalization in 1D Bose-Hubbard



PRL 102, 025302 (2009)

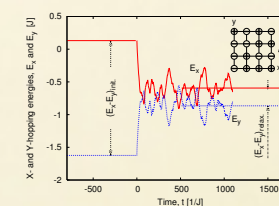
maly in 2D BEC

Quantum and

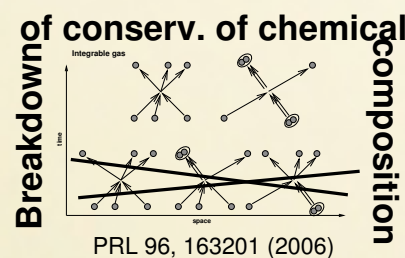


PRL 105, 095302 (2010)

Integrable to chaotic in rough quantum billiards

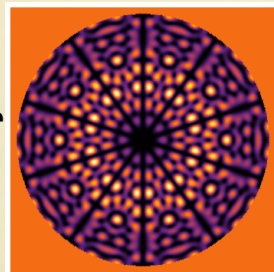


Nature Communications 3, 641 (2012)



PRL 96, 163201 (2006)

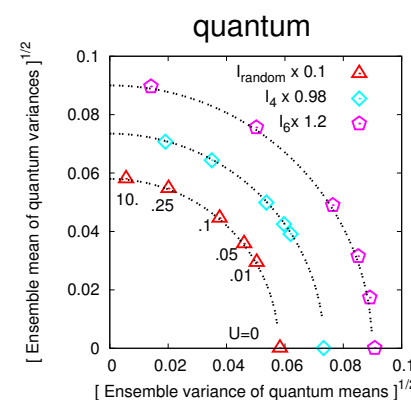
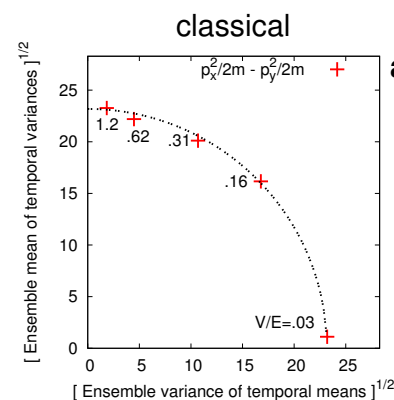
graphic Bethe



Non-crystalline

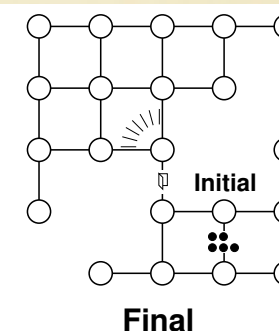
ansatz in BEC

Geometry of integrability-ergodicity



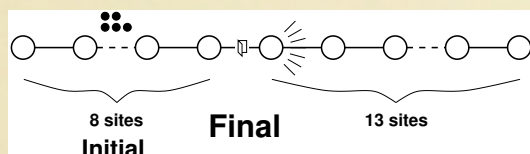
submitted to Science (2012)

Eigenstate thermalization



Nature, 452, 854 (2008)

Generalized Gibbs



PRL 98, 050405 (2007)

Integrable

Ergodic

Preview

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

- Proposition:

The sum of the ensemble variance of the temporal means and the ensemble mean of the temporal variances remains approximately constant across the integrability-to-ergodicity transition

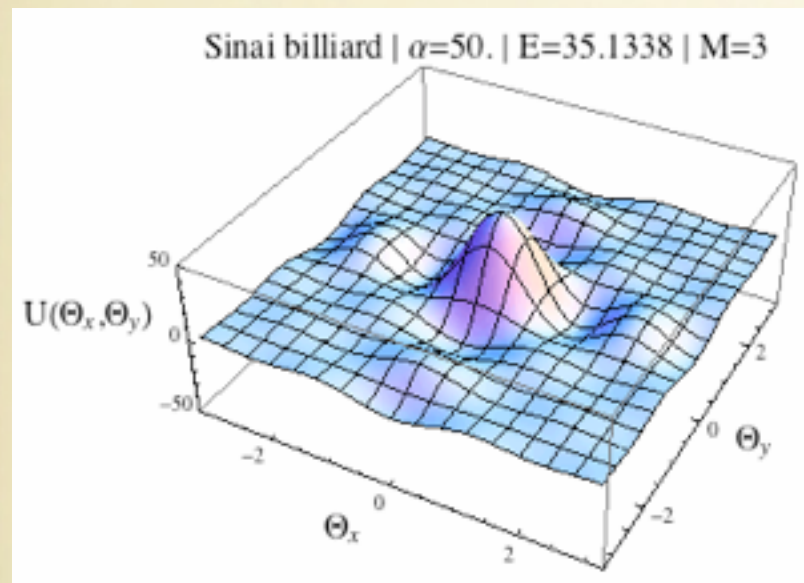
- Example of a Sinai-type billiard
- Example of long-range interacting hard-core bosons
- Ensemble variance of temporal means as a $\cos^2$ of the Hilbert-Schmidt (HS) angle between the observable and integrals of motion

HS geometry of density matrices for Quantum Information: 164 arXiv articles

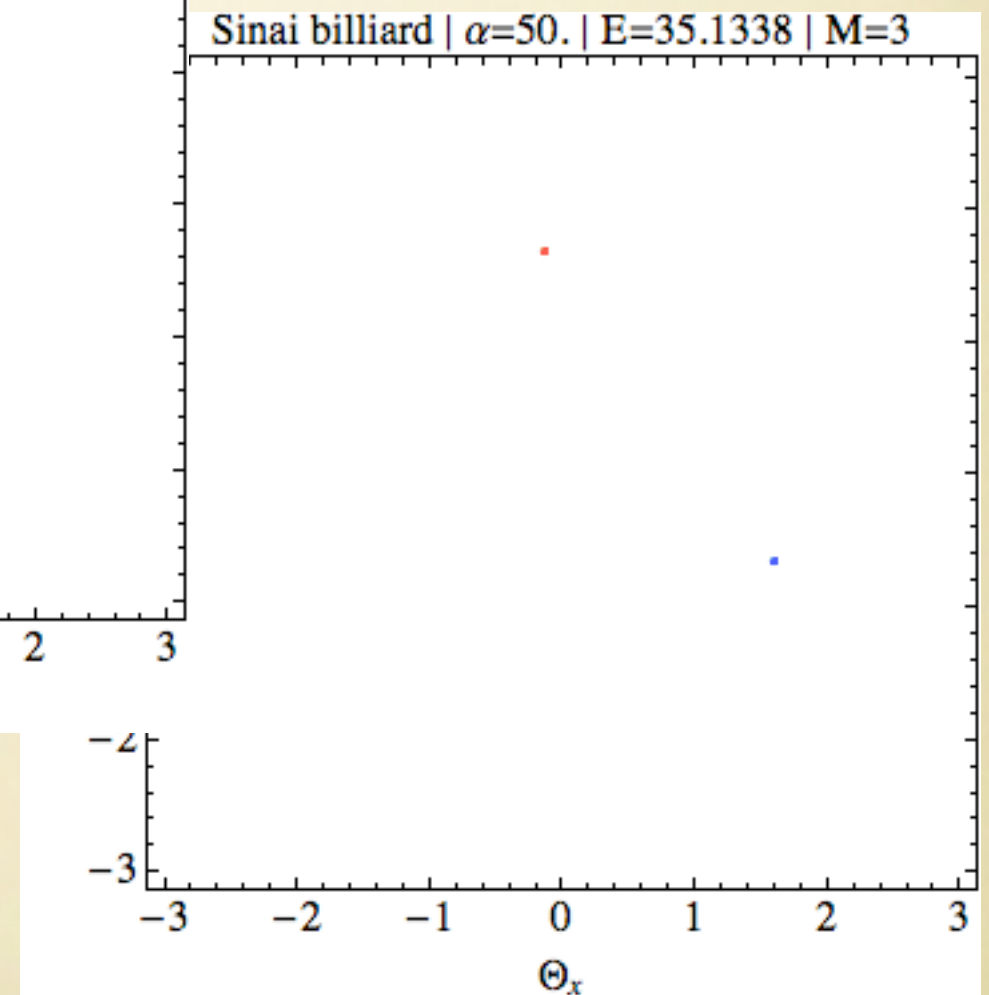
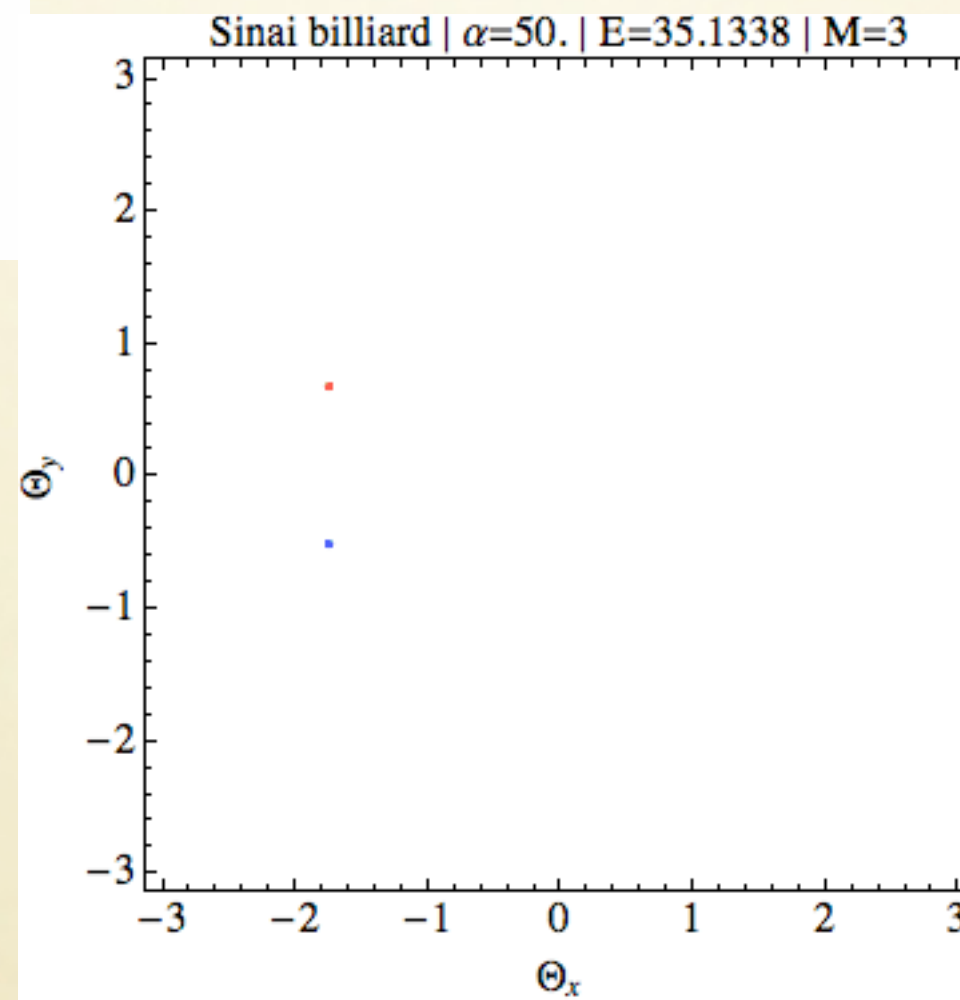
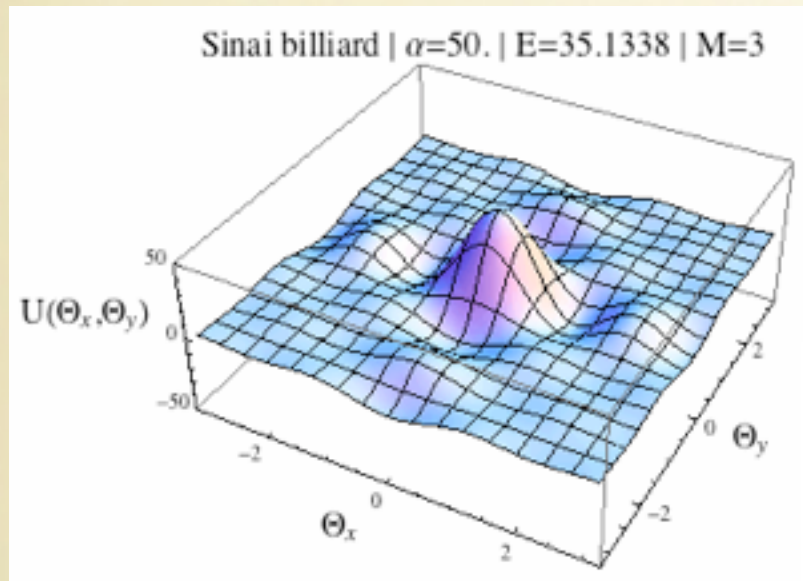
HS geometry of observables: 0 arXiv, hints in Suzuki's quantum extension of Mazur's theorem (Physica 51 (1971))

- IPR as an angle between the original and perturbed integrals of motion
- An application of the HS geometry: Optimal integrals of motion for GGE
- Mesoscopicity and integrability on the same footing → “nano-meso”

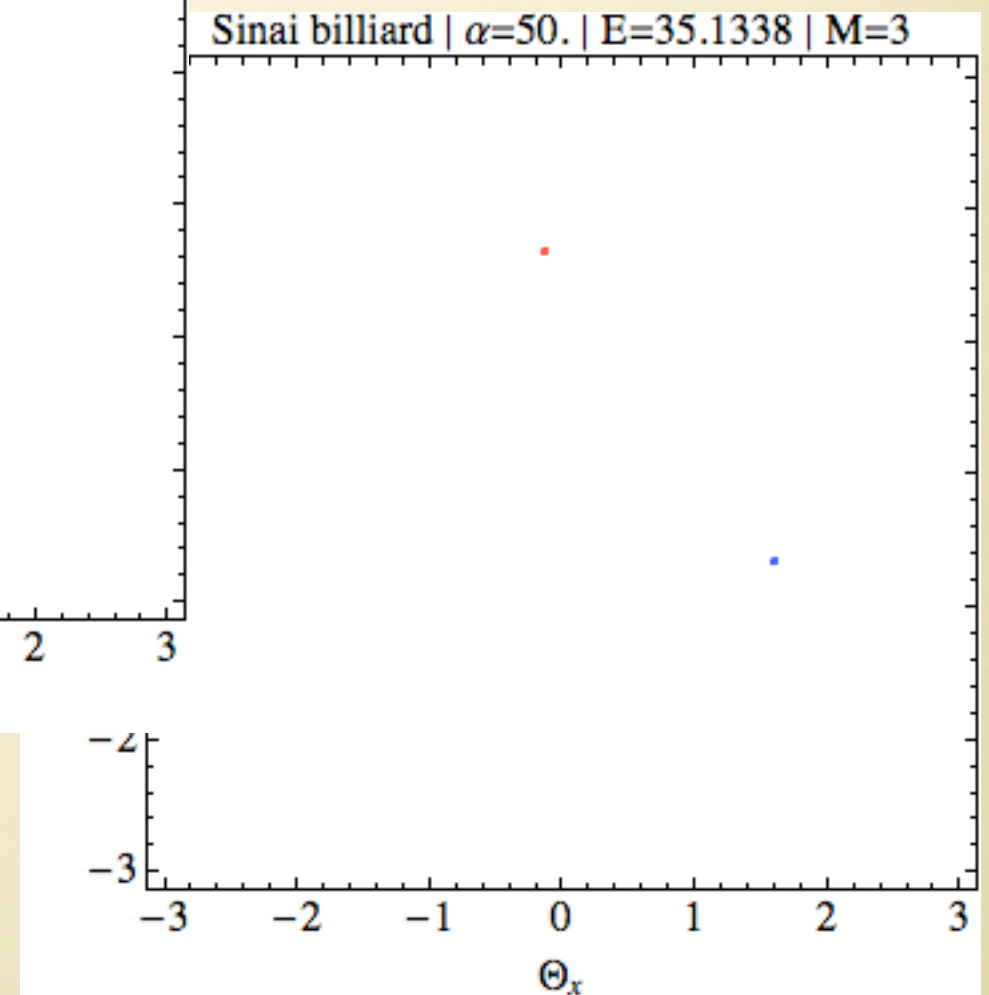
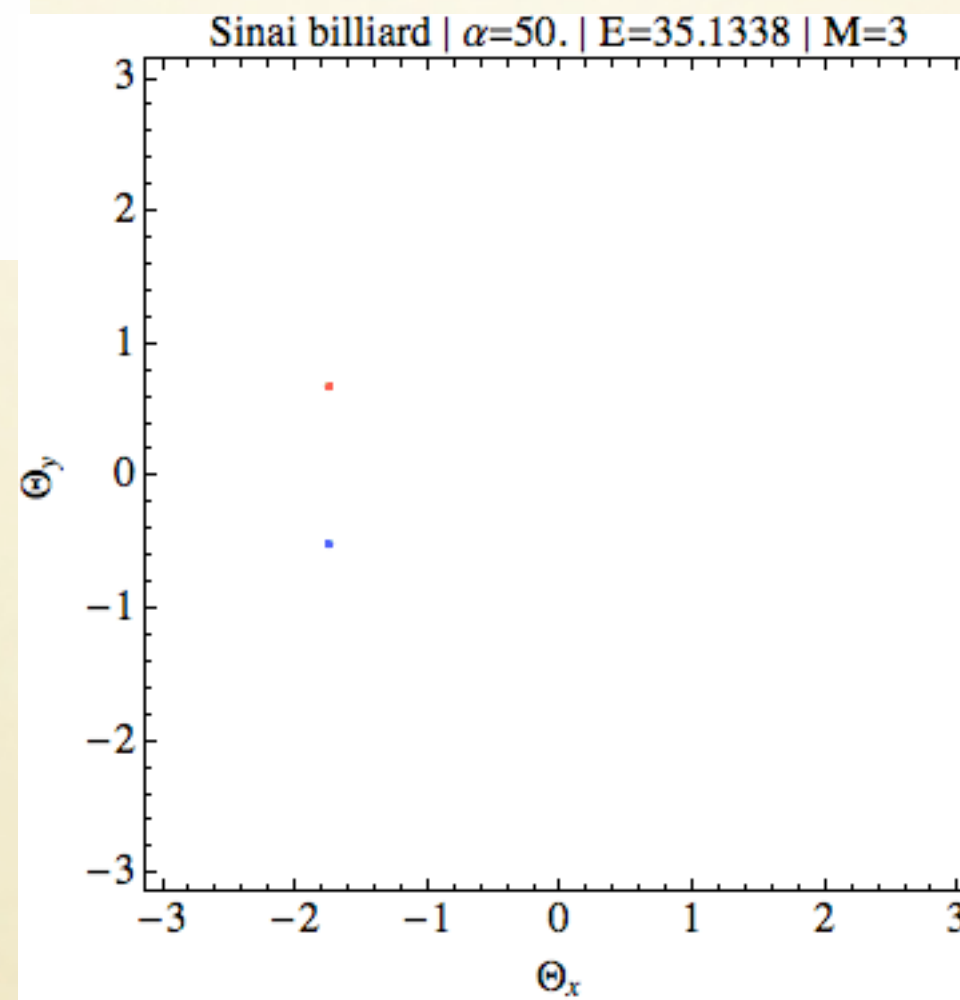
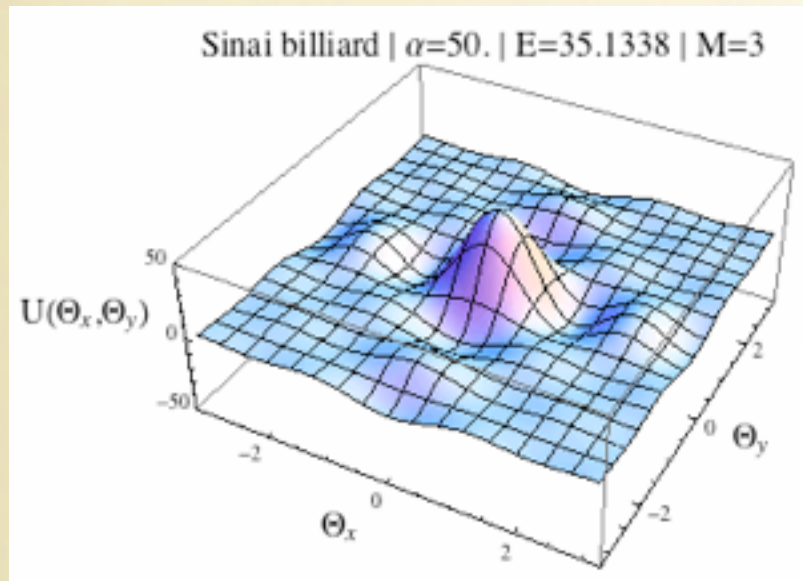
TRAJECTORIES IN A SOFT SINAI BILLIARD



TRAJECTORIES IN A SOFT SINAI BILLIARD



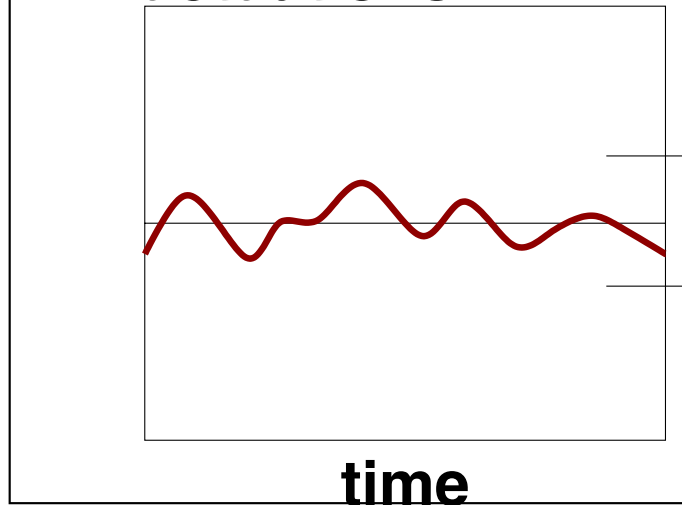
TRAJECTORIES IN A SOFT SINAI BILLIARD



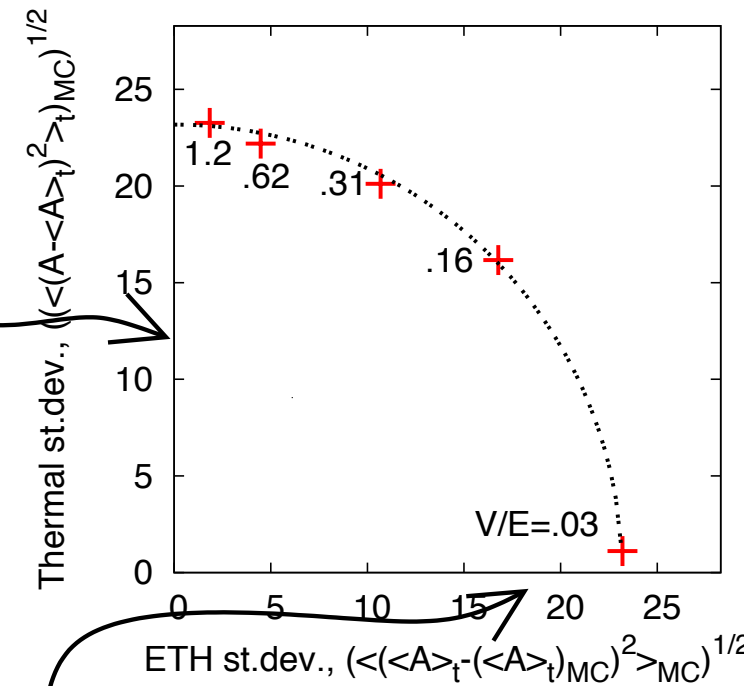
A Sinai-type billiard: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

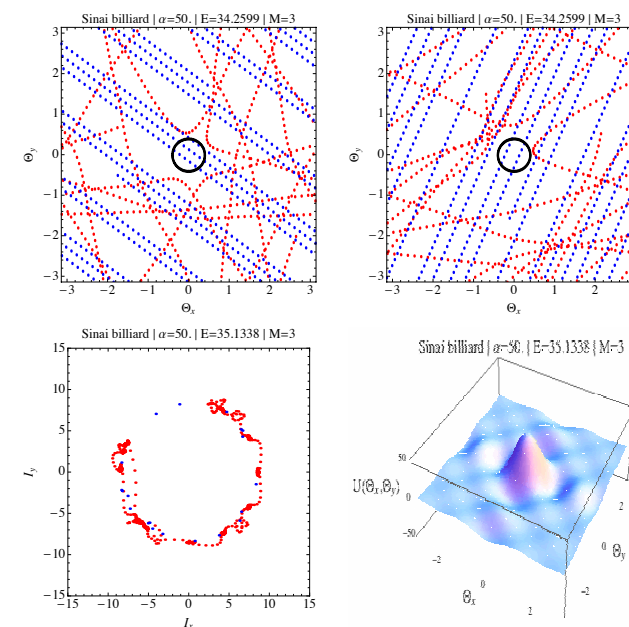
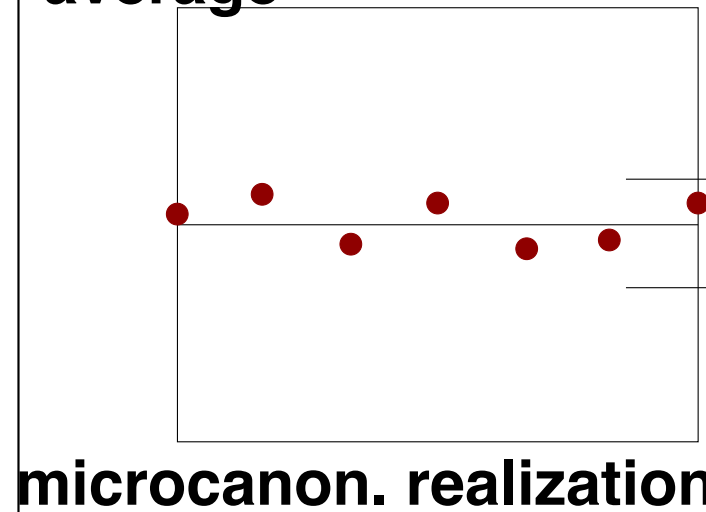
temporal/thermal fluctuations



ETH vs Thermal Variance | $A = E_x - E_y$ | 2D Sinai PBC M3



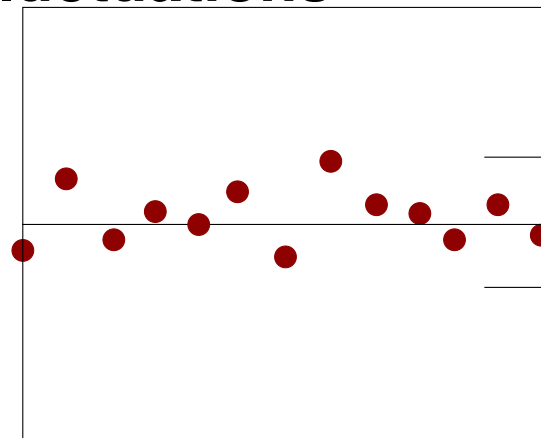
temporal average



HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

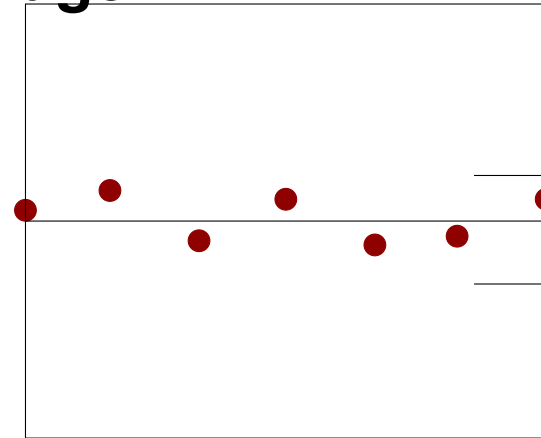
quantum/thermal
fluctuations



time

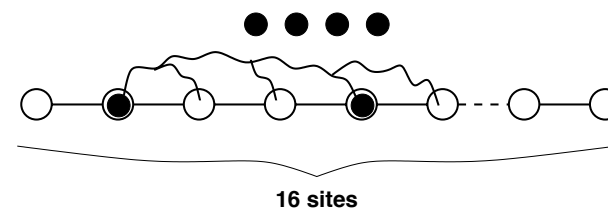
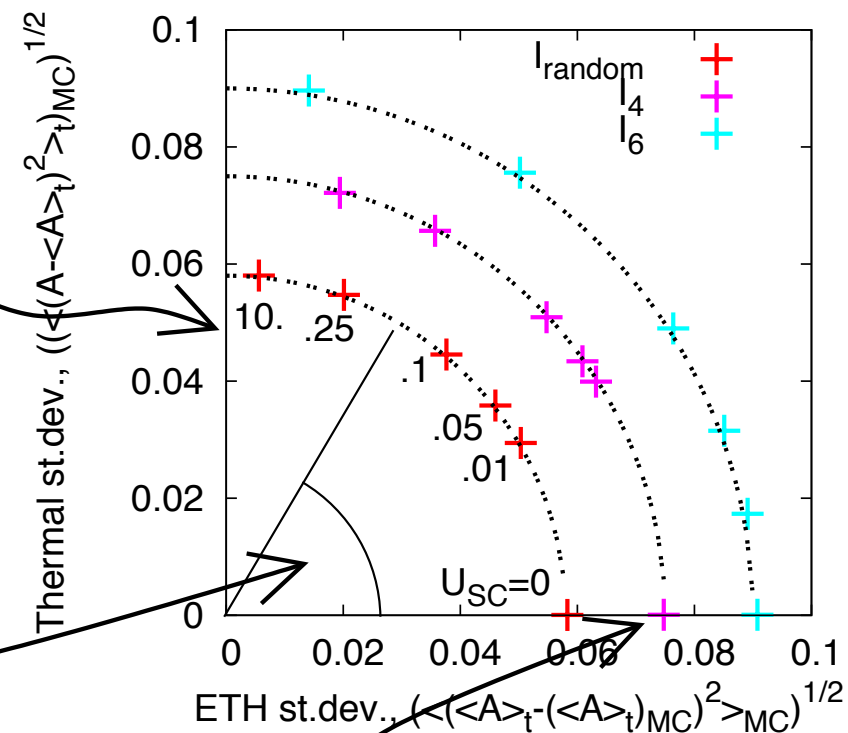
$\cos^{-1}(\sqrt{IPR})$

quantum
average

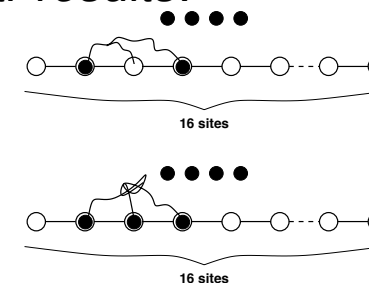


eigenstate index

ETH vs Thermal Variance | HardcoreBosons+SC_{R=4} N_{at}=4 L=16



similar results:





Hilbert-Schmidt inner product

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions



“[T]he angel of geometry and the devil of algebra share the stage, illustrating the difficulties of both.”

Hermann Weyl

The Hilbert-Schmidt (HS) inner product between two matrices:

$$(\hat{A}|\hat{B}) \equiv \text{Tr}[\hat{A}^\dagger \hat{B}] \quad .$$

HS product is invariant under unitary transformations:

$$(\hat{U} \hat{A} \hat{U}^{-1} | \hat{U} \hat{B} \hat{U}^{-1}) = (\hat{A} | \hat{B}) \quad .$$

The unitary transformations form a (small) subgroup of the group of HS rotations: the latter preserve the HS norm, defined as

$$||\hat{A}|| \equiv \sqrt{\text{Tr}[\hat{A}^2]} \quad .$$

Some definitions

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

Introduce:

(a) a microcanonical window: $\mathcal{W}_{MC} \equiv \{|\alpha\rangle \mid E_\alpha \in [E_{min}, E_{max}]\}$,
where $|\alpha\rangle$ and E_α are the eigenstates and eigenenergies of a Hamiltonian $\hat{H}$;

(b) a HS normalized identity operator: $\hat{\mathcal{I}} = (N_{MC})^{-1/2}I$;

(c) a space of the diagonal (w.r.t. $\hat{H}$) observables:
 $\mathcal{L}_{d, \hat{H}} \equiv \text{Span}[\{|\alpha\rangle\langle\alpha| \mid |\alpha\rangle \in \mathcal{W}_{MC}\}]$;

(d) a space of the off-diagonal (w.r.t. $\hat{H}$) observables:
 $\mathcal{L}_{o-d, \hat{H}} \equiv \text{Span}[\{2^{-1/2}(|\alpha\rangle\langle\beta| + h.c.)\} \cup \{i2^{-1/2}(|\alpha\rangle\langle\beta| - h.c.)\} \mid |\alpha\rangle \in \mathcal{W}_{MC}; |\beta\rangle \in \mathcal{W}_{MC}; \beta > \alpha\}]$.

The integrability-ergodicity-to-HS dictionary

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

Then:

ensemble variance of the temporal means (ETH variance) $\equiv$

$$\left(N_{MC}^{-1} \sum_{\alpha}^{\mathcal{W}_{MC}} A_{\alpha, \alpha}^2 - \langle \hat{A} \rangle_{MC} \right) / \left(\langle \hat{A}^2 \rangle_{MC} - \langle \hat{A} \rangle_{MC}^2 \right) = \cos^2(\hat{A} \hat{\mathcal{L}}_{d, \hat{H}}) - \cos^2(\hat{A} \hat{\mathcal{I}})$$

ensemble mean of the temporal (quantum) variance $\equiv$

$$N_{MC}^{-1} \left(\sum_{\alpha, \beta \neq \alpha}^{\mathcal{W}_{MC}} A_{\alpha, \beta}^2 \right) / \left(\langle \hat{A}^2 \rangle_{MC} - \langle \hat{A} \rangle_{MC}^2 \right) = \cos^2(\hat{A} \hat{\mathcal{L}}_{o-d, \hat{H}})$$

ensemble variance $\equiv$

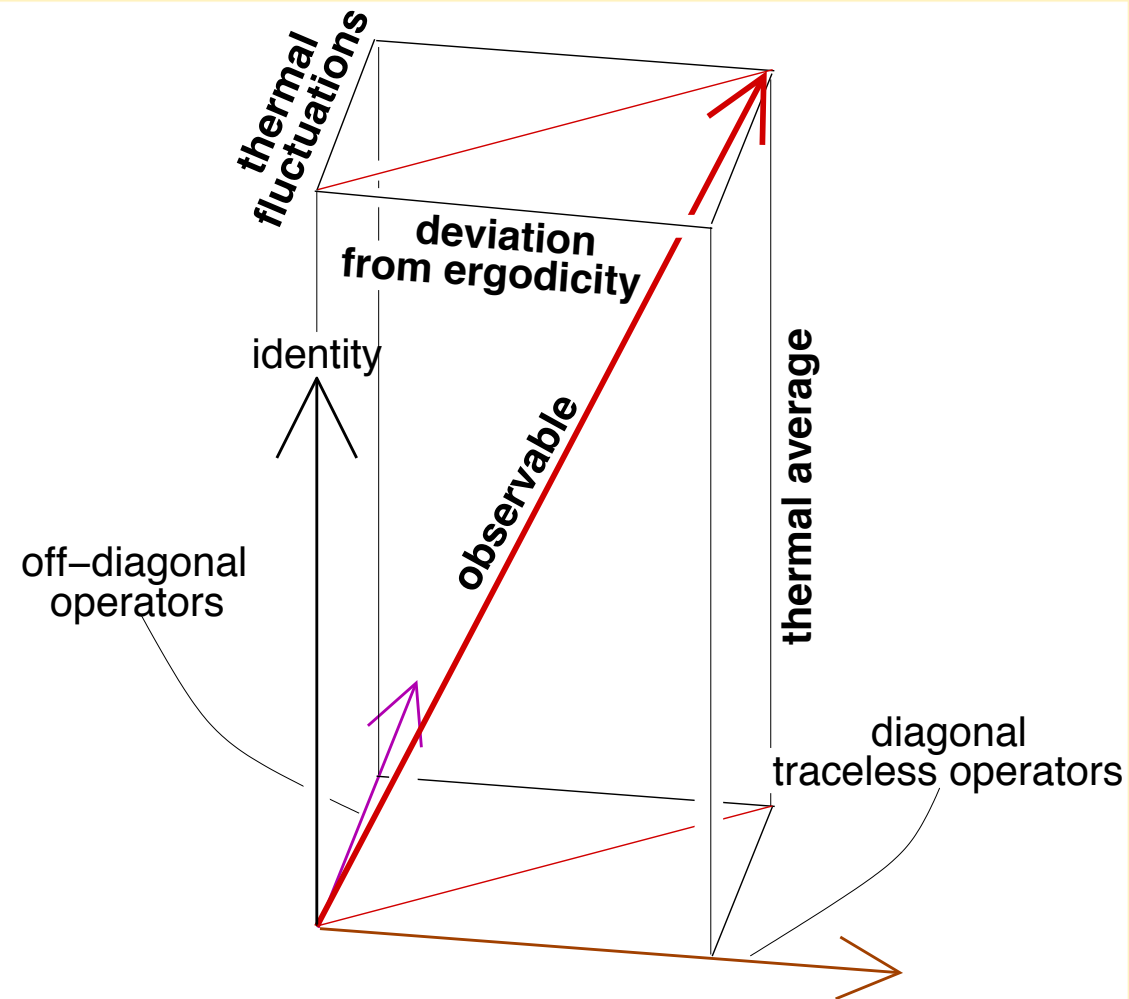
$$\langle \hat{A}^2 \rangle_{MC} - \langle \hat{A} \rangle_{MC}^2 = N_{MC}^{-1} \left(\|\hat{A}^2\| - N_{MC}^{-1} \|\hat{A}\|^2 \right)$$

inverse participation ratio (ITR) between the eigenstates of an integrable ($\hat{H}_0$)

$$N_{MC}^{-1} \sum_{\alpha, \alpha_o}^{\mathcal{W}_{MC}} |\langle \alpha_0 | \alpha \rangle|^4 = \cos^2(\mathcal{L}_{d, \hat{H}_0} \hat{\mathcal{L}}_{d, \hat{H}})$$

HS Geometry of the Integrability-Thermalizability transition

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

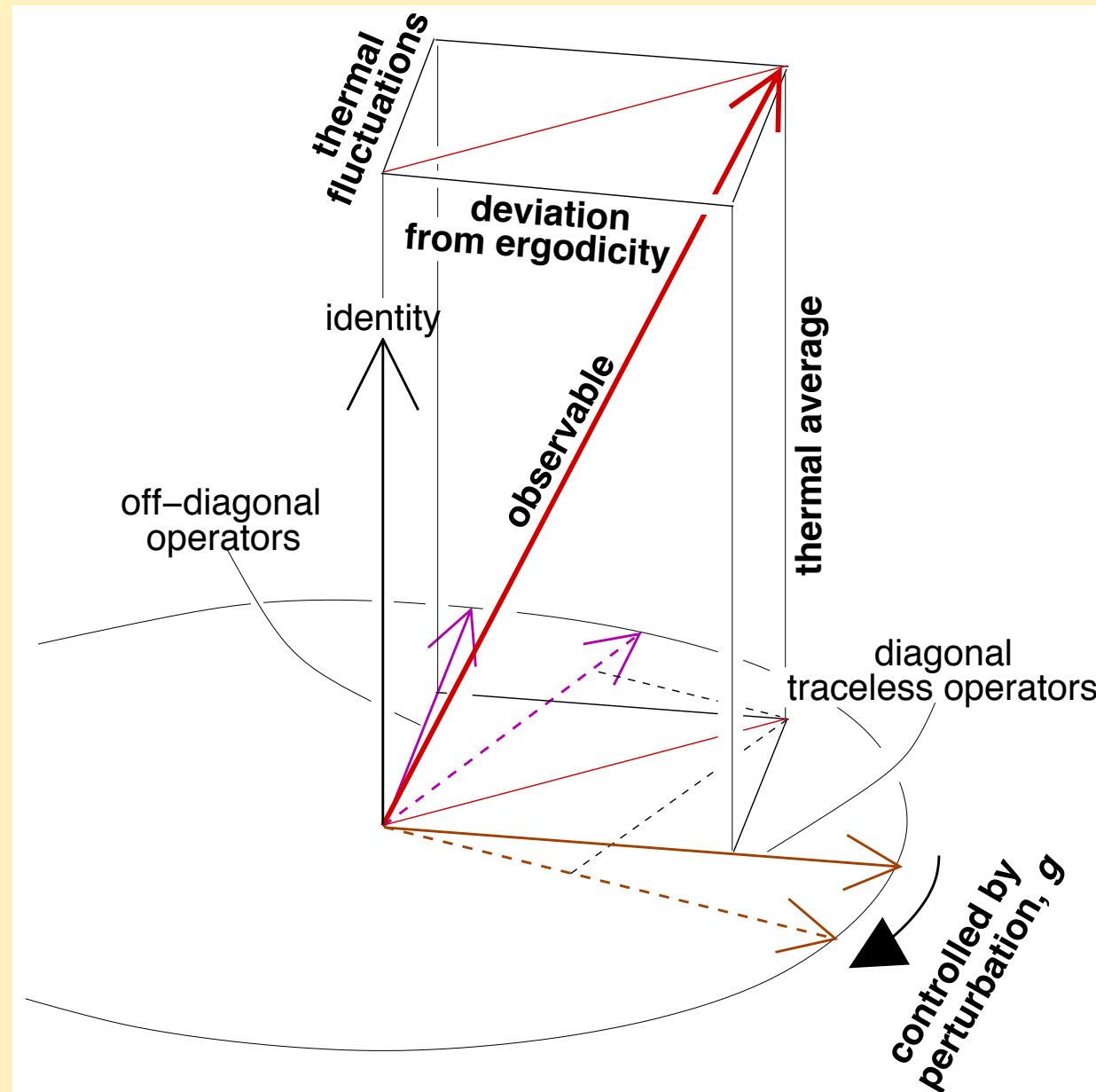


Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions



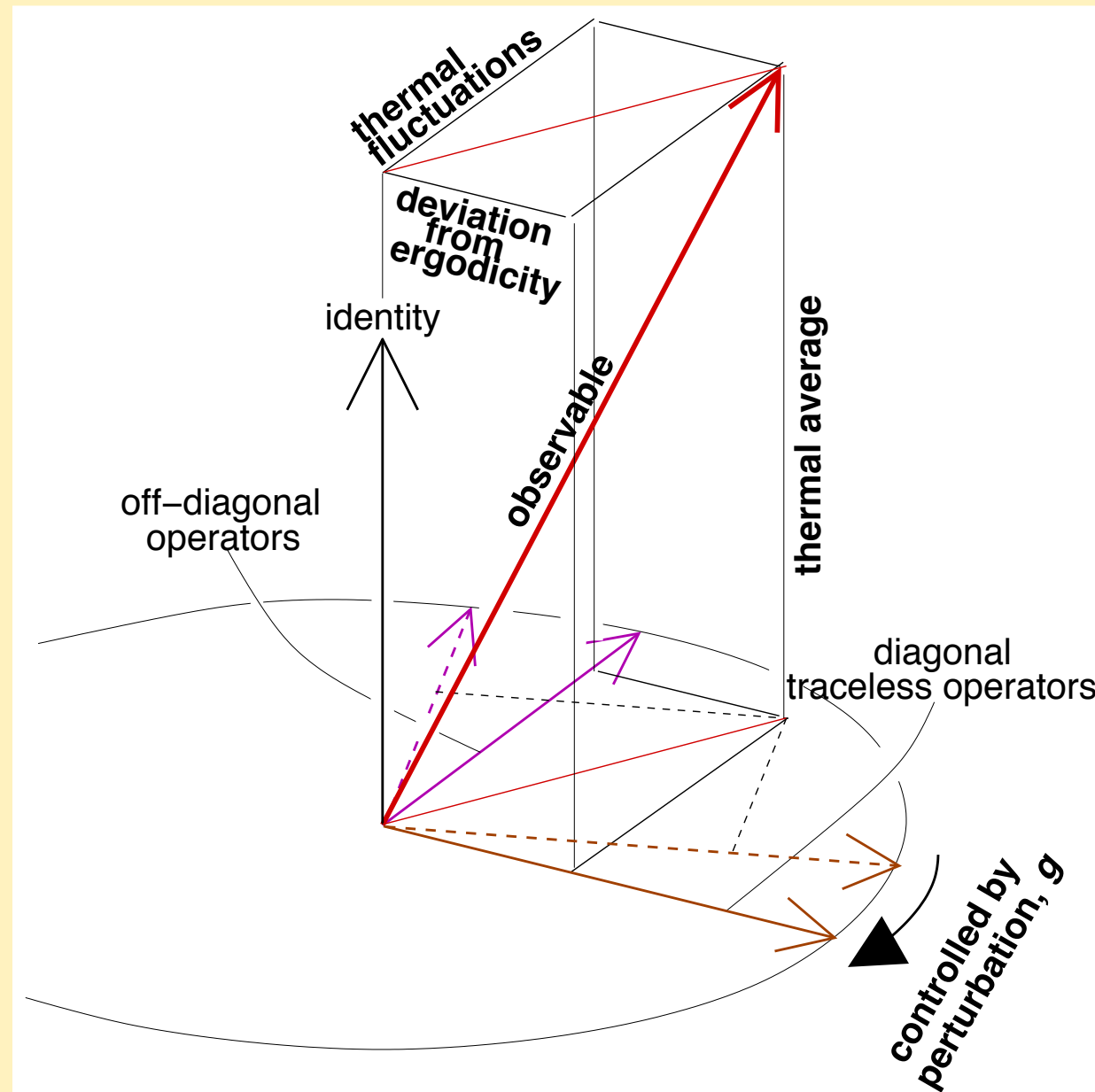
HS Geometry of the Integrability-Thermalizability transition

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions



HS Geometry of the Integrability-Thermalizability transition

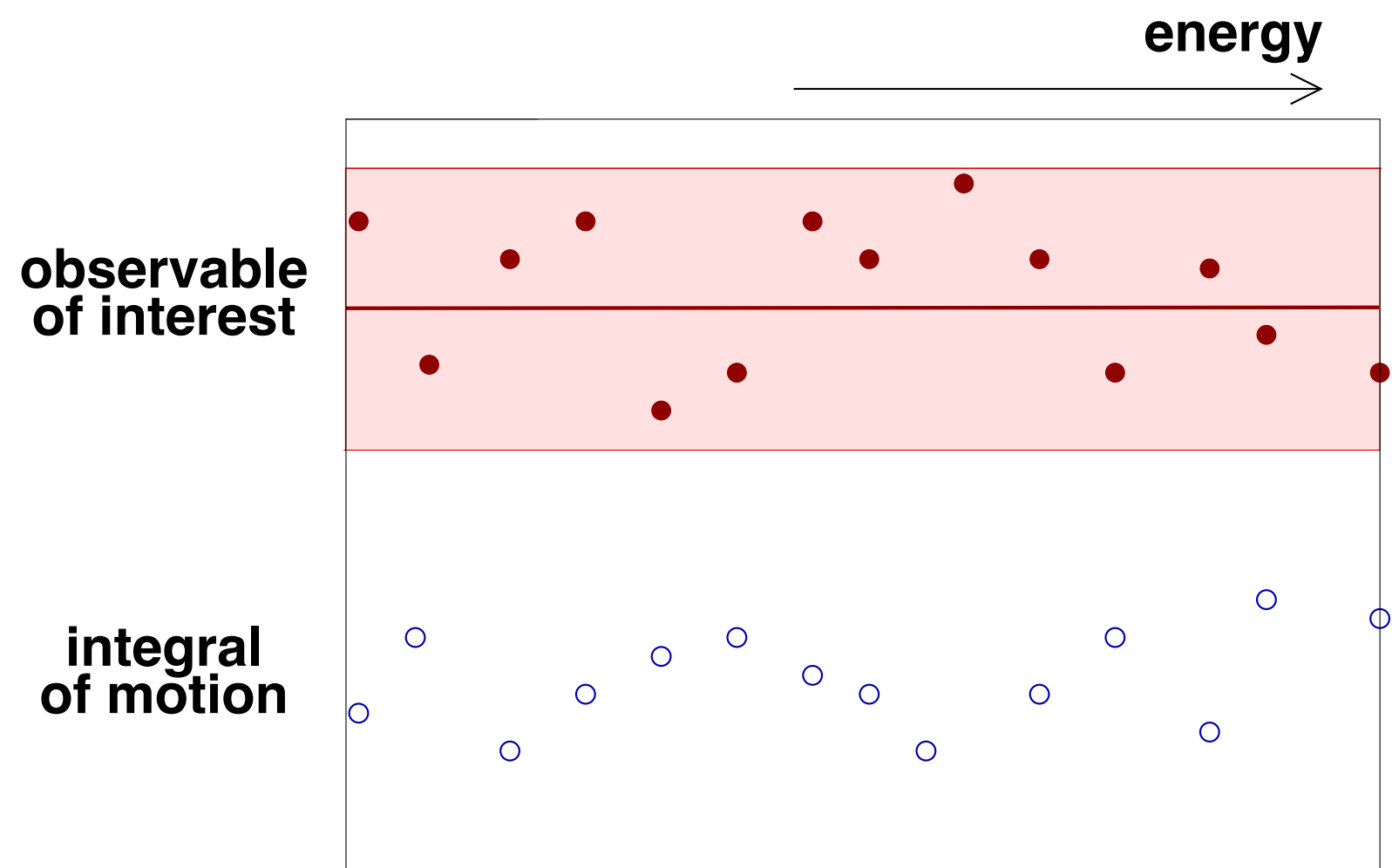
Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions



Optimizing the GGE

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Conclusions

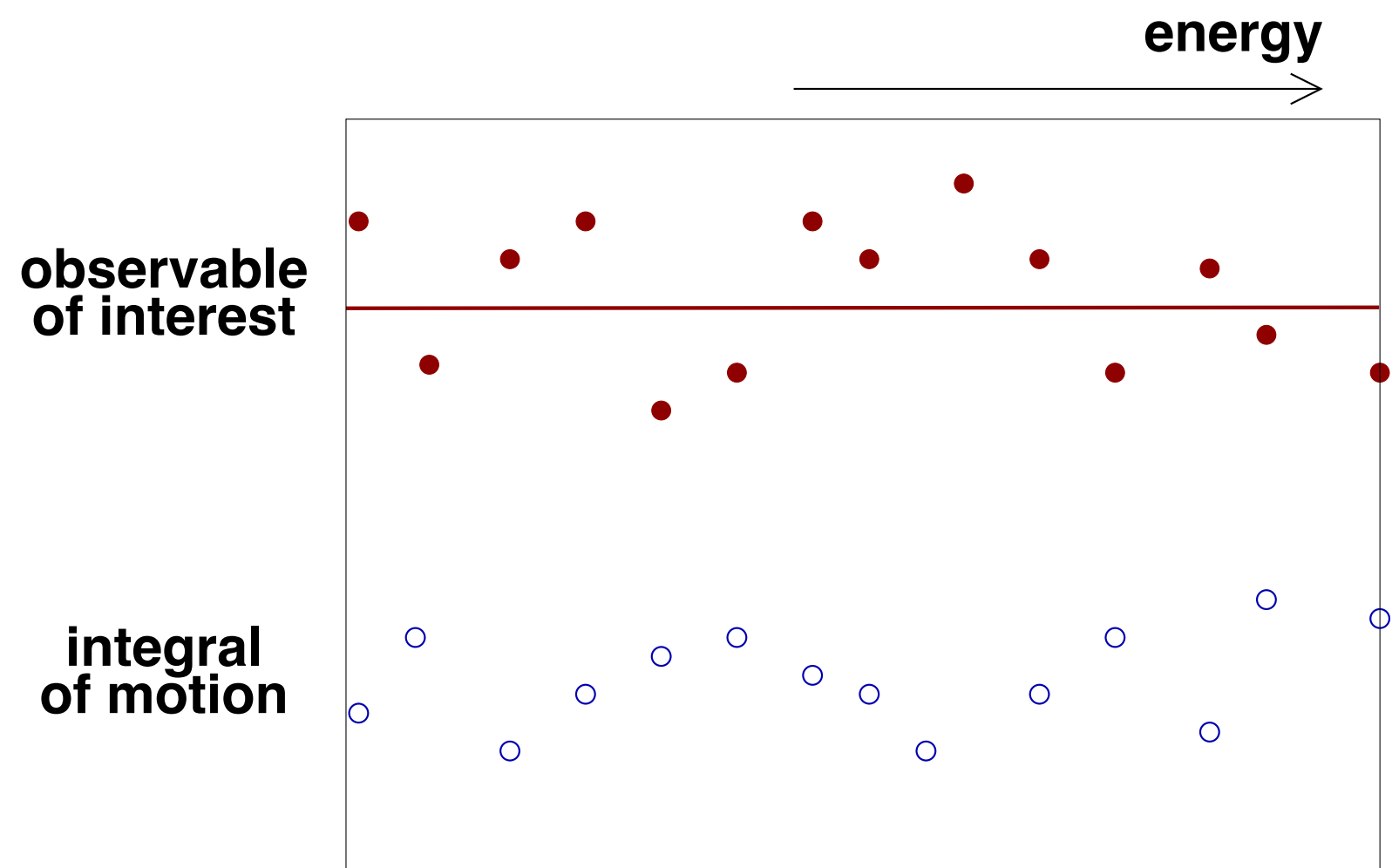
Conventional microcanonical vs generalized Gibbs microcanonical ensemble



Optimizing the GGE

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

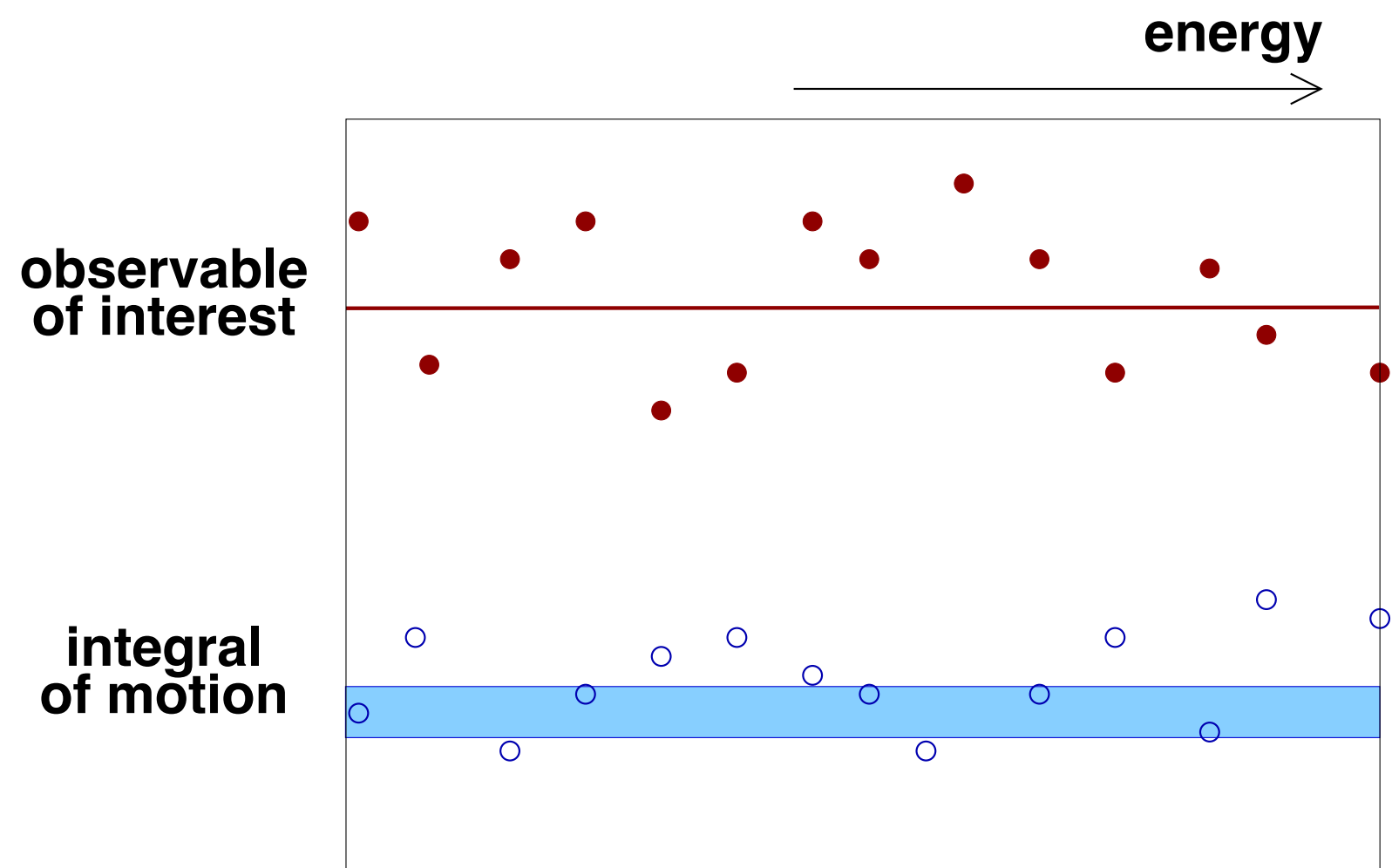
Conventional microcanonical vs generalized Gibbs microcanonical ensemble



Optimizing the GGE

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

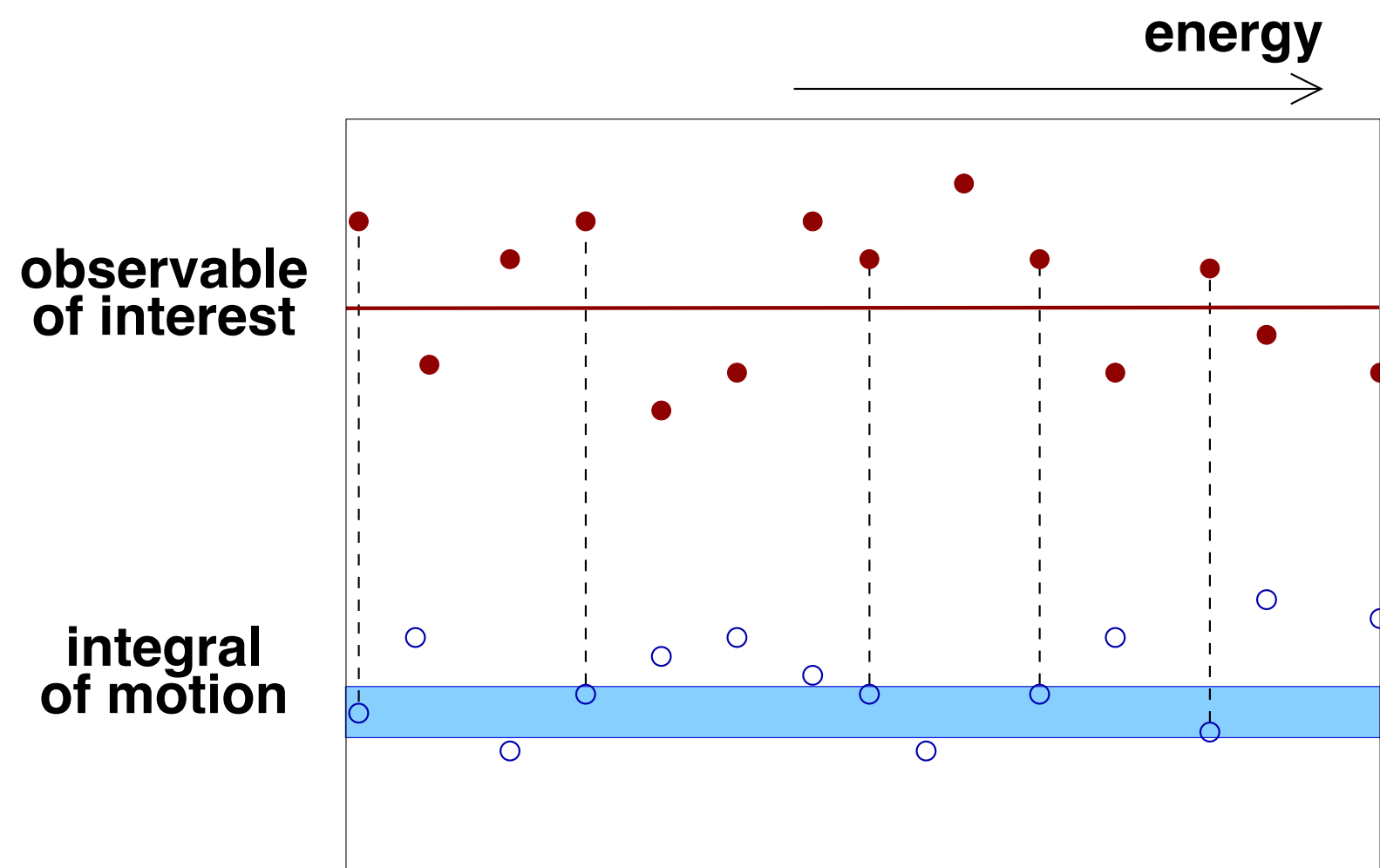
Conventional microcanonical vs generalized Gibbs microcanonical ensemble



Optimizing the GGE

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Conclusions

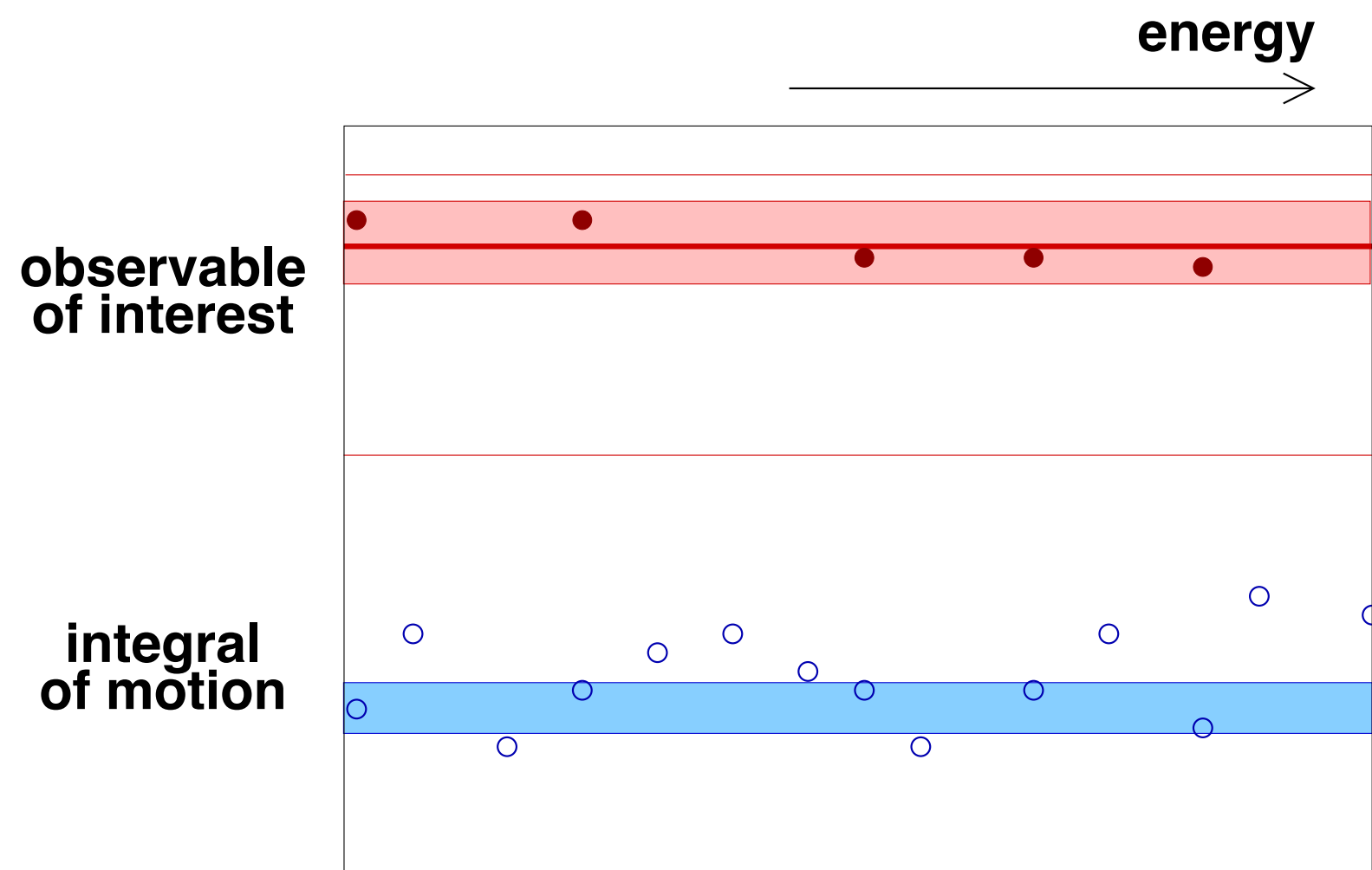
Conventional microcanonical vs generalized Gibbs microcanonical ensemble



Optimizing the GGE

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

Conventional microcanonical vs generalized Gibbs microcanonical ensemble



Optimizing the GGE: underlying exact inequality

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

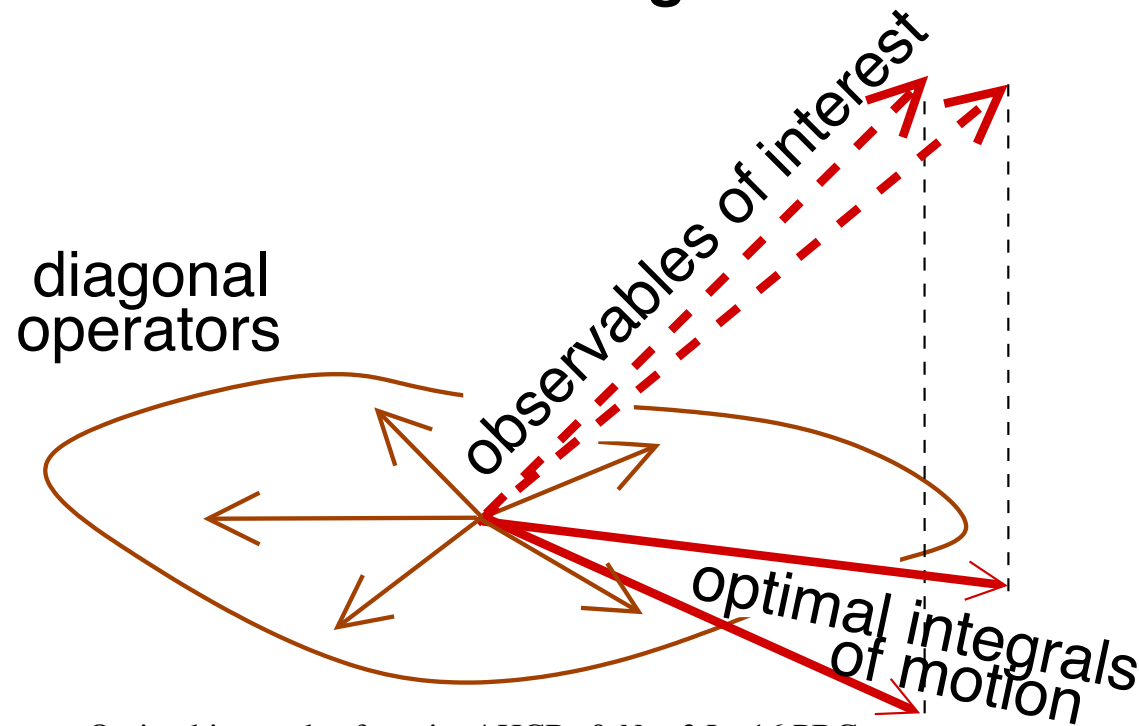
$$\frac{Var_{\text{GGE}}[\langle \alpha | \hat{A} | \alpha \rangle]}{Var_{\text{MC}}[\langle \alpha | \hat{A} | \alpha \rangle]} \leq \sin^2[\hat{I}_{tl,d} \wedge \hat{A}_{tl,d}] + 2|\cos[\hat{I}_{tl,d} \wedge \hat{A}_{tl,d}]| \underbrace{\sqrt{\frac{Var_{\text{GGE}}[\langle \alpha | \hat{I} | \alpha \rangle]}{Var_{\text{MC}}[\langle \alpha | \hat{I} | \alpha \rangle]}}}_{\mathcal{O}\left(\frac{\Delta I}{\sqrt{Var_{\text{MC}}[\langle \alpha | \hat{I} | \alpha \rangle]}}\right)},$$

where $\Delta I \equiv \max_j (I_{j+1} - I_j) =$ maximal GGE interval for $\hat{I}$,
 $\hat{B}_{tl,d} \equiv \sum_{\alpha} (\langle \alpha | \hat{B} | \alpha \rangle - Mean_{\text{MC}}[\langle \alpha | \hat{B} | \alpha \rangle]) |\alpha\rangle \langle \alpha|$

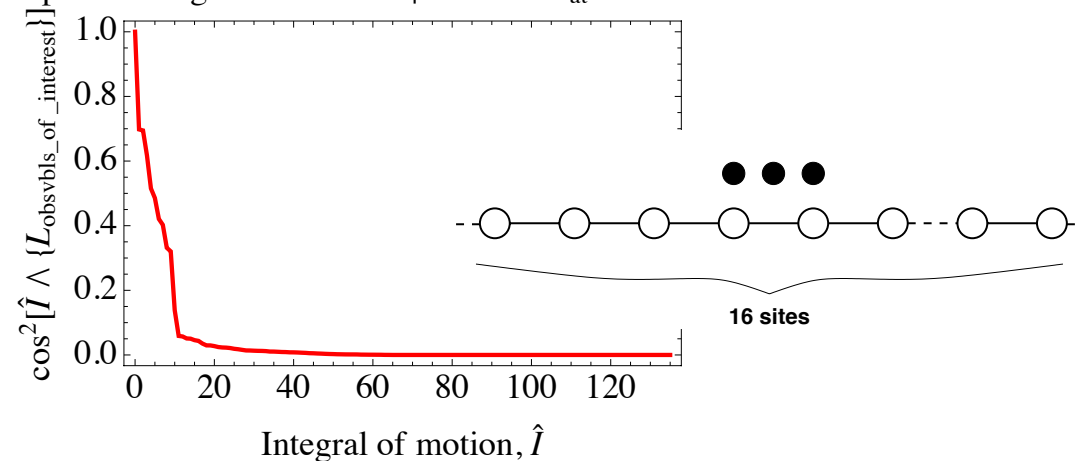
Optimizing the GGE: hard-core bosons

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

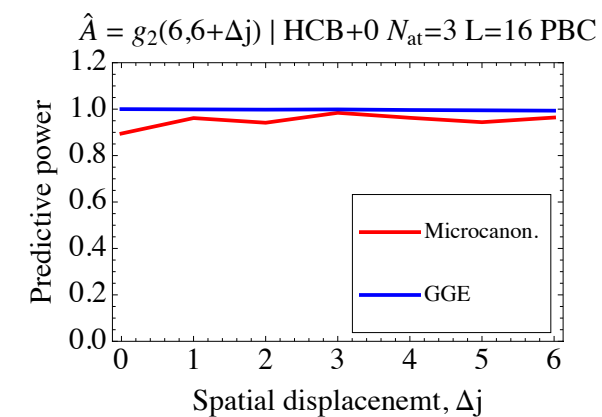
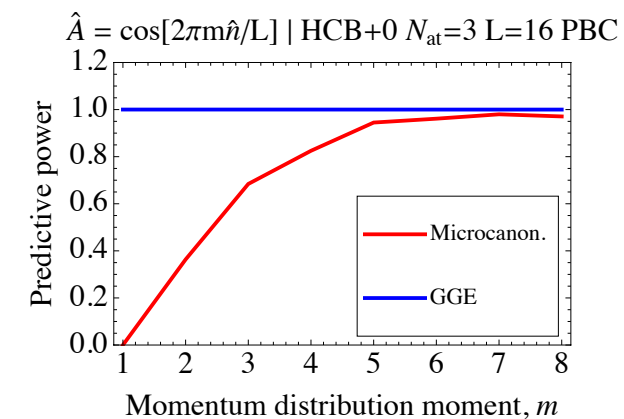
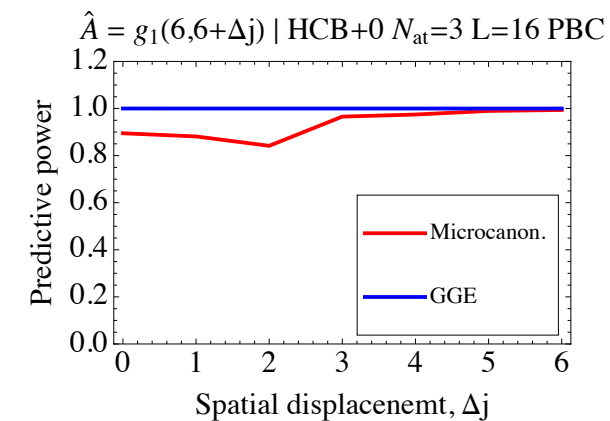
How to choose the optimal set of integrals of motion for GGE



Optimal integrals of motion | HCB+0 $N_{\text{at}}=3$ $L=16$ PBC



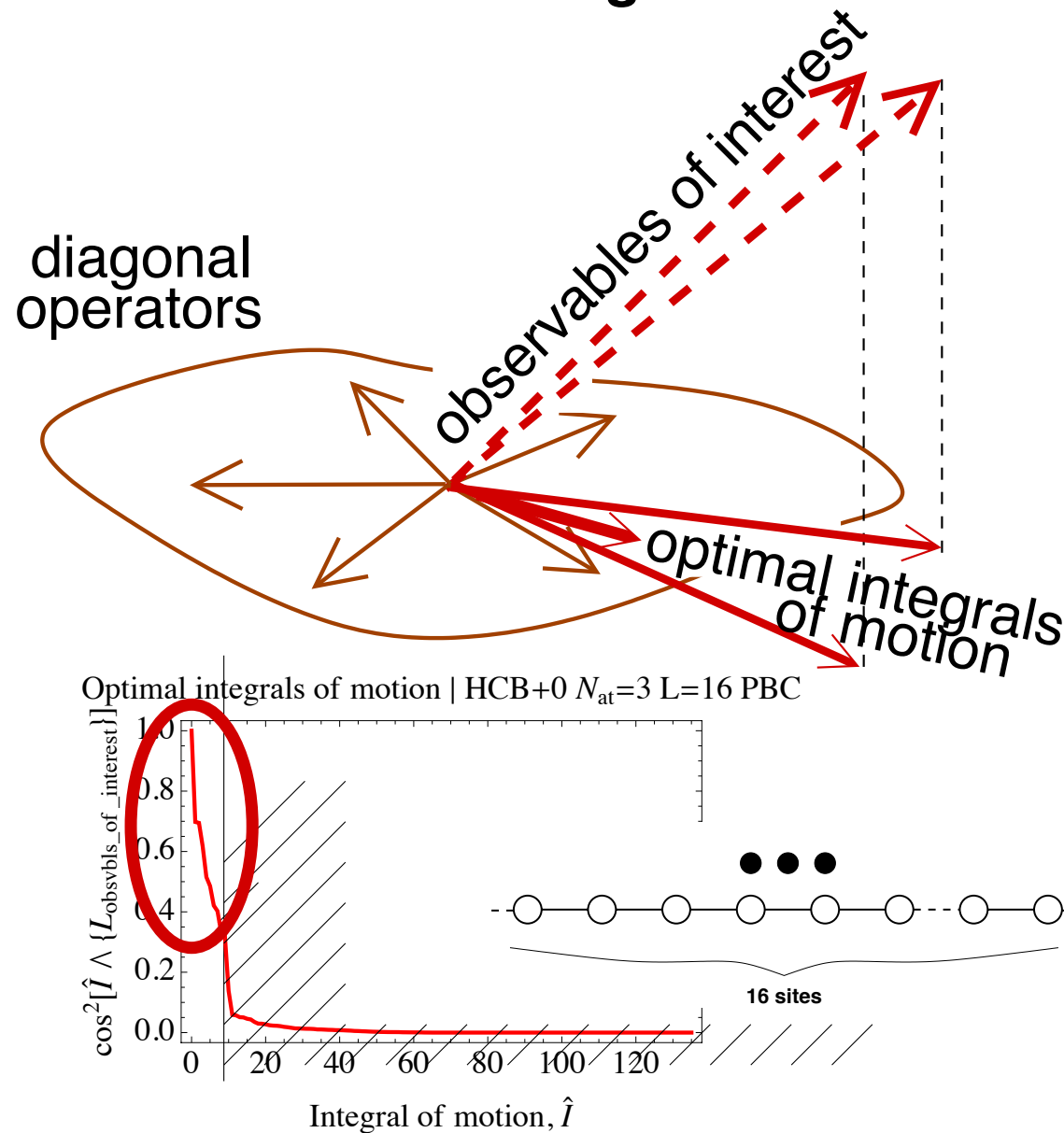
Similar ideas: Cassidy–Clark–Rigol (2011)



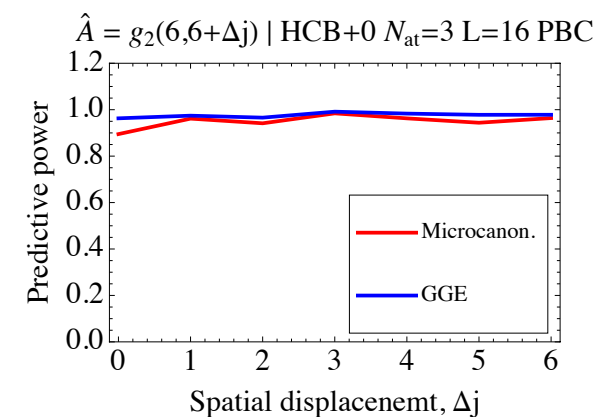
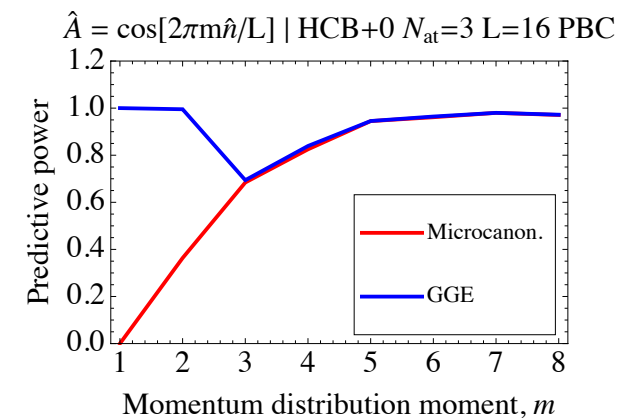
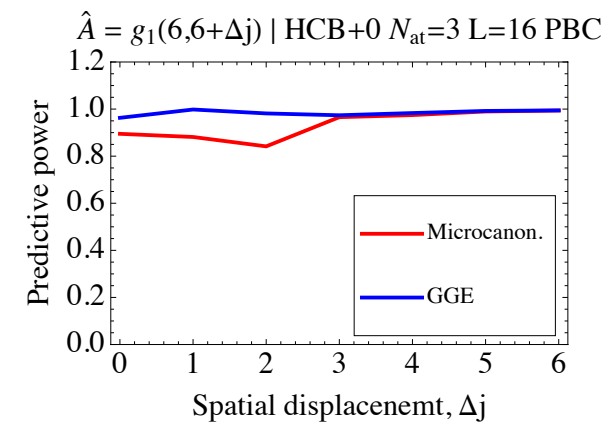
Optimizing the GGE: hard-core bosons

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

How to choose the optimal set of integrals of motion for GGE



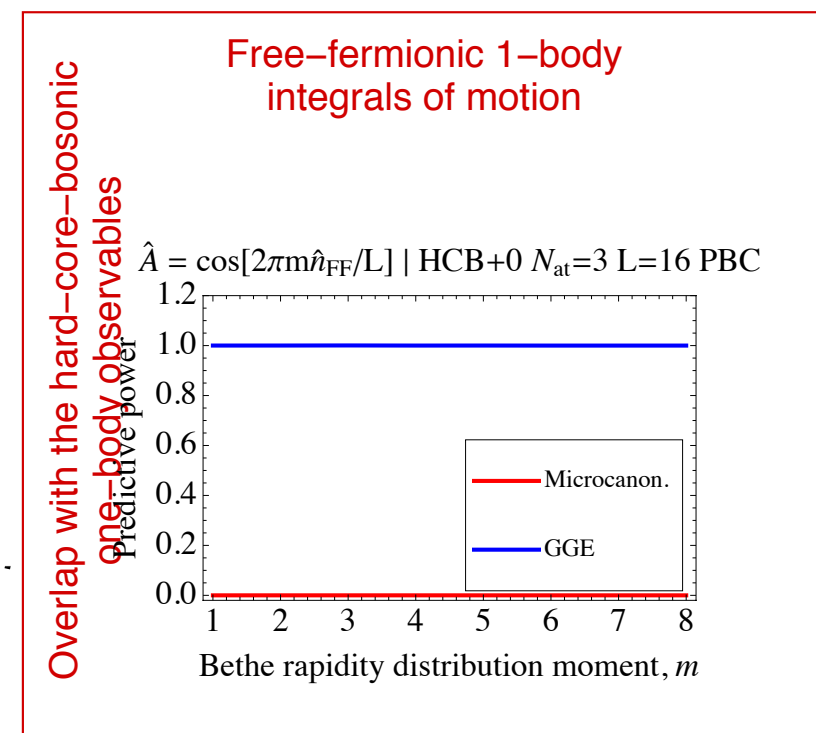
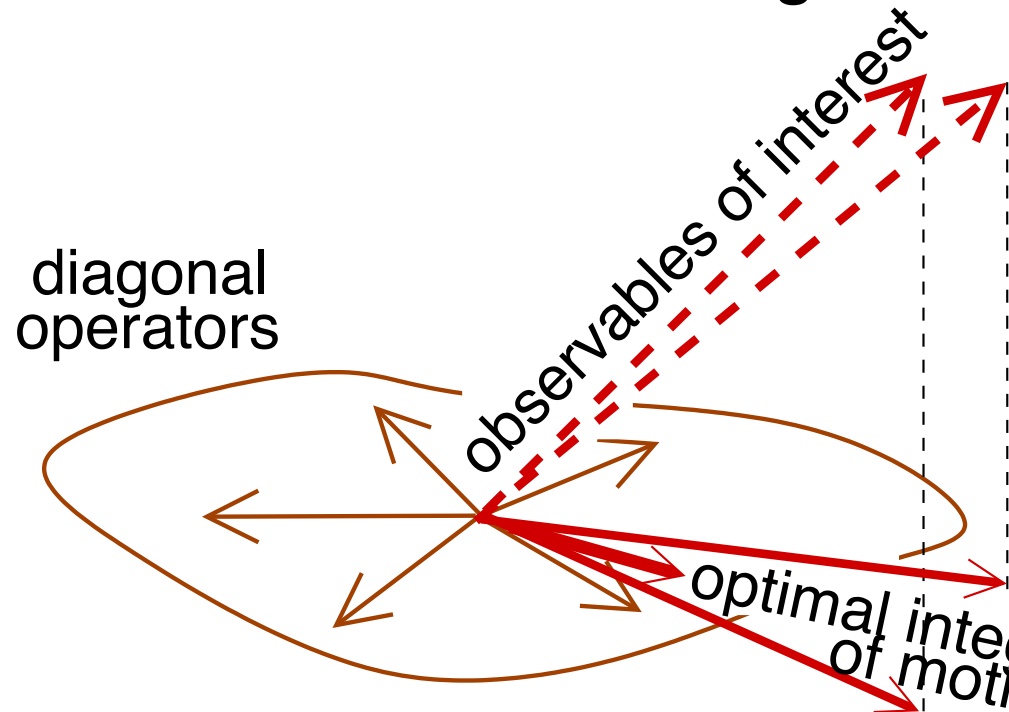
Similar ideas: Cassidy–Clark–Rigol (2011)



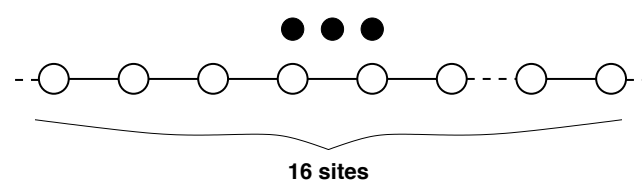
Optimizing the GGE: hard-core bosons

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Conclusions

How to choose the optimal set of integrals of motion



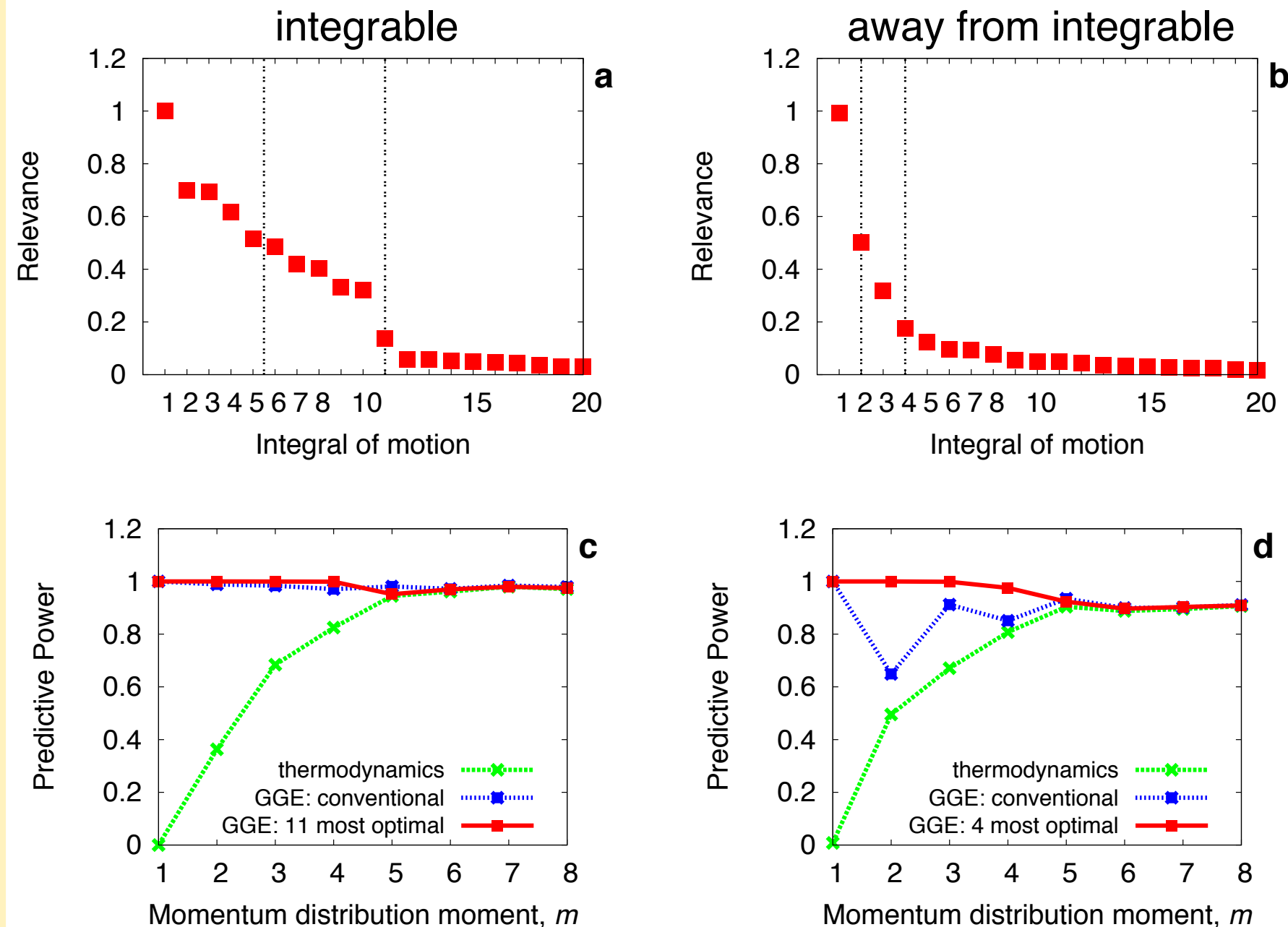
Take home:



in free-fermionic integrable systems, the Hilbert-Schmidt angle between the free-fermionic and "system proper" one-body observables is close to zero

Optimizing the GGE: beyond integrability

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions



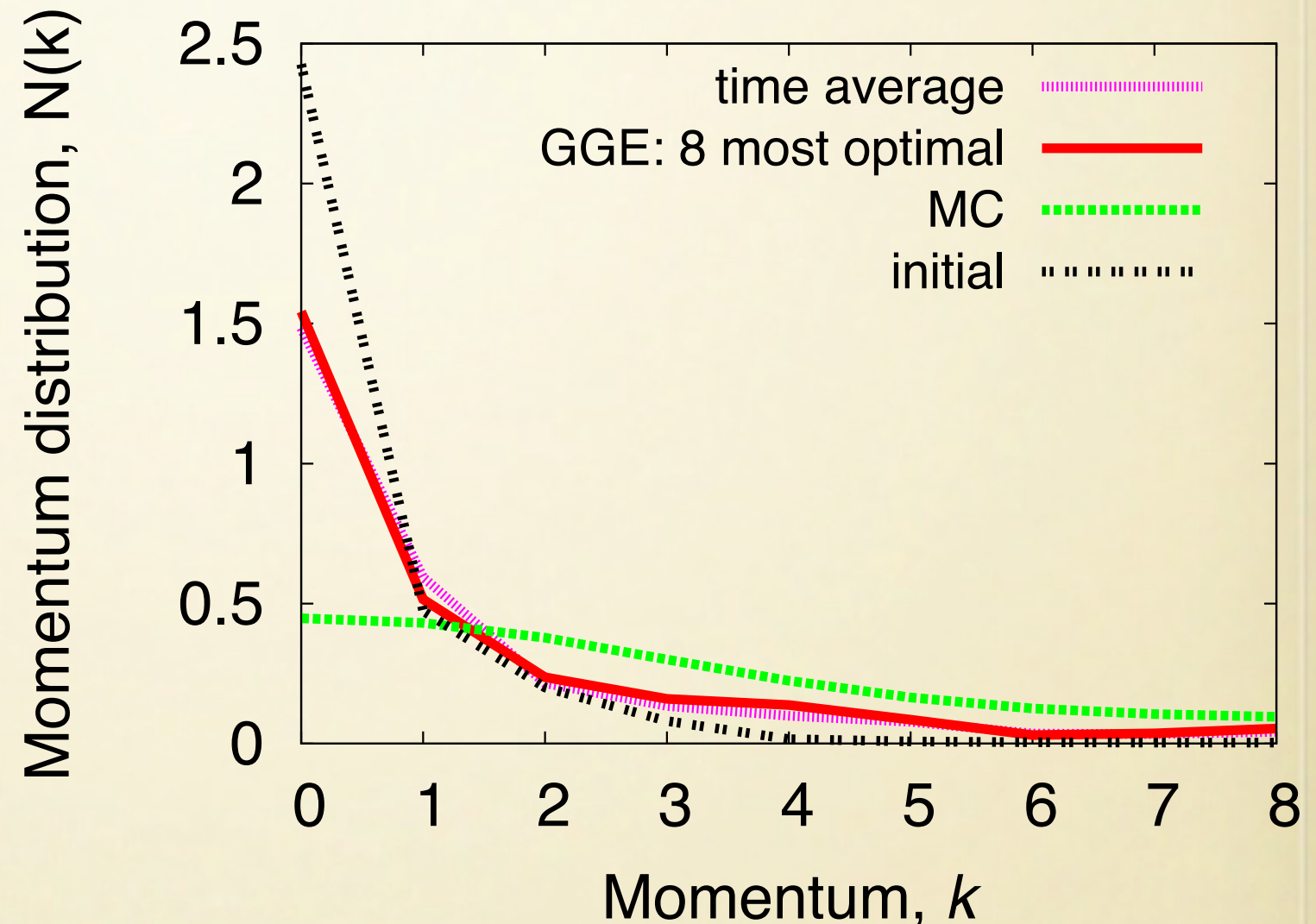
GENERALIZED THERMODYNAMICS: 4 INTERACTING BOSONS ON 16 SITES

- $N = 4 \mid L = 16 \mid \text{PBC}$
- INTERACTIONS: SOFT-CORE REPULSION OF RADIUS 4 AND STRENGTH $U=3$ + HARD-CORE

- INITIAL STATE: GROUND STATE WITH NO SOFT-CORE

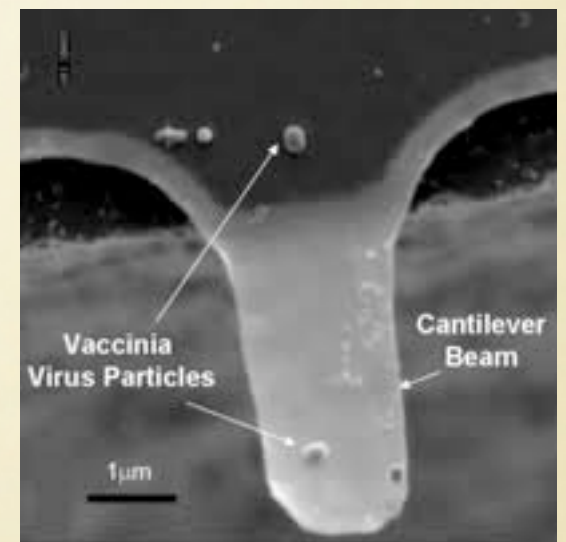
- # OF ADDITIONAL INTEGRALS OF MOTION = 7

- MC WINDOWS = 1/10 OF STATE-TO-STATE VARIANCE



OUTLOOK: MAXWELL DEMON OF NON-ERGODICITY

IDEA: IN MESOSCOPIC
SYSTEMS, USE FINITE-SIZE-
INDUCED DEVIATIONS FROM
ERGODICITY TO CONTROL
OBSERVABLES OF INTEREST



Credits: Zack Hilt*, Amit Gupta, Prof. Nick Peppas*, Prof. Rashid Bashir,
School of Electrical and Computer Engineering, Purdue University

*School of Chemical Engineering
UT Austin, Austin, TX

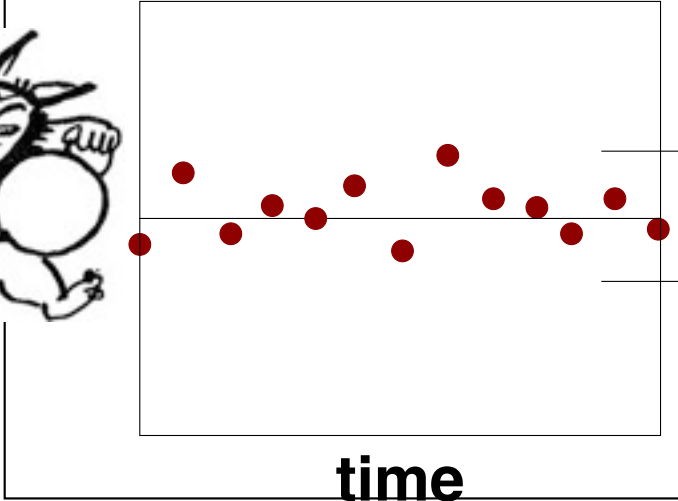
HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions



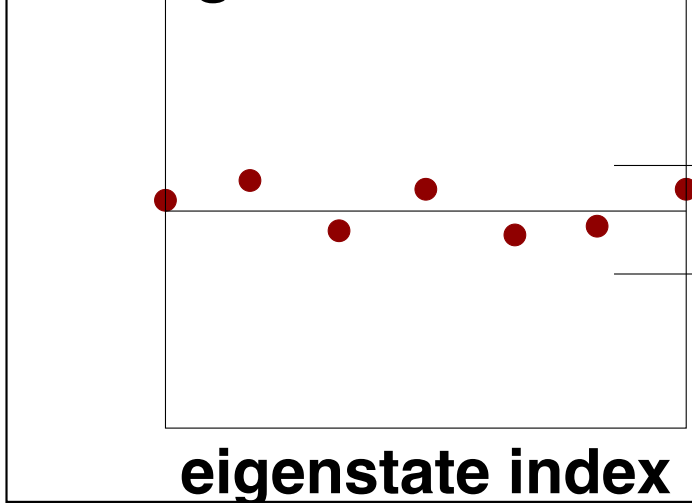
Maxwell
Demon

quantum/thermal
fluctuations

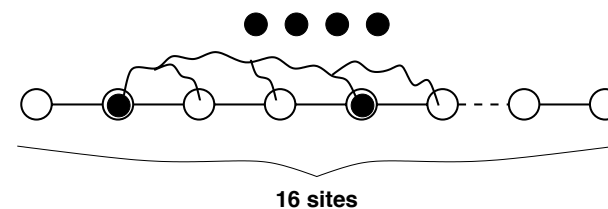
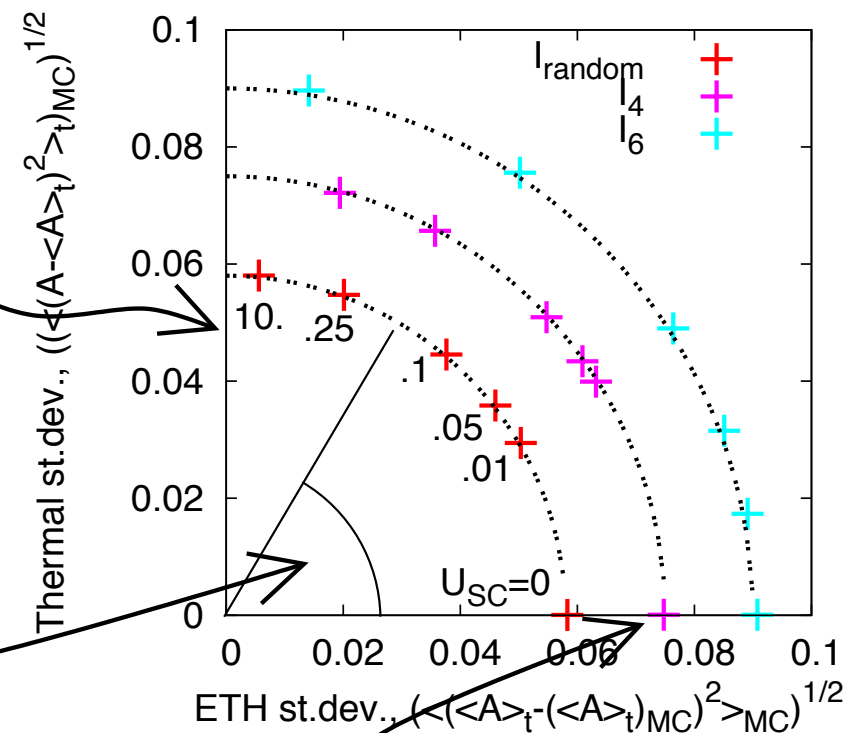


$\cos^{-1}(\sqrt{IPR})$

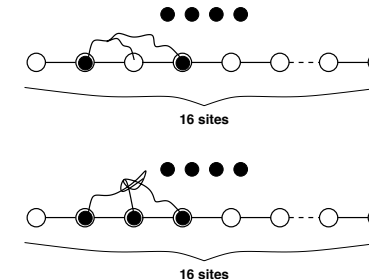
quantum
average



ETH vs Thermal Variance | HardcoreBosons+SC_{R=4} N_{at}=4 L=16

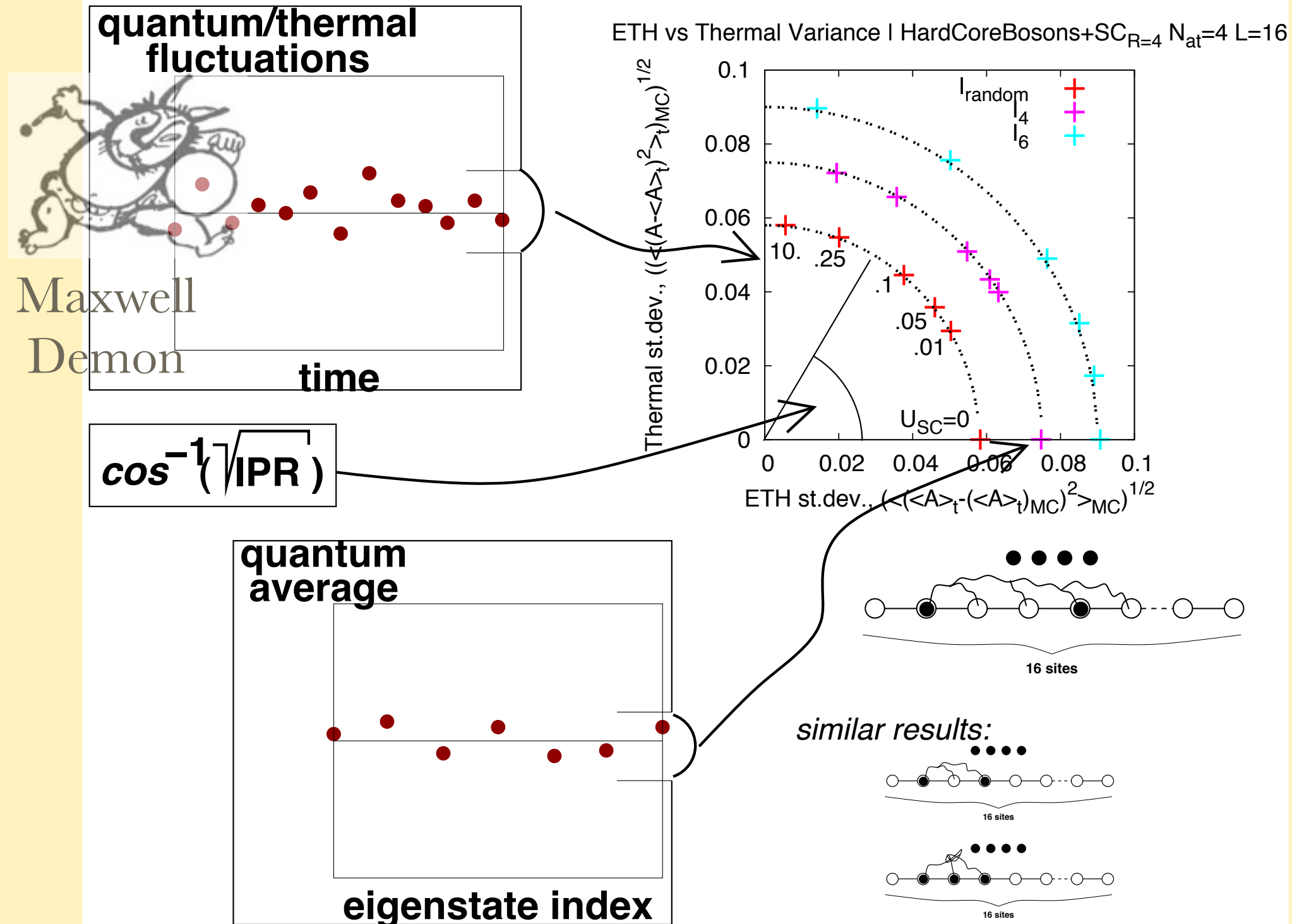


similar results:



HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

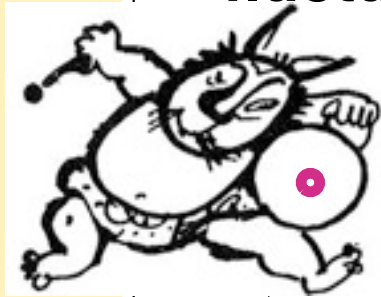
Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions



HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

quantum/thermal
fluctuations

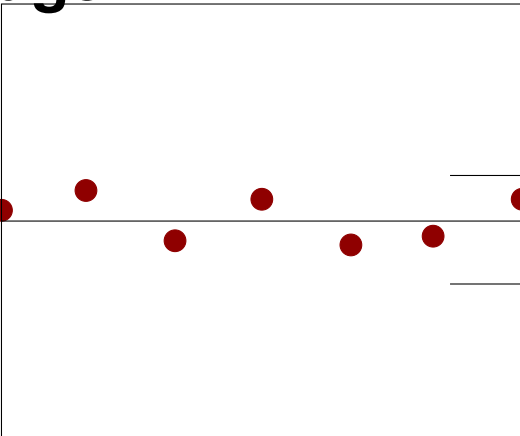


Maxwell
Demon

time

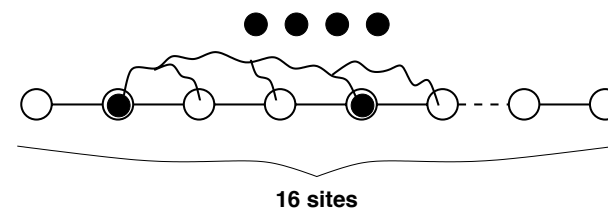
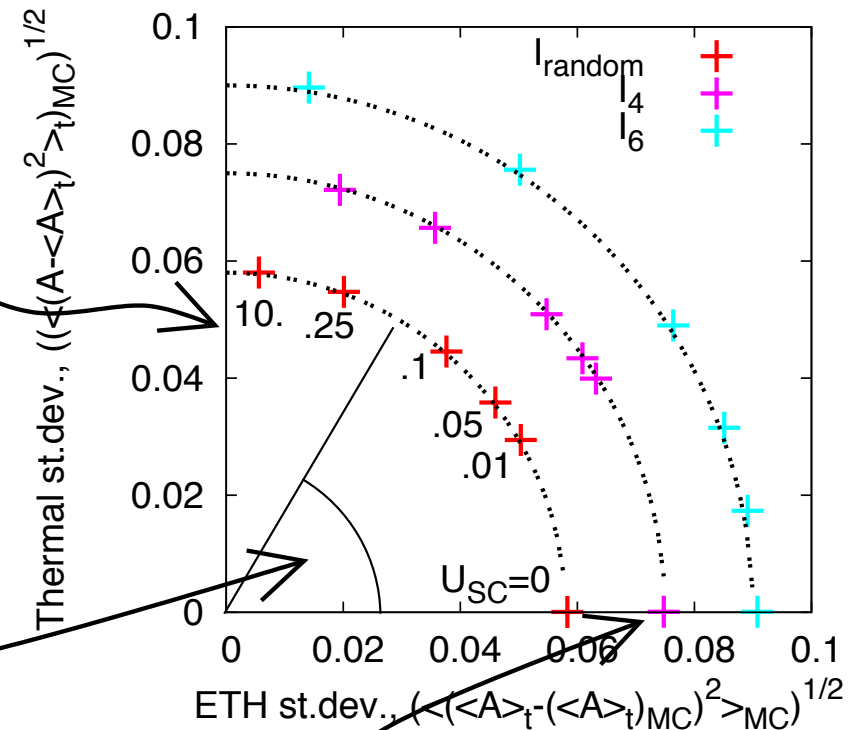
$\cos^{-1}(\sqrt{IPR})$

quantum
average

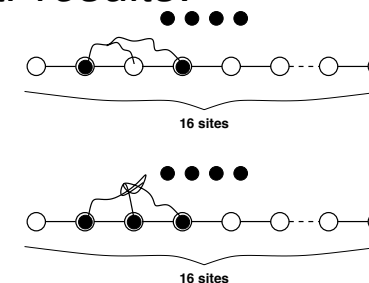


eigenstate index

ETH vs Thermal Variance | HardCoreBosons+SC_{R=4} N_{at}=4 L=16



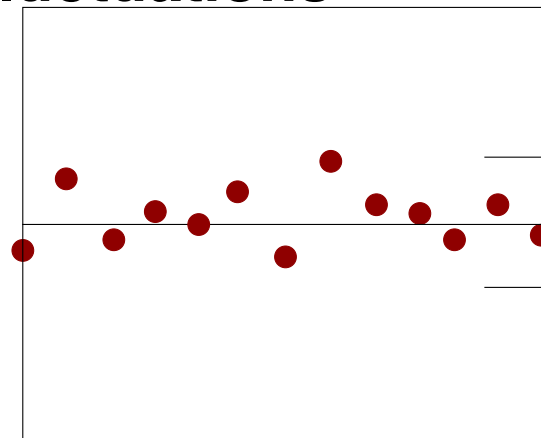
similar results:



HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

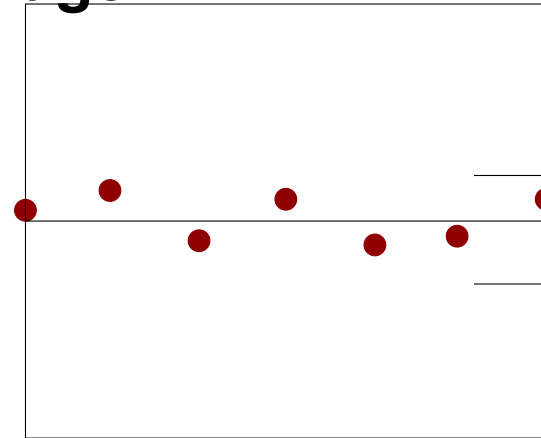
quantum/thermal
fluctuations



time

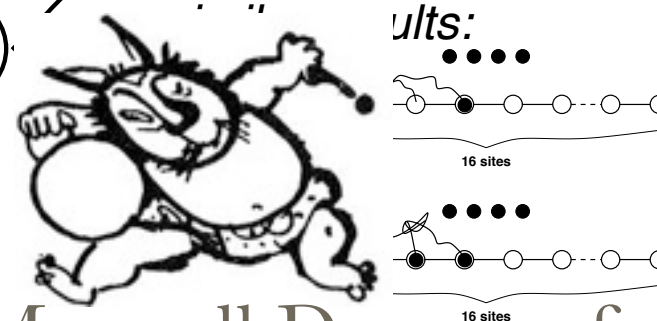
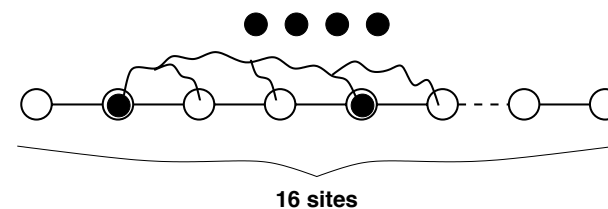
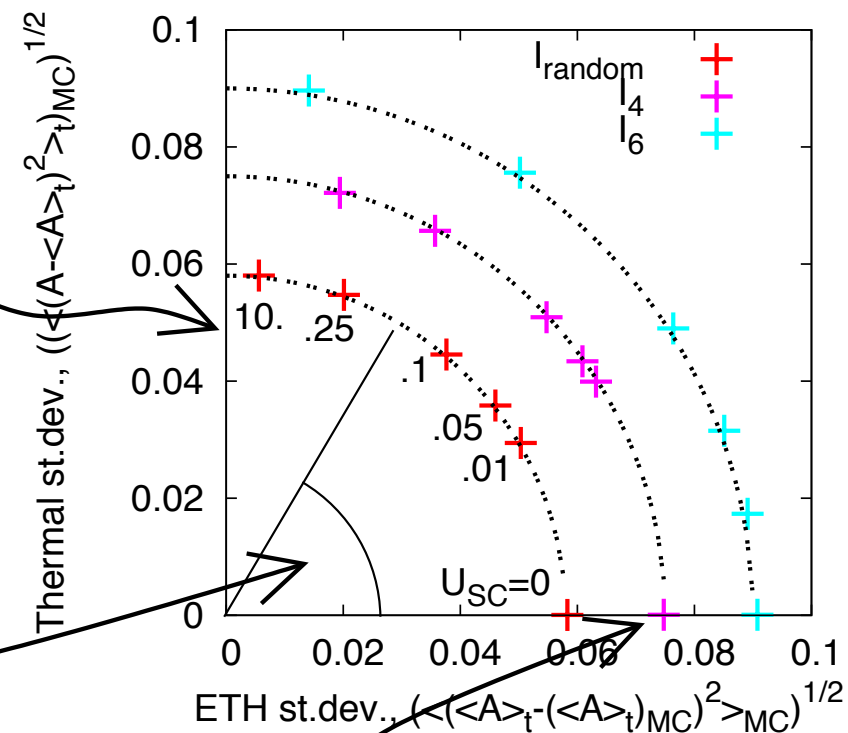
$\cos^{-1}(\sqrt{IPR})$

quantum
average



eigenstate index

ETH vs Thermal Variance | HardcoreBosons+SC_{R=4} N_{at}=4 L=16

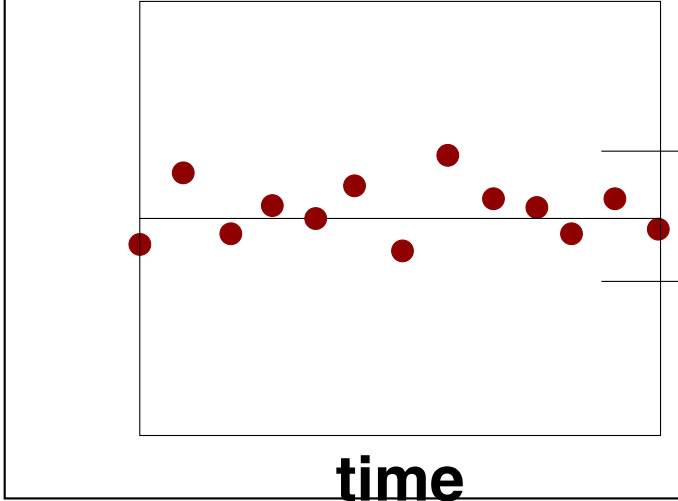


Maxwell Demon of non-ergodicity

HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

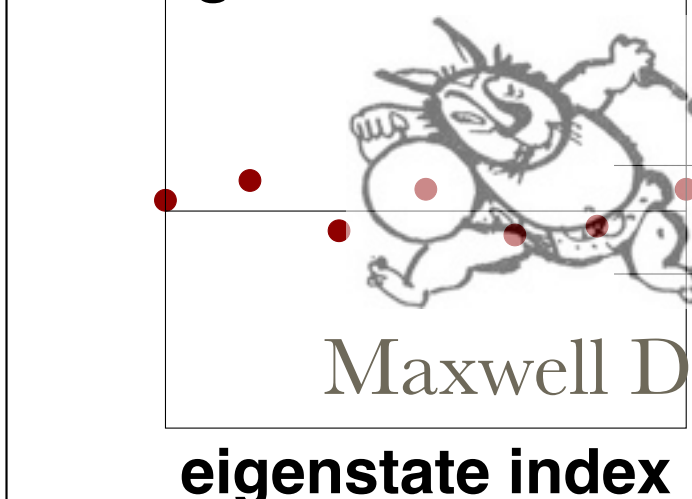
Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

quantum/thermal
fluctuations



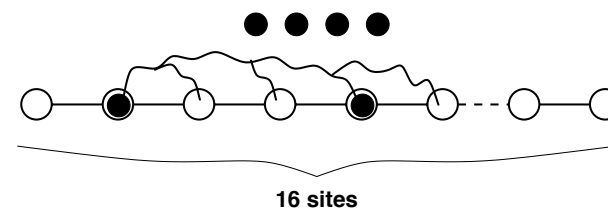
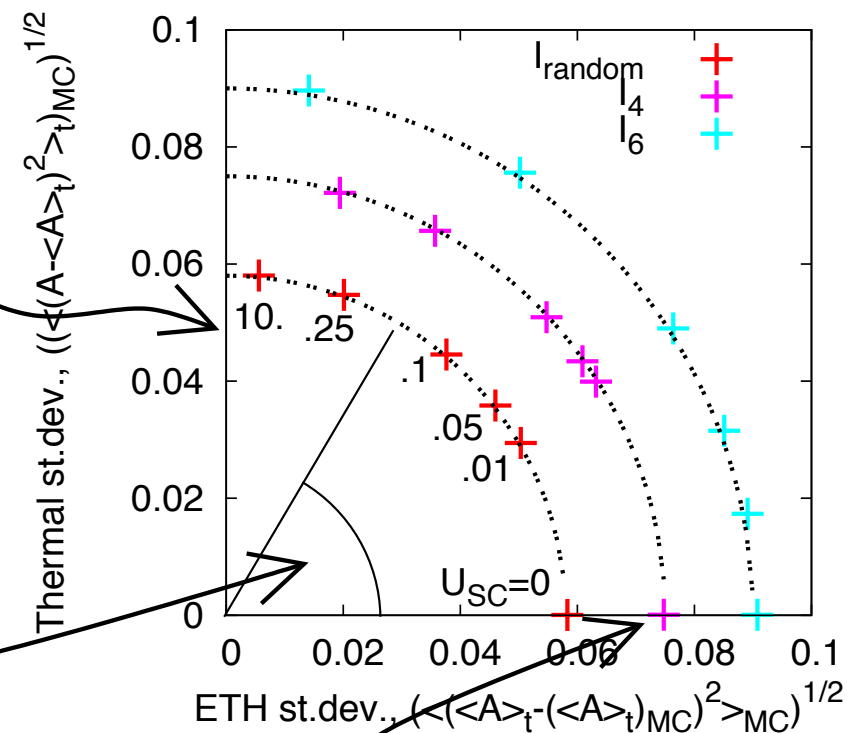
$\cos^{-1}(\sqrt{IPR})$

quantum
average

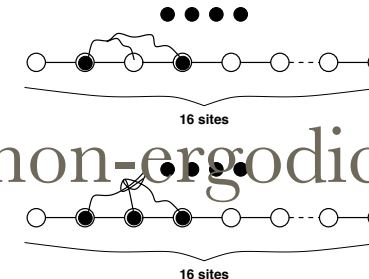


Maxwell Demon of non-ergodicity

ETH vs Thermal Variance | HardcoreBosons+SC_{R=4} N_{at}=4 L=16



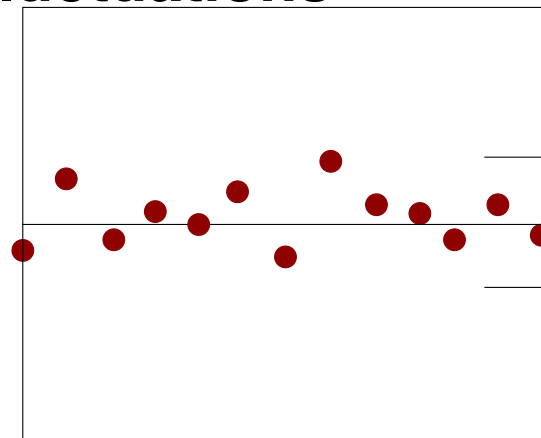
similar results:



HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

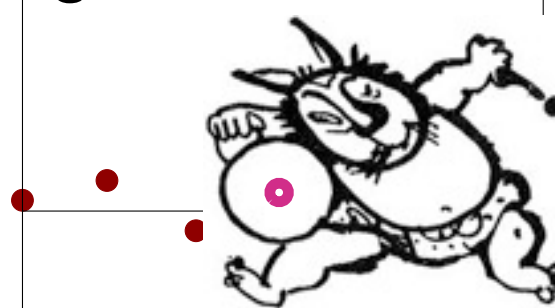
quantum/thermal
fluctuations



time

$\cos^{-1}(\sqrt{IPR})$

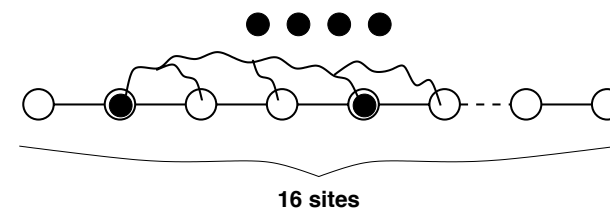
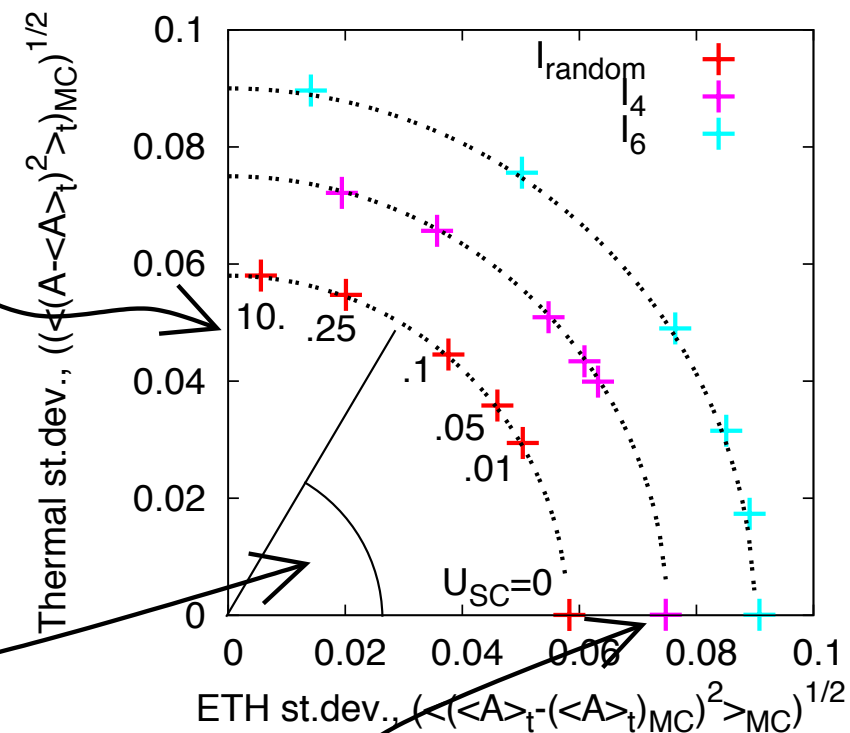
quantum
average



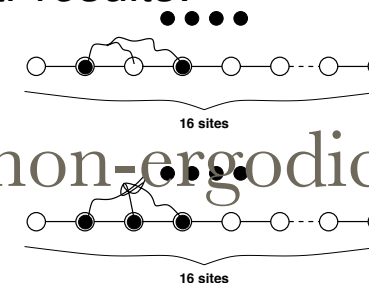
Maxwell Demon of non-ergodicity

eigenstate index

ETH vs Thermal Variance | HardcoreBosons+SC_{R=4} N_{at}=4 L=16



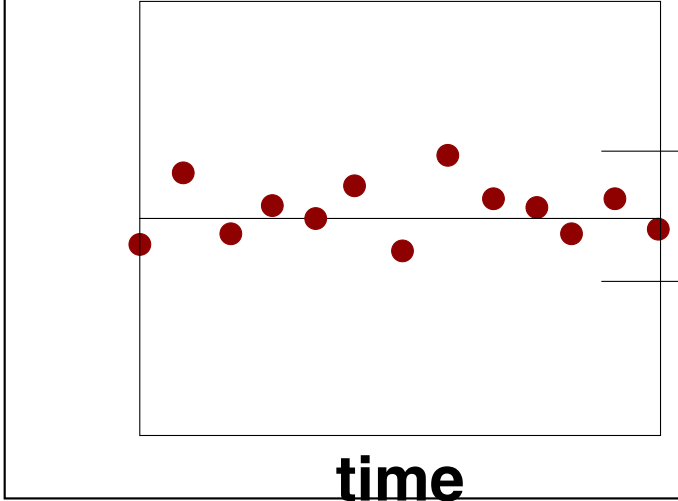
similar results:



HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

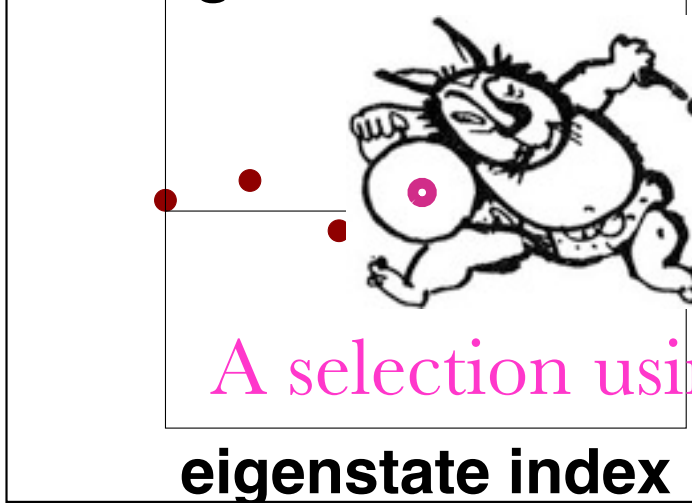
Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

quantum/thermal
fluctuations

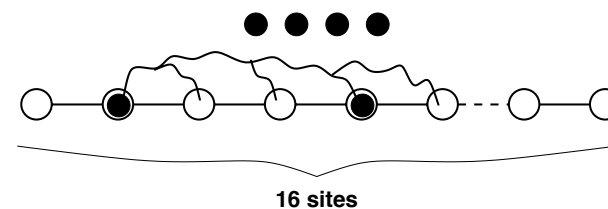
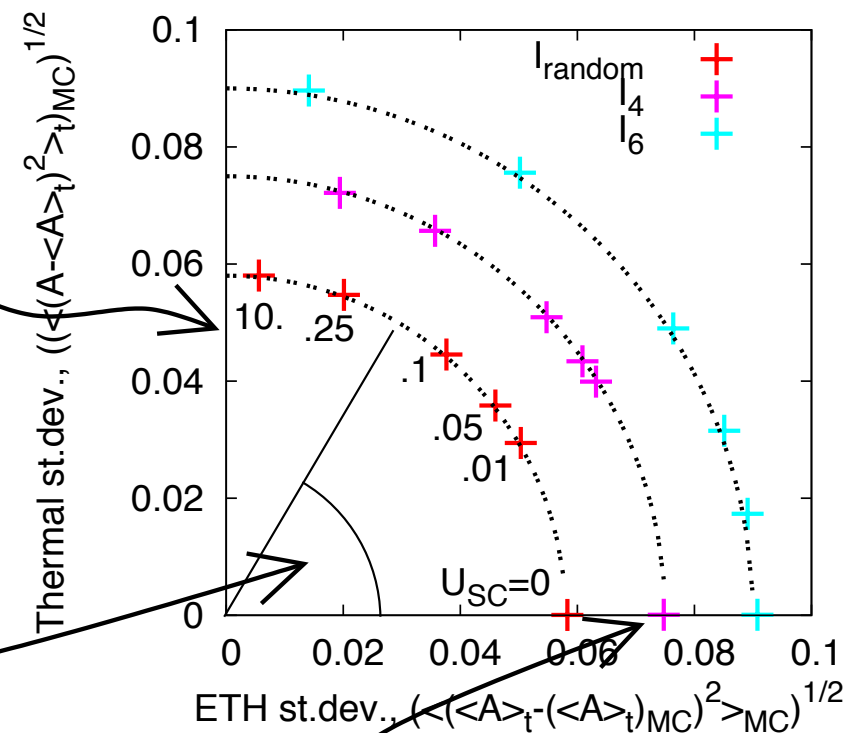


$\cos^{-1}(\sqrt{IPR})$

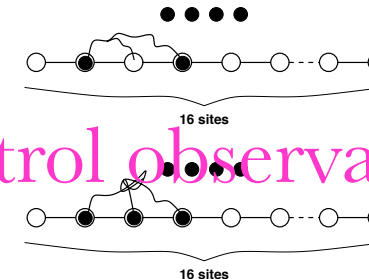
quantum
average



ETH vs Thermal Variance | HardcoreBosons+SC_{R=4} N_{at}=4 L=16



similar results:

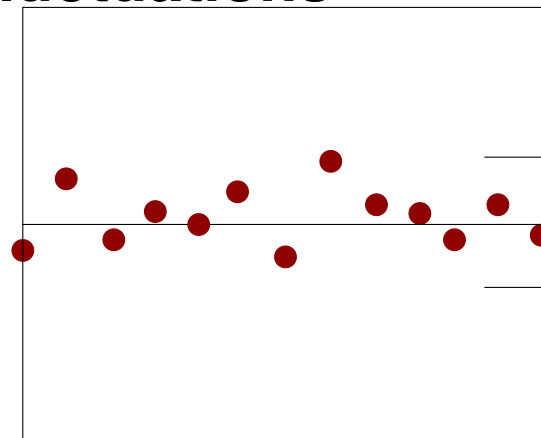


A selection using a “control observable”...

HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

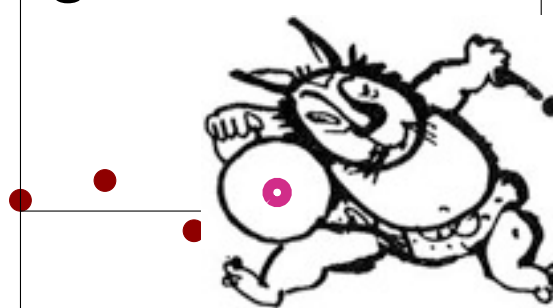
quantum/thermal
fluctuations



time

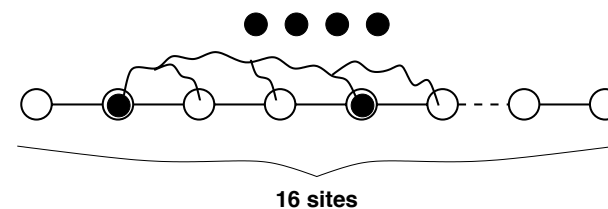
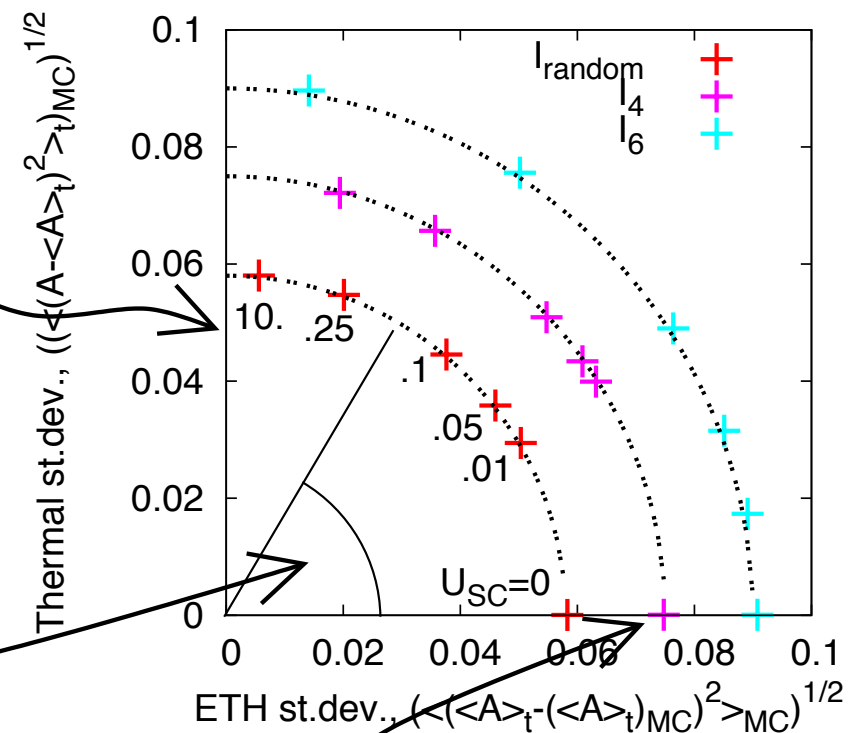
$\cos^{-1}(\sqrt{IPR})$

quantum
average

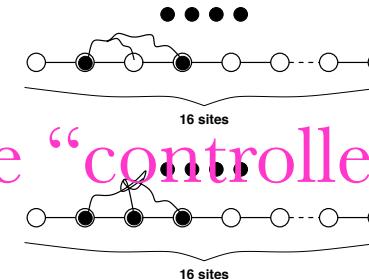


eigenstate index

ETH vs Thermal Variance | HardcoreBosons+SC_{R=4} N_{at}=4 L=16



similar results:

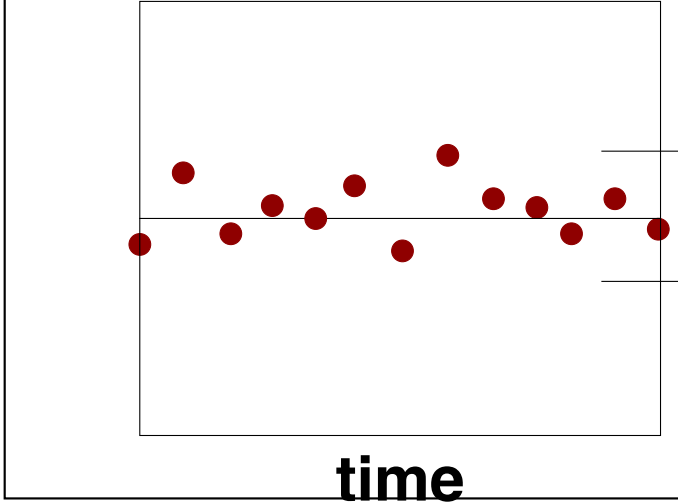


... maximally correlated with the “controlled observable”

HCB+NNNNN: $Var_{MC}[Mean_t[A]]$ vs. $Mean_{MC}[Var_t[A]]$

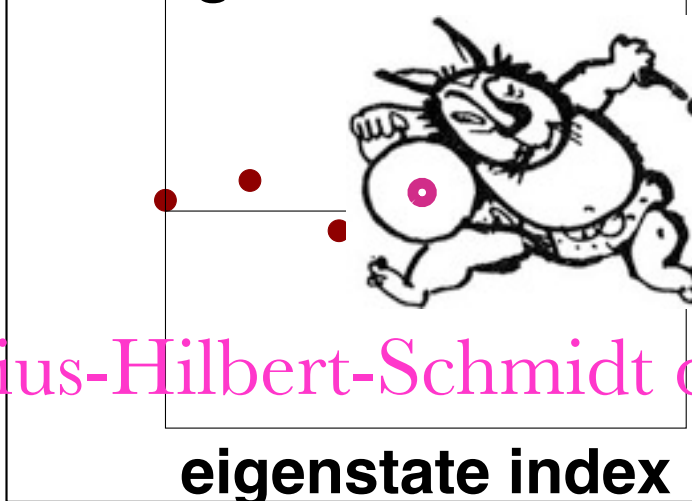
Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concussions

quantum/thermal
fluctuations

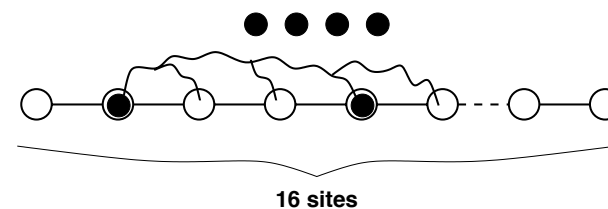
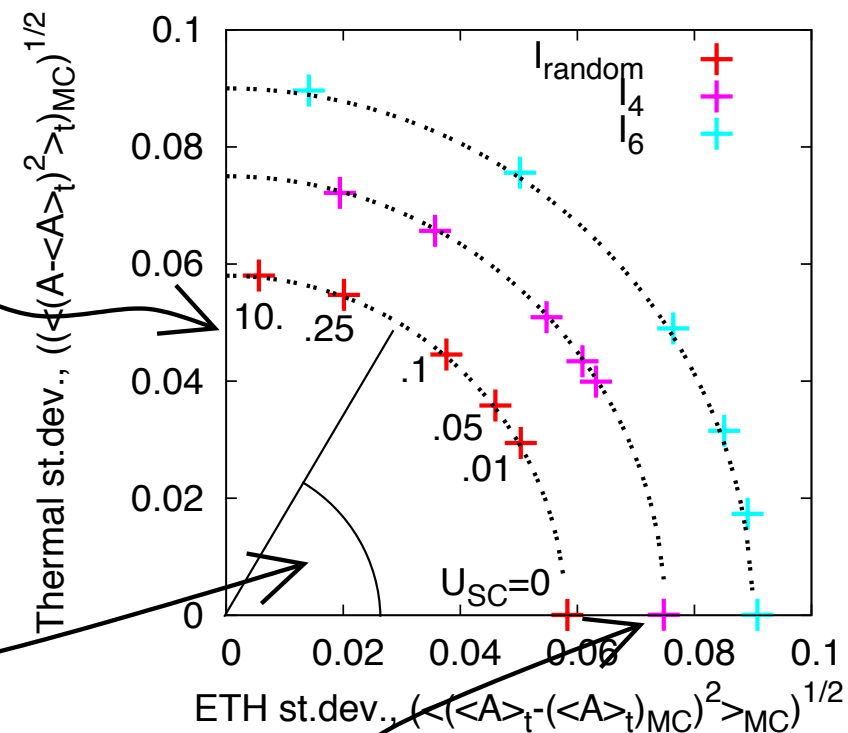


$\cos^{-1}(\sqrt{IPR})$

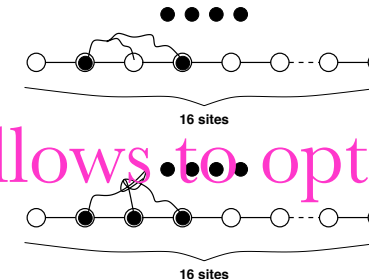
quantum
average



ETH vs Thermal Variance | HardcoreBosons+SC_{R=4} N_{at}=4 L=16



similar results:



Frobenius-Hilbert-Schmidt distance allows to optimize the “controls”

Summary

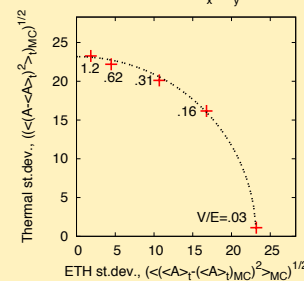
Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

In this presentation we

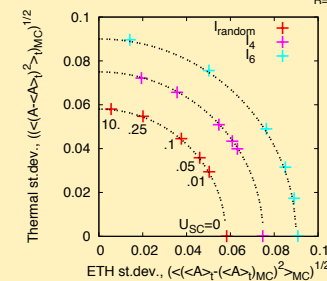
- suggested the following proposition:

The sum of the ensemble variance of the temporal means and the ensemble mean of the temporal variances remains approximately constant across the integrability-to-ergodicity transition

ETH vs Thermal Variance | $A = E_x - E_y$ | 2D Sinai PBC M3



ETH vs Thermal Variance | HardCoreBosons+SC $R=4$ $N_{at}=4$ $L=16$



- linked the proposition to the **Hilbert-Schmidt (HS) geometry of the observables**: $\text{ETH variance} = \cos^2(\text{HS angle between the observable and integrals of motion})$; $\text{IPR} = \cos^2(\text{HS angle between the original and perturbed integrals of motion})$;
- found a way to identify the **optimal integrals of motion for GGE**;
- found a way to treat the integrability and mesoscopicity under the same umbrella, with possible applications in nano-systems

CREDITS



Preview

Preview Sinai billiard Hard-Core Bosons Optimizing the GGE Concusions

We suggest

$$\tan^2[\Theta_A] \equiv \frac{\text{Var}_{MC}[\text{Mean}_t[A]]}{\text{Mean}_{MC}[\text{Var}_t[A]]}$$

as a measure of the position of an observable A on the (Integral of Motion)-(Thermalizable Observable) continuum.