Generalized Microcanonical Ensemble: From Quantum to Classical

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Dynamics of Isolated Quantum System

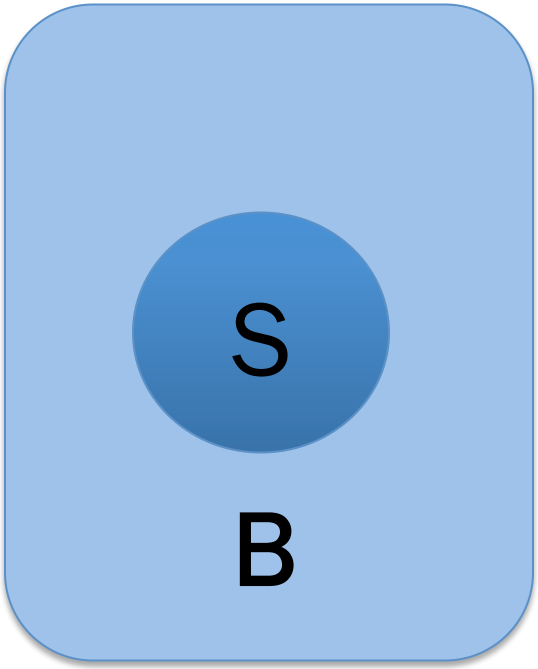
$$|\psi(0)\rangle = \sum_n c_n |n\rangle$$: Initial nonequilibrium state

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle = \sum_n c_n e^{-iE_n t}|n\rangle$$: State at time t

- As a whole, a state can never thermalize
  - Never approaches a stationary state

Thermalization of isolated system: Local thermalization

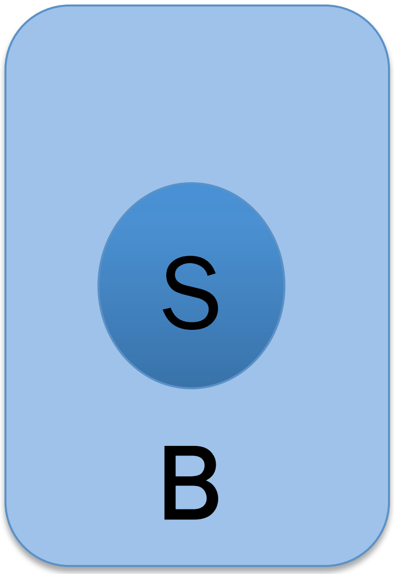
- What we observe: local system



- Universe : S (system) + B (bath)
- Look at $\langle \psi(t) | O_s | \psi(t) \rangle$
- When |S|>>1 & |B|>>|S|, (similar to von Neumann's macroscopic operator) O_S can reach stationary value for a long time

Ref: Linden, Popescu, Short, Winter, PRE 2009

Local Thermaliztion (formal)



$$\langle\psi(t)|O_S|\psi(t)\rangle = \mathrm{Tr}_S(O_S\rho_S(t))$$

$$\begin{aligned}\rho_S(t) &= \mathrm{Tr}_B(|\psi(t)\rangle\langle\psi(t)|) \\ &= \mathrm{Tr}_B(\sum_{n,m} e^{i(E_m-E_n)t} c_m^* c_n |n\rangle\langle m|) \\ &= \sum_n |c_n|^2 \mathrm{Tr}_B(|n\rangle\langle n|) \quad \text{for most t}\end{aligned}$$

$$\rho_S(\infty) \equiv \sum_n |c_n|^2 \mathrm{Tr}_B(|n\rangle\langle n|)$$: "Stationary State" ("Diagonal Ensemble")

Q: How to efficiently describe the stationary state?

Thermal Ensembles (ME & GE)

- Thermal ensemble: fixed by Energy conservation

$$\langle \psi(0)|H|\psi(0)\rangle = \langle \psi(t)|H|\psi(t)\rangle = E$$

- Microcanonical Ensemble (ME):

$$\rho_S(\infty) = \frac{1}{N}\mathrm{Tr}_B\Big(\sum_{|E_n - E|<\delta} |n\rangle\langle n|\Big)$$

Rigol, et. al., Nature '08
Popescu, et al, Nature phys. '06

- Gibbs Ensemble (GE):

$$\rho_S(\infty) = \frac{1}{Z}\mathrm{Tr}_B(e^{-\beta H}) \simeq \frac{1}{Z}e^{-\beta H_S}$$

Tasaki, PRL '96
Goldstein et. al, PRL '06

Common feature: Use only energy conservation

More conservation laws: Integrable systems

- Integrability:
  - # of "nontrivial" conservation laws $\propto$ L

$$\langle\psi(t)|H_1|\psi(t)\rangle = \mu_1$$
$$\langle\psi(t)|H_2|\psi(t)\rangle = \mu_2$$
$$\langle\psi(t)|H_3|\psi(t)\rangle = \mu_3$$
$$\cdots$$
$$\langle\psi(t)|H_L|\psi(t)\rangle = \mu_L$$

- More conserved quantities
- More constrained dynamics
- No reason to relax to a simple canonical form

Subsystem can still reach a stationary state (Linden et. al, PRE '09)

Extension of GE: Generalized Gibbs Ensemble (GGE)

- Natural extension of Gibbs ensemble with more conservation laws

$$\rho_{GGE} = \frac{1}{Z} e^{-\sum_i \lambda_i H_i}$$

λ_i : Lagrange multipliers : $\langle \psi(0) | H_i | \psi(0) \rangle = \mathrm{Tr}(\rho_{GGE} H_i)$

$$\rho_S(\infty) = \mathrm{Tr}_B(\rho_{GGE})$$

- Only in thermodynamic limit
- Short range interaction
- Known to be correct for free fermions

Refs: Rigol, PRL '07, Gurarie, J Stat Mech '13, Ilievski, et. al, arXiv:1507.02993

Extension of ME: Generalized Microcan. Ensemble (GME)

- In principle (Popescu, et. al, Nat. Phys. '06):

$$H_R : \text{Restricted Hilbert Space}$$

$$\rho_{GME} = \frac{1}{d_R}\mathbf{I}_R \quad (\mathbf{I}_R : \text{Identity on } H_R)$$

$$\rho_S(\infty) = \mathrm{Tr}_B(\rho_{GME})$$

- Natural Choice:

$$\rho_{GME} = \frac{1}{N}\sum_n |n\rangle\langle n| \qquad (|n\rangle : \text{Eigenstate of } H)$$

$$\sum_n : |\langle n|H_i|n\rangle - \mu_i| < \delta \text{ for all } i = 1, \ldots, L$$

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- Natural Choice:

$$\rho_{GME} = \frac{1}{\ } \sum |n\rangle\langle n| \qquad (|n\rangle : \text{Eigenstate of } H)$$

However, VERY hard to construct in practice...

$$\sum_n : |\langle n|H_i|n\rangle - \mu_i| < \delta \text{ for all } i = 1, \ldots, L$$

Outline

- Difficulties of construction of GME
  - Discrete spectra
  - Finite gap
  - Long-range interaction
- Proposal of GME: Gaussian GME
  - Properties
  - Case studies

Difficulties of GME construction: I. Discrete spectra

Free fermions:

- Natural conserved quantities: $\hat{n}_k$ (momentum occupation number)
- Each eigenstate: $\langle n|\hat{n}_k|n\rangle = 0 \text{ or } 1$
- Initial state: $\langle \psi(0)|\hat{n}_k|\psi(0)\rangle \in [0, 1]$

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- Possibility: no eigenstate matches all occupation numbers => which state to include in GME?

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- A construction of free fermions: Cassidy et. al, PRL ’11,
- Local Hamiltonian: Caux & Essler, PRL ’13

  - explicit construction of free fermions

Difficulties of GME construction: II. Finite gap

- Central Spin Model:

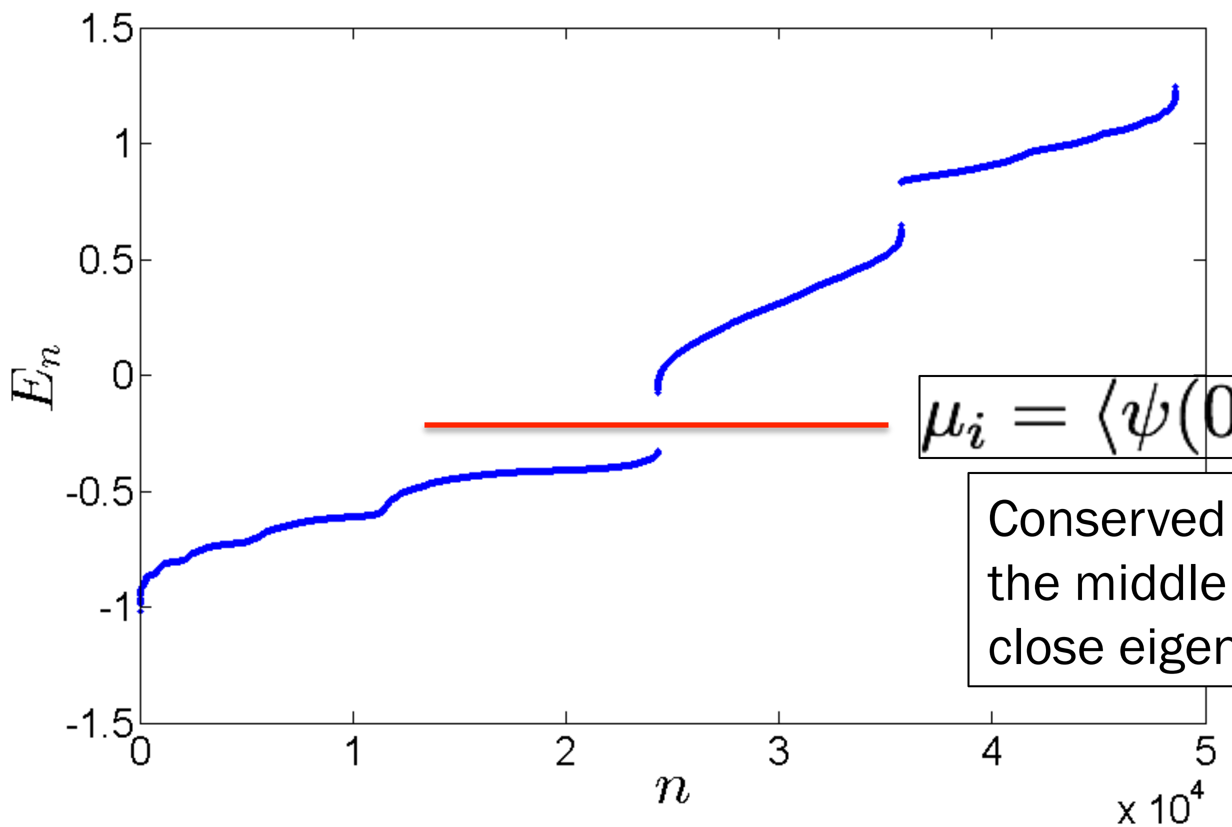
$$H_i = BS_i^z + \sum_{j \neq i}^{N} \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{\epsilon_i - \epsilon_j}$$

$$[H_i, H_j] = 0 \text{ for all } i = 1, 2, \ldots, N$$

  – Finite gap in the middle of spectrum
  – Long-range interaction
    - previous remedy is not applicable

Difficulties of GME construction: II. Finite gap

- Central Spin Model:



$$\mu_i = \langle \psi(0) | H_I | \psi(0) \rangle$$

Conserved quantity in the middle of gap: no close eigenstate

Begin from classical physics

- Classical integrable system: Yuzbashyan, arXiv:1509.06351

$$\rho_{GME}^{cl} = \frac{1}{V} \prod_{i=1}^{N} \delta(H_i(\mathbf{p}, \mathbf{q}) - \mu_i)$$

$$\lim_{T \to \infty} \int_0^T dt O(\mathbf{p}(t), \mathbf{q}(t)) = \int d\mathbf{p} d\mathbf{q} O(\mathbf{p}, \mathbf{q}) \rho_{GME}^{cl}$$

- Phase space average over invariant tori
- Valid for
  - Any deg. of freedom (thermodynamic limit NOT required)
  - Any interaction (long-range & short-range)

Quantize Classical GME

- From function to operator

$$\delta(H_i(\mathbf{p},\mathbf{q}) - \mu_i) \rightarrow \delta(\hat{H}_i - \mu_i)$$

  - Broaden delta functions
  - Need nontrivial way of broadening
  - Naïve equal-weight eigenstate broadening does not work

Proposal: Gaussian GME

$$\rho_{GME} = \frac{1}{Z} \exp\left[-\sum_{i,j} (H_i - \mu_i)(C^{-1})_{i,j}(H_j - \mu_j) \right]$$

$\mu_i, (C^{-1})_{i,j}$ fixed by

$$\langle \psi(0) | H_i | \psi(0) \rangle = \mathrm{Tr}(\rho_{GME} H_i)$$

$$\langle \psi(0) | H_i H_j | \psi(0) \rangle = \mathrm{Tr}(\rho_{GME} H_i H_j)$$

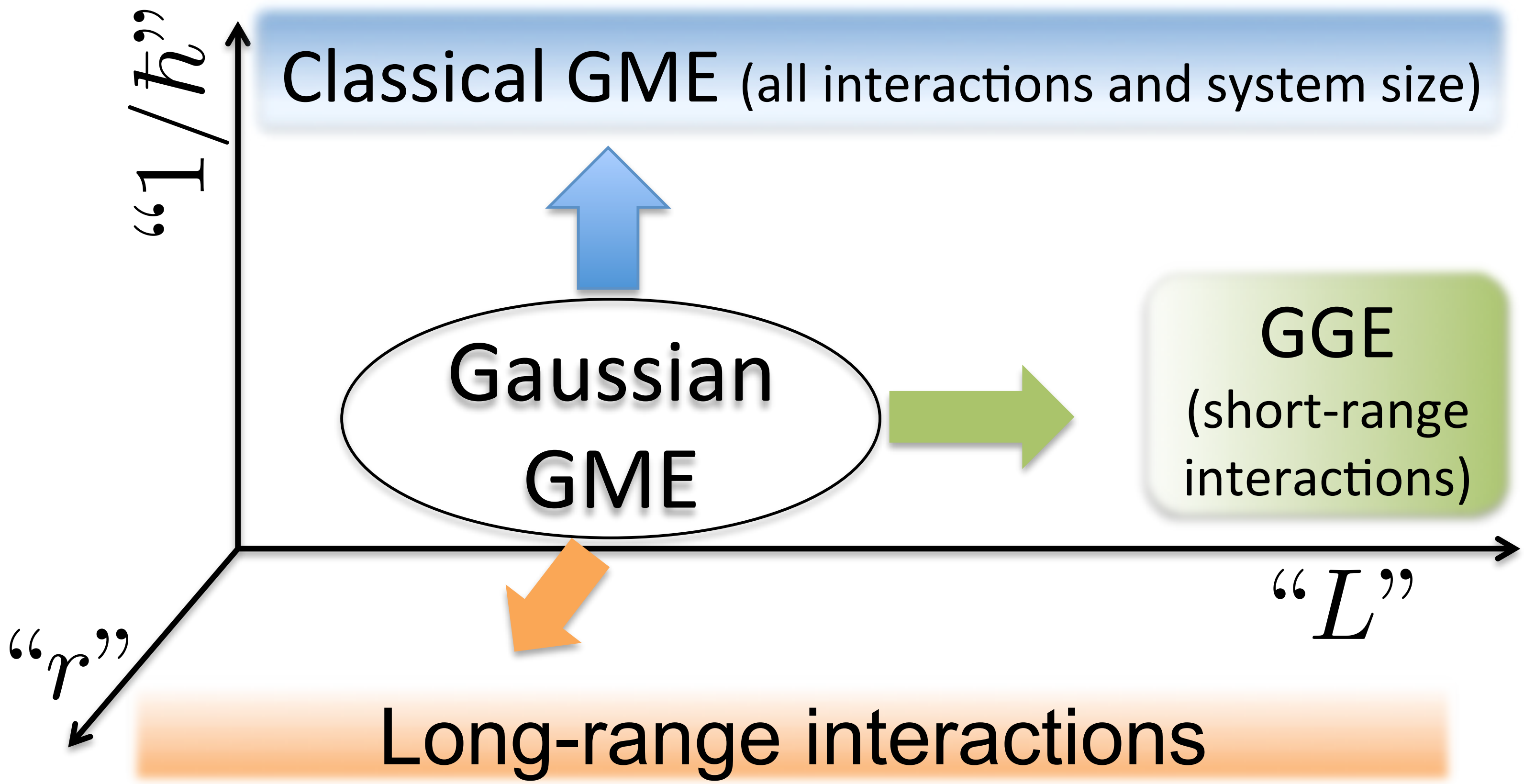
Construct in energy eigenstates but discard equal-weight ensemble

Properties of Gaussian GME

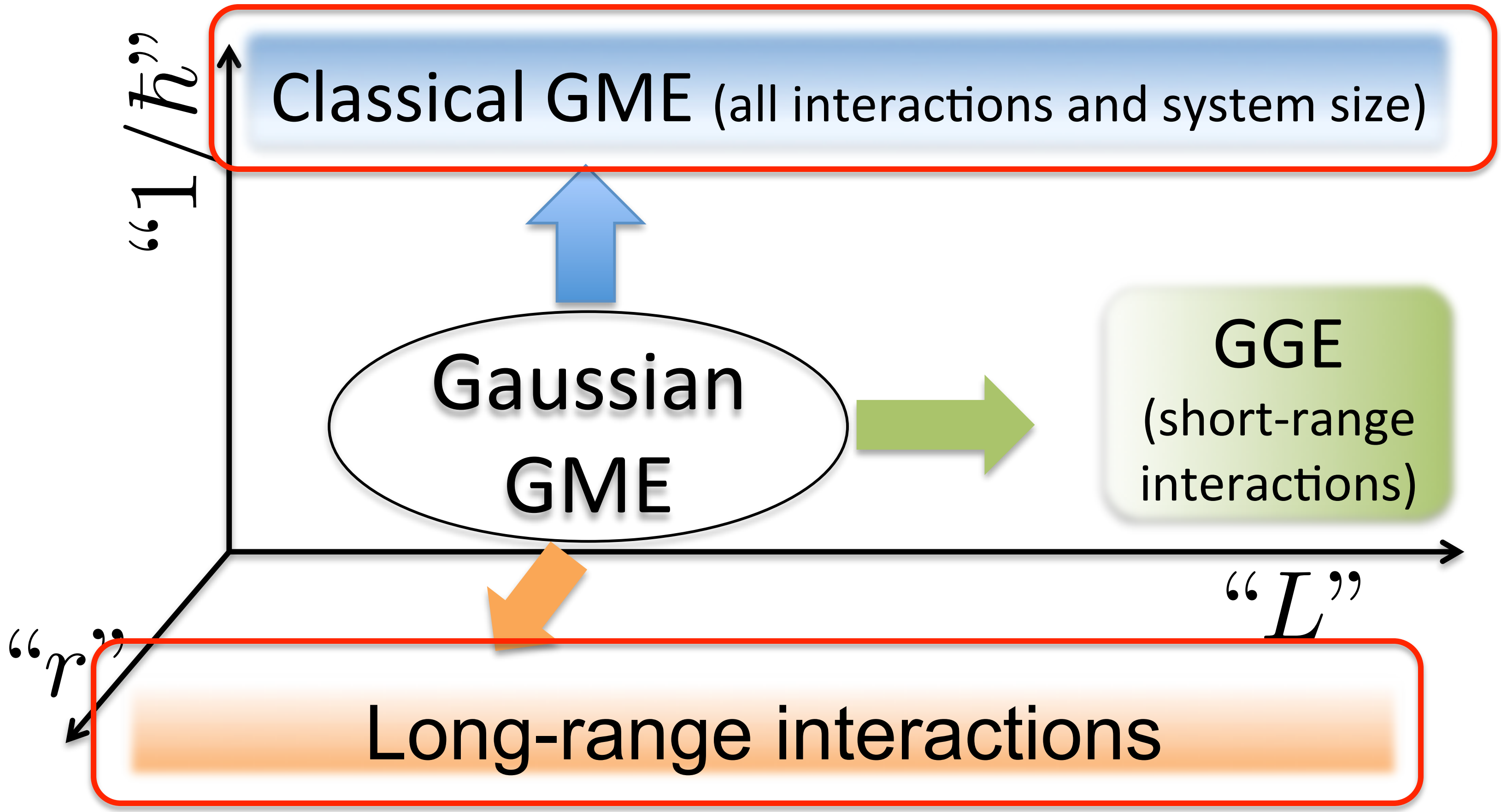
$$\rho_{GME} = \frac{1}{Z} \exp\left[-\sum_{i,j} (H_i - \mu_i)(C^{-1})_{i,j}(H_j - \mu_j) \right]$$

- More accurate than GGE (fixing second moments)
- Smooth connection to exact classical GME
  - Captures first quantum correction in classical limit
- Can be defined for any type of interaction & spectrum
- Operationally simple

Properties of Gaussian GME



Properties of Gaussian GME



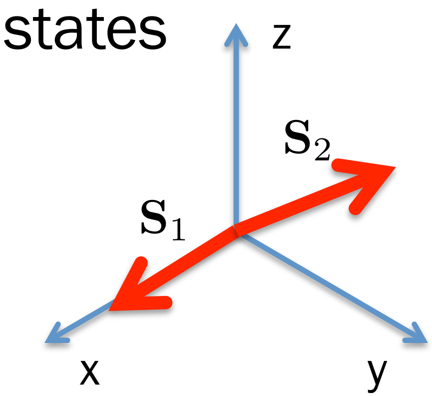
Application: Two Interacting Spins

Model:
$$H_1 = BS_1^z + \gamma \mathbf{S}_1 \cdot \mathbf{S}_2$$
$$H_2 = BS_1^z - \gamma \mathbf{S}_1 \cdot \mathbf{S}_2$$
$$[H_1, H_2] = 0$$

5 conservation laws in GME:
$$H_1, H_2, (H_1)^2, (H_2)^2, H_1 H_2$$

Initial state:
$$|\psi(0)\rangle = |\mathbf{S}_1\rangle \otimes |\mathbf{S}_2\rangle$$

Product of two spin coherent states
Minimal uncertainty state
Classical limit: $|\mathbf{S}| \to \infty$



Parameters: $\gamma = 1, B = |\mathbf{S}_2|$

Results of Two Interacting Spins

Observable: S_1^z

$$H_1 = BS_1^z + \gamma \mathbf{S}_1 \cdot \mathbf{S}_2$$
$$H_2 = BS_1^z - \gamma \mathbf{S}_1 \cdot \mathbf{S}_2$$

Two cases: $|\mathbf{S}_1| = |\mathbf{S}_2|$ Both spins become classical as $|\mathbf{S}_2|$ increases

$\text{Increase } |\mathbf{S}_2|$

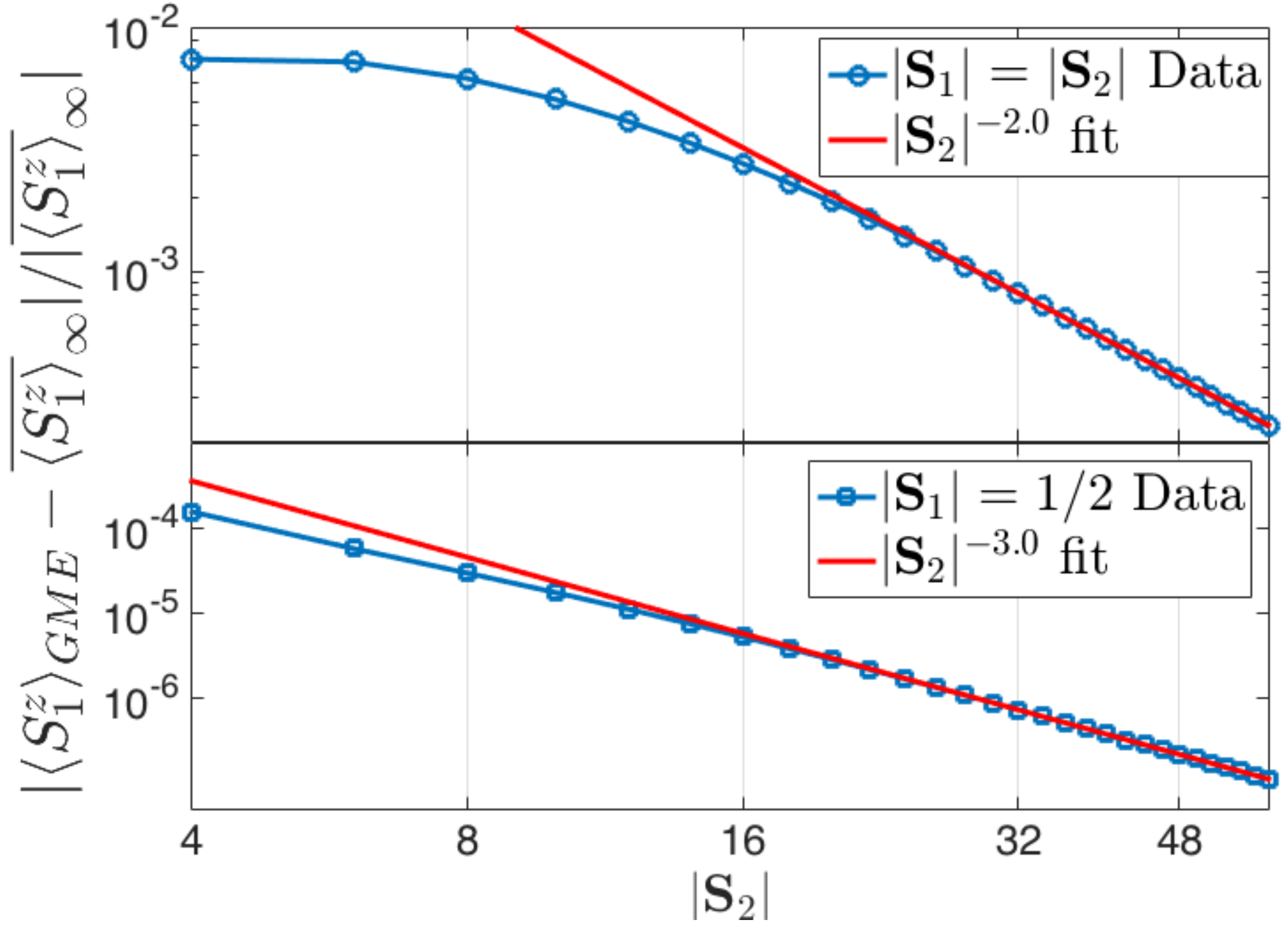
$$\langle S_1^z \rangle \sim S_1(a + b/S_1 + c/(S_1)^2 + \ldots)$$

$|\mathbf{S}_1| = 1/2$ Spin 1 remains quantum, Spin 2 becomes classical

$\text{Increase } |\mathbf{S}_2|$

Classical limit is not evident

Results of Two Interacting Spins



- GME results converge to classical results
- Captures leading quantum correction

Application: Central Spin Model

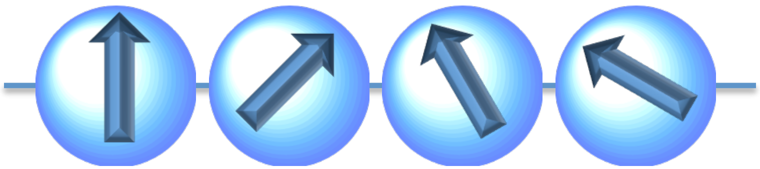
$$H_i = BS_i^z + \sum_{j \neq i}^{N} \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{\epsilon_i - \epsilon_j}$$

$$[H_i, H_j] = 0 \text{ for all } i = 1, 2, \ldots, N$$

- Model for electron spin decoherence due to nuclear spins
- Long-range interaction (GGE has not been applied)
- Energy is NOT extensive
- All spins are 1/2

Setup of Central Spin Model

Initial state: $|\psi(0)\rangle = \prod_{i=1}^{N} \otimes |\mathbf{S}_1\rangle$



Product of spins pointing random directions
(average over 100 random realizations)

Observable: S_1^z

Compare three ensembles

- Conventional equal weight GME
- Gaussian GME
- GGE

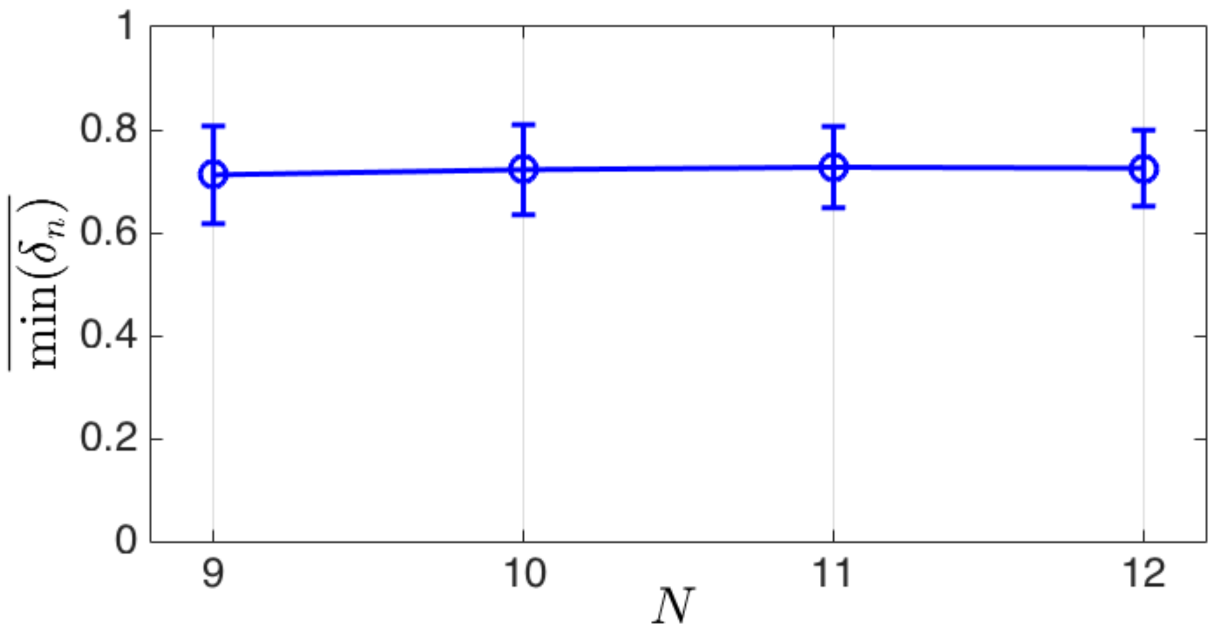
Equal Weight GME

GME criterion: Include eigenstate $|n\rangle$ of small δ_n

$$\delta_n = \frac{1}{N}\sum_{i=1}^{N} |h_i - \mu_i|$$

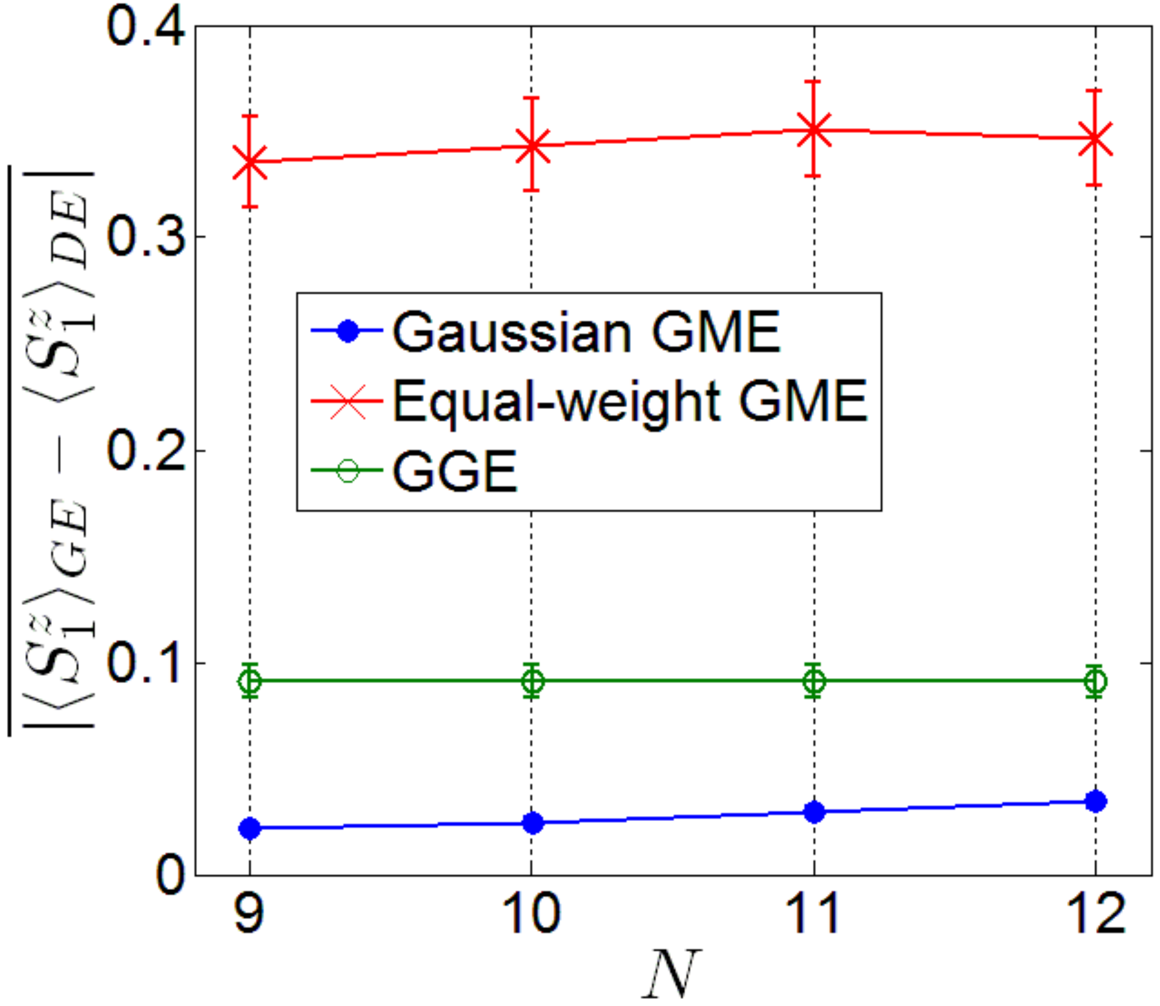
$$\langle n|H_i|n\rangle = h_i$$

$$\langle \psi(0)|H_i|\psi(0)\rangle = \mu_i$$



- No single eigenstate matches all conserved quantities

Expectation Value Comparison



- GME works better than the other two ensembles!

Summary & Outlook

- Practical Construction of Generalized Microcanonical Ensemble is hard
  - Discrete spectra
  - No eigenstate may match conserved quantities
- Gaussian GME
  - Guided by exact classical GME
  - Works well for a few case studies
- More detailed comparison with GGE
- Complete connection to classical GME for many-body system

Collaborations:

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Rutgers University

Anatoli Polkovnikov,
Boston University

Feeds me