

# Generalized Microcanonical Ensemble for Quantum Integrable Dynamics

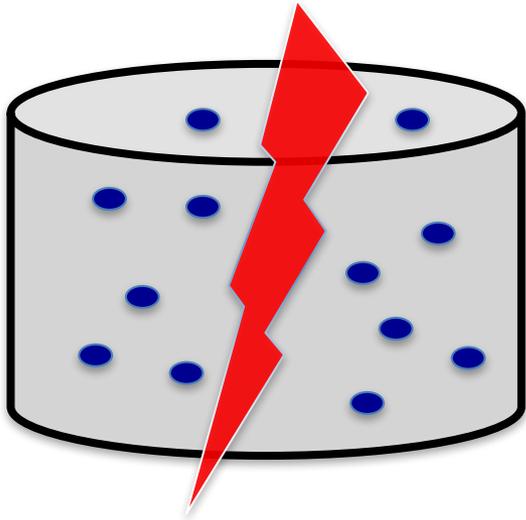
Emil Yuzbashyan



Dynamics and Hydrodynamics of Certain Quantum Matter  
*March 20, 2017 – March 23, 2017*

# Quantum Quench

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$$



1. Many-body system initially in equilibrium
2. **Strong** perturbation pulse drives the system far from equilibrium. *Easy*
3. But **not too strong**. No dissipation, unwanted interactions. The system evolves **coherently** with desired Hamiltonian for long time. *very difficult*

**Coherent** Many-Body Dynamics:

$$i \frac{\partial |\psi\rangle}{\partial t} = \left( \hat{H}_0 + \hat{H}_{\text{int}} \right) |\psi\rangle$$

# Quantum Quench: Coherent Many-Body Dynamics

**Q:** What happens to the system in time? Where does it end up as a result of unitary evolution? Does it equilibrate?

$$|\psi(t \rightarrow \infty)\rangle =? \quad \langle \hat{O}(t \rightarrow \infty) \rangle =?$$

**A:** Depends on the system (on  $H$ ) and on the initial condition

a. Equilibration (thermalization) with some effective  $T$

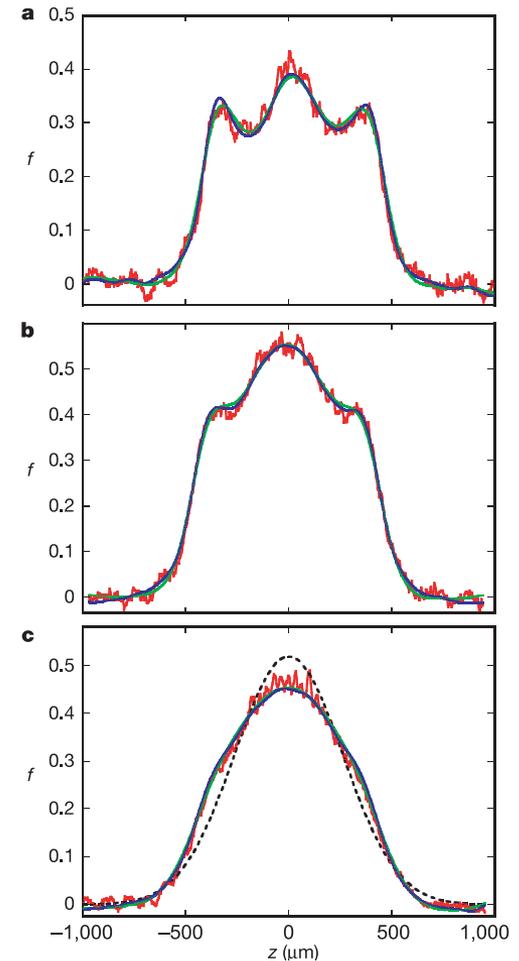
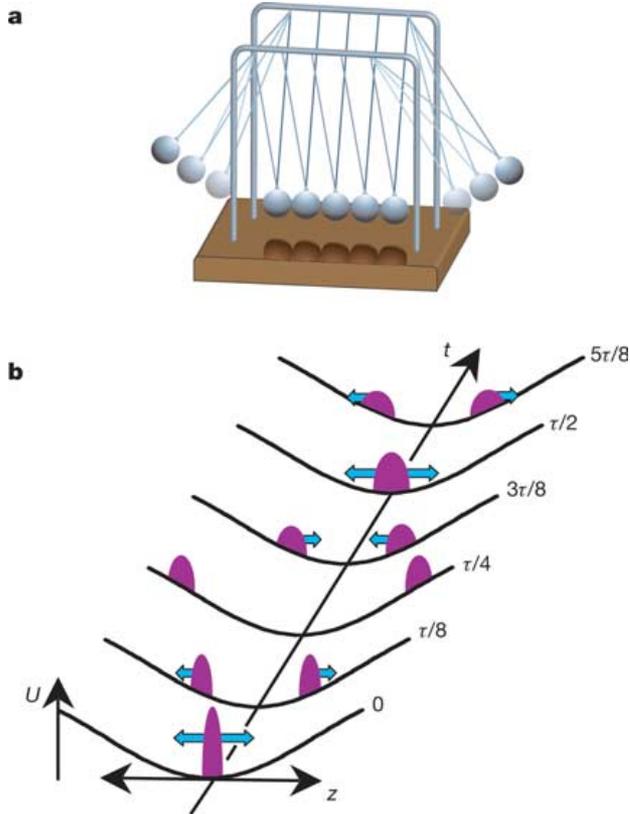
$$\langle \hat{O}(t \rightarrow \infty) \rangle = \text{Tr} \hat{O} e^{-\hat{H}/T_{\text{eff}}}$$

b. *No thermalization - asymptotic state - nonequilibrium "phase" with new properties*

$$\langle \hat{O}(t \rightarrow \infty) \rangle =?$$

# A quantum Newton's cradle

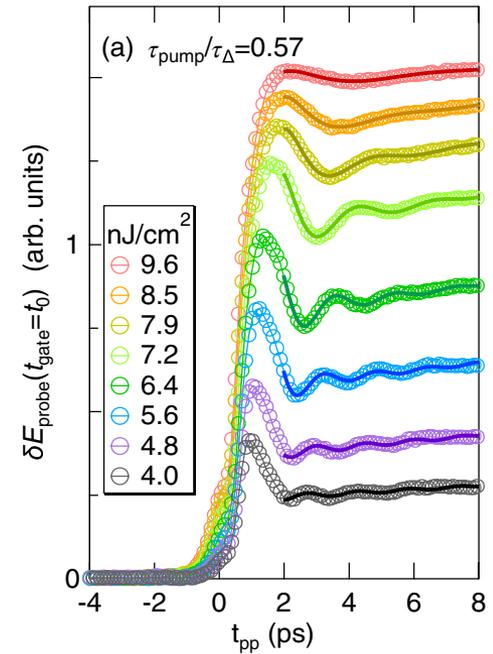
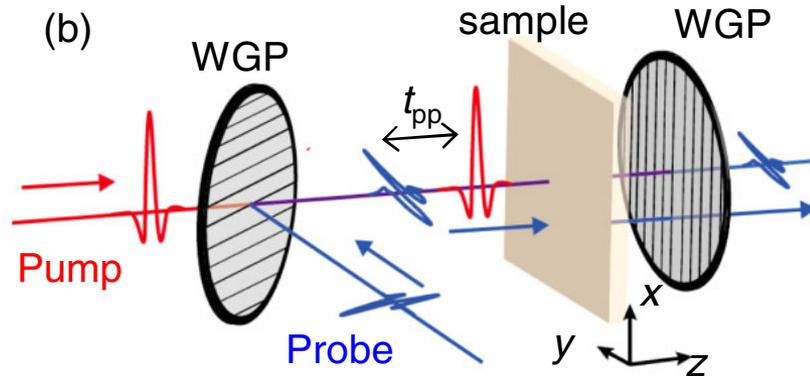
T. Kinoshita, T. Wenger, D. Weiss Nature (2006)



“<sup>87</sup>Rb atoms ... do not noticeably equilibrate even after thousands of collisions. Our results are probably explainable by the well-known fact that a homogeneous 1D Bose gas with point-like collisional interactions is *integrable*.”

## Higgs Amplitude Mode in the BCS Superconductors $\text{Nb}_{1-x}\text{Ti}_x\text{N}$ Induced by Terahertz Pulse Excitation

Ryusuke Matsunaga,<sup>1</sup> Yuki I. Hamada,<sup>1</sup> Kazumasa Makise,<sup>2</sup> Yoshinori Uzawa,<sup>3</sup>  
Hiroataka Terai,<sup>2</sup> Zhen Wang,<sup>2</sup> and Ryo Shimano<sup>1</sup>



$|\psi(0)\rangle = |\text{noneq. state produced by the pulse}\rangle$

$$\hat{H}_{\text{BCS}} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} - g \sum_{\mathbf{k}, \mathbf{p}} \hat{c}_{\mathbf{k}\uparrow}^{\dagger} \hat{c}_{-\mathbf{k}\downarrow}^{\dagger} \hat{c}_{-\mathbf{p}\downarrow} \hat{c}_{\mathbf{p}\uparrow}$$

$$i \frac{d|\psi\rangle}{dt} = \hat{H}_{\text{BCS}} |\psi\rangle$$

Higgs mode  
(order parameter)

$$\Delta(t) = g \sum_{\mathbf{p}} \langle \hat{c}_{-\mathbf{p}\downarrow} \hat{c}_{\mathbf{p}\uparrow} \rangle$$

# Long time dynamics of a BCS superconductor in response to a sudden perturbation (quantum quench)

$$\hat{H}_{\text{BCS}} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} - g \sum_{\mathbf{k}, \mathbf{p}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \hat{c}_{-\mathbf{p}\downarrow} \hat{c}_{\mathbf{p}\uparrow}$$

$$i \frac{d|\psi\rangle}{dt} = \hat{H}_{\text{BCS}} |\psi\rangle$$

Higgs mode  
(order parameter)  $\Delta(t) = g \sum_{\mathbf{p}} \langle \hat{c}_{-\mathbf{p}\downarrow} \hat{c}_{\mathbf{p}\uparrow} \rangle$

**Q:**  $|\psi(t \rightarrow \infty)\rangle = ? \quad \Delta(t \rightarrow \infty) = ?$

**A:** For moderate perturbation strength:  $|\Delta(t)| = \Delta_\infty + a \frac{\cos(2\Delta_\infty t + \alpha)}{\sqrt{\Delta_\infty t}}$

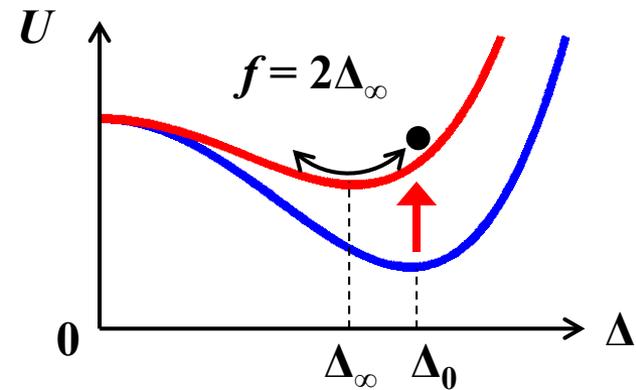
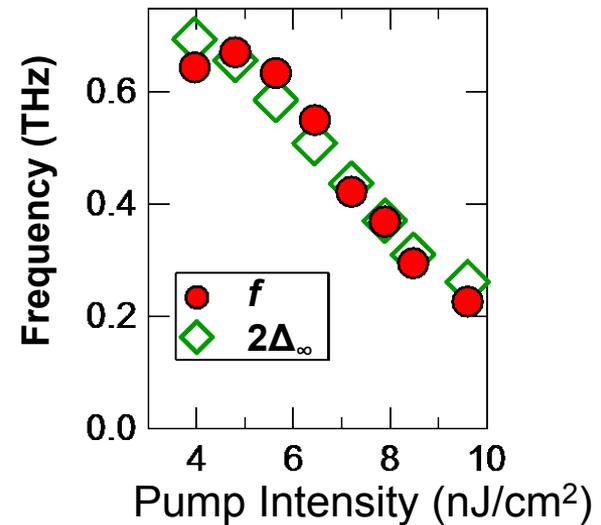
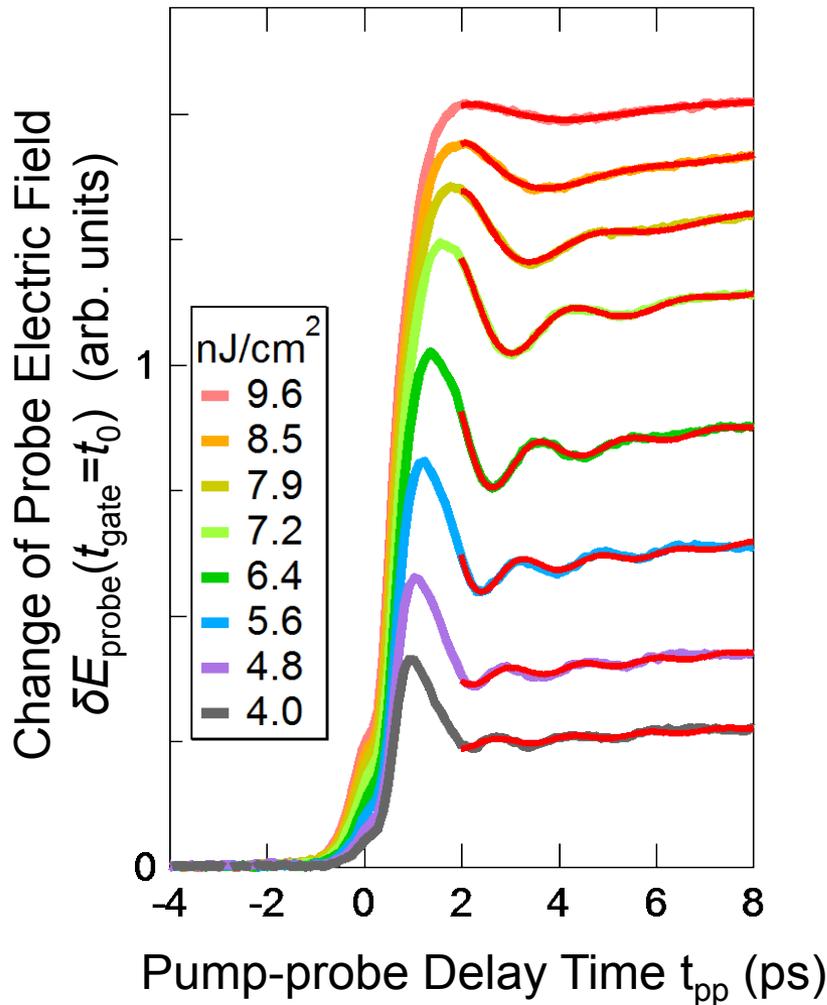
Yuzbashyan, Tsypliyev, Altshuler, PRL (2006)

For stronger perturbations  $|\Delta(t)|$  either vanishes or oscillates persistently at large times. In all cases the superconductor does NOT thermalize.

# Order parameter dynamics

$$\delta\Delta(t_{pp}) = C_1 + C_2 t_{pp} + \frac{a}{(t_{pp})^b} \cos(2\pi f t_{pp} + \phi)$$

E. Yuzbashyan et al.,  
PRL **96**, 230404 (2006).



R. Matsunaga et al., PRL**111**, 057002 (2013)

# Long time dynamics of a BCS superconductor in response to a sudden perturbation (quantum quench)

$$H_{\text{BCS}} = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} s_{\mathbf{k}}^z - g \sum_{\mathbf{k}, \mathbf{p}} s_{\mathbf{k}}^+ s_{\mathbf{p}}^-$$

$$i \frac{d|\psi\rangle}{dt} = \hat{H}_{\text{BCS}} |\psi\rangle$$

Higgs mode  
(order parameter)  $\Delta(t) = g \sum_{\mathbf{p}} \langle s_{\mathbf{p}}^-(t) \rangle$

$H_{\text{BCS}}$  is integrable, Richardson (1964), Gaudin (1983)

Integrals of motion for  $H_{\text{BCS}}$  – Gaudin magnets/ central spin models

$$H_{\mathbf{k}} = \sum_{\mathbf{p}} \frac{\vec{s}_{\mathbf{k}} \cdot \vec{s}_{\mathbf{p}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} - \frac{s_{\mathbf{k}}^z}{g}, \quad [H_{\mathbf{k}}, H_{\mathbf{p}}] = 0, \quad H_{\text{BCS}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} H_{\mathbf{k}} \quad \Rightarrow \quad [H_{\text{BCS}}, H_{\mathbf{k}}] = 0$$

# of integrals = # of pseudospins = # of pairs of states ( $\mathbf{k} \uparrow, -\mathbf{k} \downarrow$ )

# Integrable systems do NOT thermalize

Do they follow Generalized Gibbs Ensemble (GGE)?

$$[H, H_i] = 0, \quad [H_i, H_j] = 0 \quad \rho = C \exp\left(-\sum_i \beta_i H_i\right) \quad \beta_i \text{ are determined from:}$$
$$\langle \psi(0) | H_i | \psi(0) \rangle = \text{Tr } \rho H_i$$

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle O(t) \rangle dt = \text{Tr } \rho O$$

*When does it work?*

Not for finite size, long range interactions or global observables

For local interactions & observables and thermodynamic limit – sometimes **YES**, sometimes **NO** – depends on the set of available integrals (and also on  $H$  and the initial state)

- GGE fails for 1D Heisenberg spin chains  
Goldstein & Andrei, Phys. Rev. A (2014); Pozsgay et. al. PRL (2014)
- Does work for 1D Heisenberg spin chains if newly discovered integrals are added  
Ilievski et. al. PRL (2015)

# Integrable systems do NOT thermalize

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$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle O(t) \rangle dt = \text{Tr } \rho O$$

*When does it work?*

How do we determine if we have the “right” set of integrals and the criteria for the validity of GGE?

**Problem:** quantum integrability is NOT well-defined!

See e.g. Sutherland, *Beautiful Models* (2004), Caux & Mossel (2011), Yuzbashyan & Shastry (2013)

No natural notion of a **nontrivial** integral of motion, let alone of a complete set

For example, for any set of  $H_k$  such that  $[H, H_k]=0$ , can find  $H_0$  so that:

$$H_k = \sum_n a_{kn} H_0^n$$

i.e. always only one functionally independent integral –  $H$  itself

# Integrable systems do NOT thermalize

Do they follow **Generalized Gibbs Ensemble (GGE)**?

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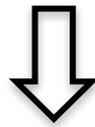
Without an independent notion of a complete set of nontrivial integrals of motion GGE is **essentially unfalsifiable** in Quantum Mechanics

## Classical Integrability is well-defined

$H(p, q)$ , where  $q = (q_1, \dots, q_n)$ ;  $p = (p_1, \dots, p_n)$ ; i.e.  $n$  degrees of freedom

**Definition:**  $H(p, q)$  is integrable if it has  $n$  (maximum possible number) of functionally independent Poisson-commuting integrals

$$\{H_i(p, q), H_j(p, q)\} = 0, \quad i, j = 0, \dots, n - 1; \quad H_0(p, q) \equiv H(p, q)$$



- ✓ *Unambiguous separation between integrable and not integrable*
- ✓ *Clear notion of a complete set of integrals to construct GGE*

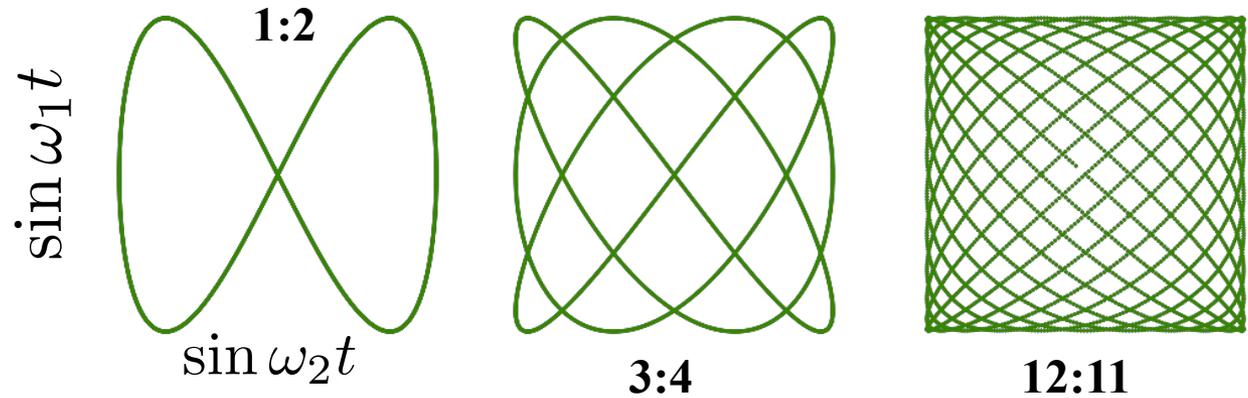
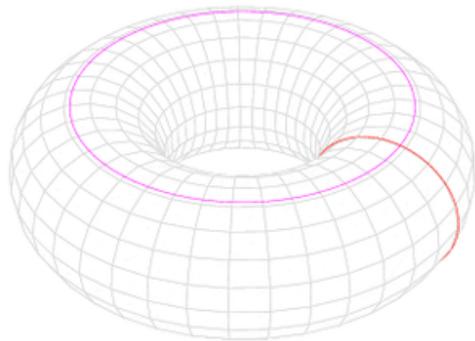
Do Classical Mechanics before going Quantum?!

# Generalized Gibbs Ensemble DeMystified in Classical Mechanics

Dynamics is on “invariant torus” –  $n$ -dim portion of  $2n$ -dim phase-space cut out by integrals of motion  $H_1(p,q)=\text{const}, H_2(p,q)=\text{const}, \dots, H_n(p,q)=\text{const}$

There are  $n$  typically incommensurate frequencies  $\omega_1, \omega_2, \dots, \omega_n$  (non-resonant torus)

Lissajous figures



**Theorem about averages** (Arnold, *Math. Methods of CM*):

For a non-resonant torus and any “reasonable” observable  $O(p,q)$   
*time average = phase-space average over the torus*

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T O(t) dt = \int O(\varphi) \frac{d\varphi}{(2\pi)^n}$$

# Generalized Gibbs Ensemble DeMystified in Classical Mechanics

**Theorem about averages** (Arnold, *Math. Methods of CM*):

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Going back to the original variables  $p$  &  $q$  and using the fact that this is a canonical transform can prove **Generalized Microcanonical Ensemble (GME)**

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T O(t) dt = \int O(p, q) \rho(p, q) dp dq$$

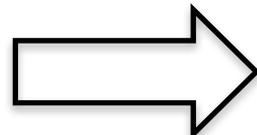
E.Y., Ann. Phys. (2016)

$$\rho(p, q) = V^{-1} \prod_{k=1}^n \delta(H_k(p, q) - \alpha_k)$$

Works for any system size (any  $n$ )  
Exceptions: resonant tori

Additive integrals,  
thermodynamic limit

$$H_k \propto n$$
$$n \rightarrow \infty$$



See e.g. Ruelle, Stat. Mech.:  
Rigorous Results (1999)

**Generalized (canonical) Gibbs**

$$\rho(p, q) = C \exp \left[ - \sum_k \beta_k H_k(p, q) \right]$$

**Not always the case**

# Going Quantum

$$\rho(p, q) = V^{-1} \prod_{k=1}^n \delta(H_k(p, q) - \alpha_k)$$

Note: microcanonical ensemble doesn't work for finite  $n$

Works for any system size (any  $n$ )

non-integrable CM  $\neq V^{-1} \delta(H(p, q) - E)$

**Q:** What is Generalized Microcanonical Ensemble (GME) in the quantum case, i.e. a quantum analog of  $\rho(p, q)$ ?

Consider a system where we can gradually go from quantum to classical while maintaining integrability (e.g. Gaudin magnets)

- ✓ Is GME similarly exact in the quantum case for a finite system? If not, how does it improve as  $\hbar \rightarrow 0$ ?
- ✓ How does GME compare to GGE?

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$$H_k(p, q) \rightarrow \hat{H}_k \text{ works for GGE, } \exp\left[-\sum_k \beta_k H_k(p, q)\right] \rightarrow \exp\left[-\sum_k \beta_k \hat{H}_k\right]$$

Doesn't work for GME because  $\langle \hat{H}_i \hat{H}_k \rangle \neq \langle \hat{H}_i \rangle \langle \hat{H}_k \rangle$

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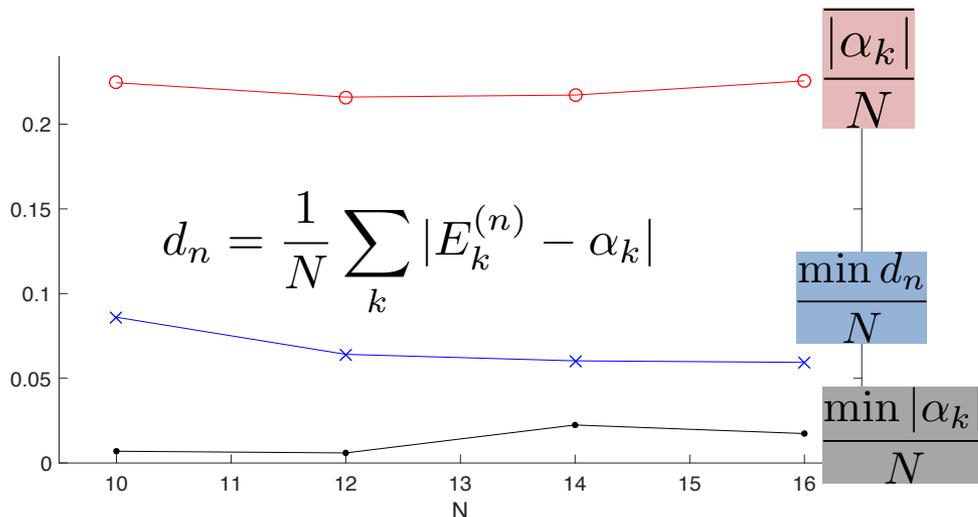
Need to broaden  $\delta$ -functions.

$$\alpha_k = \langle \hat{H}_k \rangle, \quad \hat{H}_k |\psi_n\rangle = E_k^{(n)} |\psi_n\rangle,$$

“Windows”, i.e. equal weight GME?

$$\mathcal{S} : |E_k^{(n)} - \alpha_k| < \delta_k, \quad \langle \hat{O} \rangle = \sum_{n \in \mathcal{S}} \langle \psi_n | \hat{O} | \psi_n \rangle$$

Doesn't work well for many integrals!



$$H_{\text{BCS}} = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} s_{\mathbf{k}}^z - g \sum_{\mathbf{k}, \mathbf{p}} s_{\mathbf{k}}^+ s_{\mathbf{p}}^-$$

$\alpha_k$  for quench  $g_i = 0.5\delta \rightarrow g_f = 2\delta$

$$H_{\mathbf{k}} = \sum_{\mathbf{p}} \frac{\vec{s}_{\mathbf{k}} \cdot \vec{s}_{\mathbf{p}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} - \frac{s_{\mathbf{k}}^z}{g}$$

NO states sufficiently close to all  $\alpha_k$

# Going Quantum

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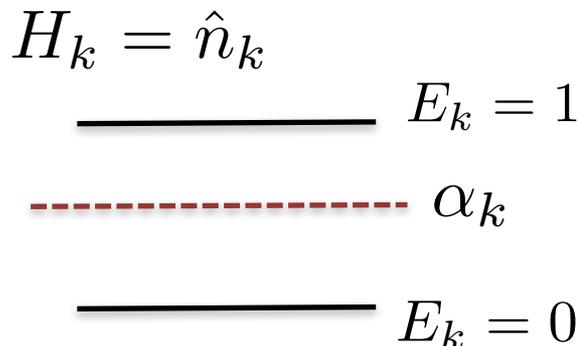
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Doesn't work well for many integrals!

Or suppose integrals take discrete values, e.g. fermion occupation #s



Unlike GGE or Classical Mechanics, NO viable generalization of the microcanonical ensemble for a quantum integrable system!

Forget about comparing it to GGE

See also Cassidy et. al. PRL (2011)

# Going Quantum

$$\rho(p, q) = V^{-1} \prod_{k=1}^n \delta(H_k(p, q) - \alpha_k)$$

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Functional broadening, e.g. Gaussian?

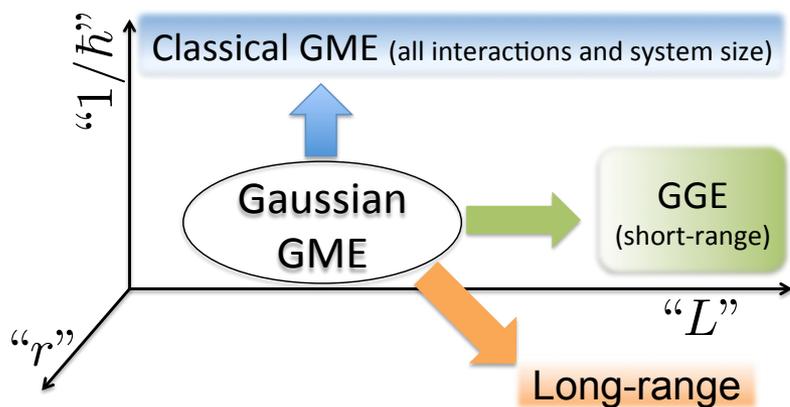
$$\hat{\rho} = C \exp \left[ - \sum_{ik} (\hat{H}_i - \mu_i) M_{ik} (\hat{H}_k - \mu_k) \right]$$

Classical limit:

$$\langle \hat{H}_i \hat{H}_k \rangle \rightarrow \langle \hat{H}_i \rangle \langle \hat{H}_k \rangle \implies \hat{\rho} \rightarrow \rho(p, q)$$

$\mu_i, M_{ik}$  are determined from:  
 $\langle \hat{H}_i \rangle_0 = \text{Tr}(\hat{\rho} \hat{H}_i)$  and  $\langle \hat{H}_i \hat{H}_k \rangle_0 = \text{Tr}(\hat{\rho} \hat{H}_i \hat{H}_k)$

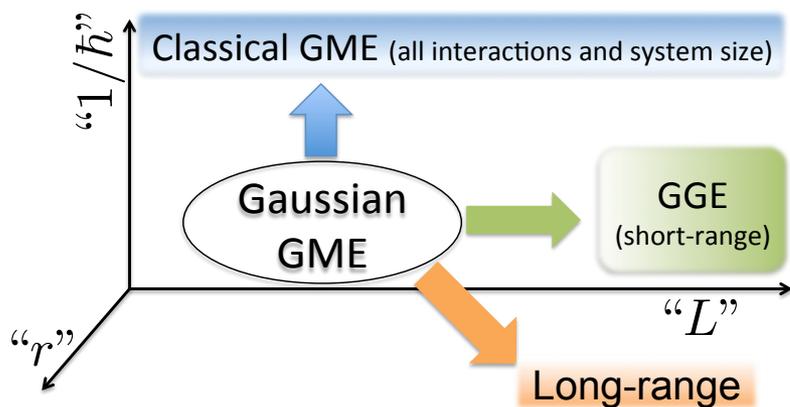
Quantum Generalized Microcanonical Ensemble =  
Gaussian GME



$$\hat{\rho} = C \exp \left[ - \sum_{ik} (\hat{H}_i - \mu_i) M_{ik} (\hat{H}_k - \mu_k) \right]$$

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1. Well defined and straightforward to implement for any system/size
2. Guaranteed exact in classical limit,  $\hbar \rightarrow 0$  (any system size)
3. Captures leading quantum correction ( $\propto \hbar$ ) (any system size)
4. Works whenever GGE does and converges faster ( $1/L^2$ ) than GGE ( $1/L$ ) with system size,  $L$ , i.e. captures leading finite size correction
5. Works well for systems with long-range interactions
6. Unlike GGE, also captures fluctuations of local & global observables



$$\hat{\rho} = C \exp \left[ - \sum_{ik} (\hat{H}_i - \mu_i) M_{ik} (\hat{H}_k - \mu_k) \right]$$

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Exact in classical limit and, moreover, captures the leading quantum correction

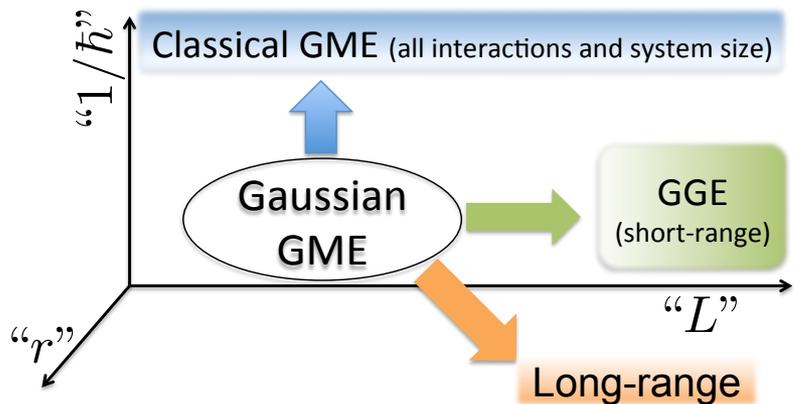
**Ex 1:** harmonic oscillator  $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{q}^2}{2}$

$|\psi(0)\rangle = |z\rangle = \text{coherent state}, a|z\rangle = z|z\rangle$

**Classical limit:**  $\hbar \rightarrow 0, E_0 = \hbar\omega|z|^2 = \text{fixed}$

$$\overline{\langle \hat{n}^k \rangle}_\infty \equiv \lim_{T \rightarrow \infty} \int_0^T \langle \hat{n}^k(t) \rangle dt = |z|^{2k} \left[ 1 + k(k-1) \frac{\hbar\omega}{E_0} + \dots \right], \quad (\hat{n} = a^\dagger a)$$

$$\langle \hat{n}^k \rangle_{\text{GME}} \equiv \text{Tr}(\hat{\rho} \hat{n}^k) = |z|^{2k} \left[ 1 + k(k-1) \frac{\hbar\omega}{E_0} + \dots \right]$$



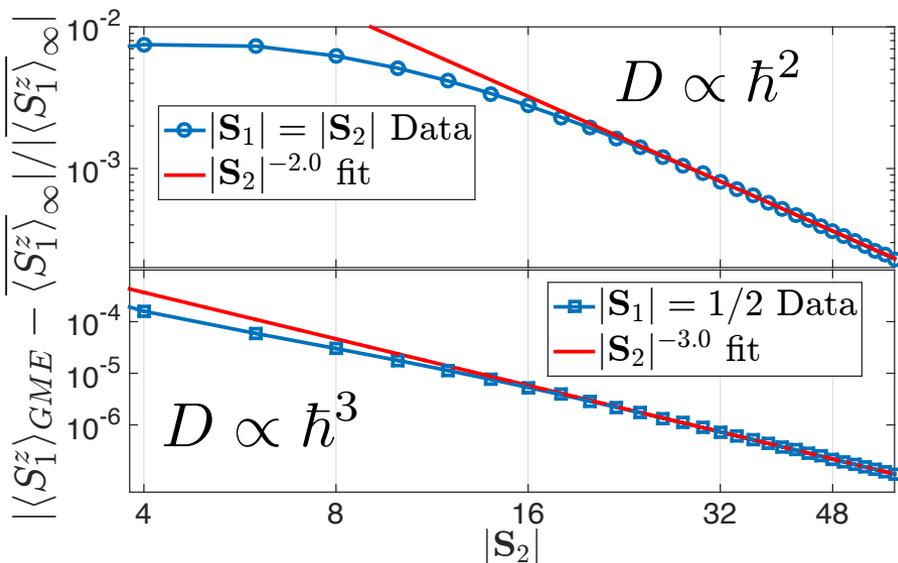
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Exact in classical limit and, moreover, captures the leading quantum correction

**Ex 2: 2-spin Gaudin magnet**

$$H_1 = BS_1^z + \gamma \vec{S}_1 \cdot \vec{S}_2, \quad H_2 = BS_2^z - \gamma \vec{S}_1 \cdot \vec{S}_2, \\ [H_1, H_2] = 0$$



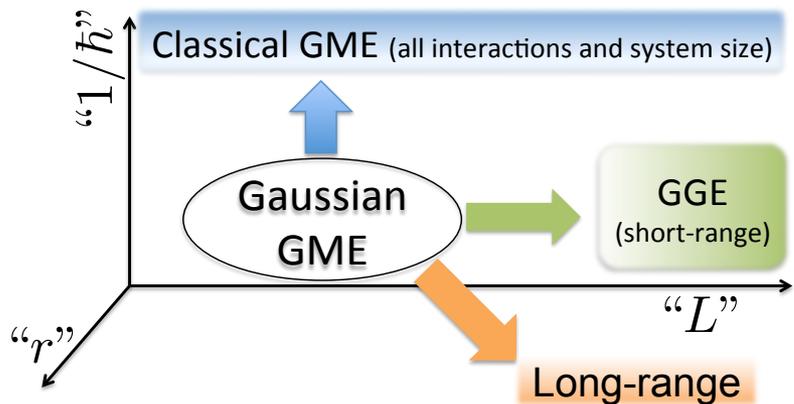
$|\psi(0)\rangle = |\theta_1, \varphi_1\rangle \otimes |\theta_2, \varphi_2\rangle$  (coherent st.)

Two scenarios: both spins classical or only  $S_2$

(a)  $\hbar \rightarrow 0, \hbar S_1 = \hbar S_2 = \text{fixed}$

(b)  $\hbar \rightarrow 0, \hbar S_2 = \text{fixed}, S_1 = 1/2$

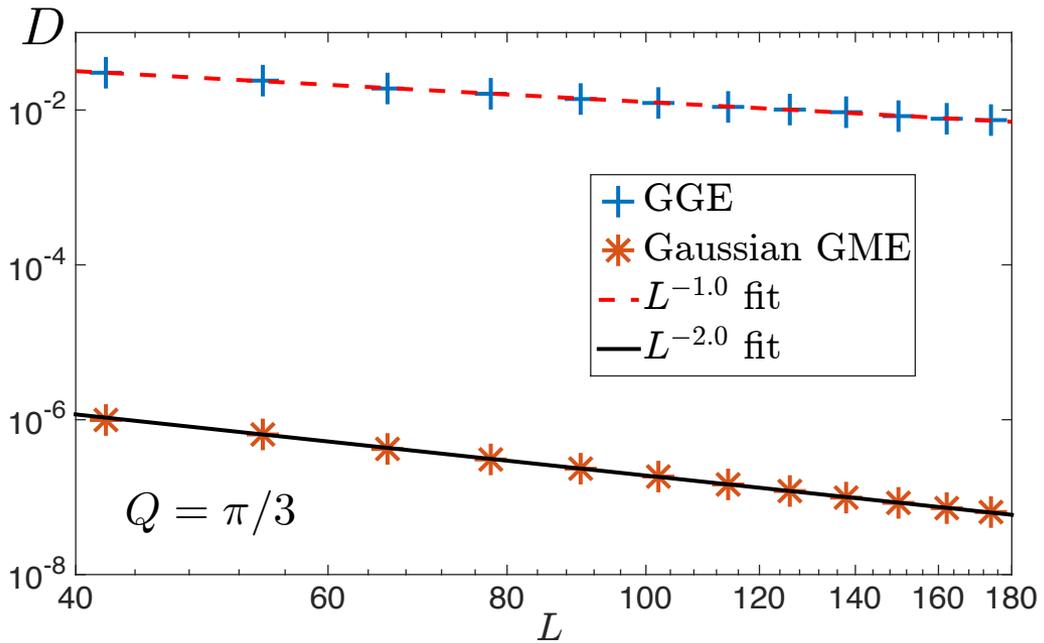
$$D = \frac{\langle S_1^z \rangle_{\text{GME}} - \overline{\langle S_1^z \rangle}_\infty}{\overline{\langle S_1^z \rangle}_\infty}$$



$$\hat{\rho} = C \exp \left[ - \sum_{ik} (\hat{H}_i - \mu_i) M_{ik} (\hat{H}_k - \mu_k) \right]$$

Works whenever GGE does and converges faster ( $1/L^2$ ) than GGE ( $1/L$ ) as system size,  $L$ , grows

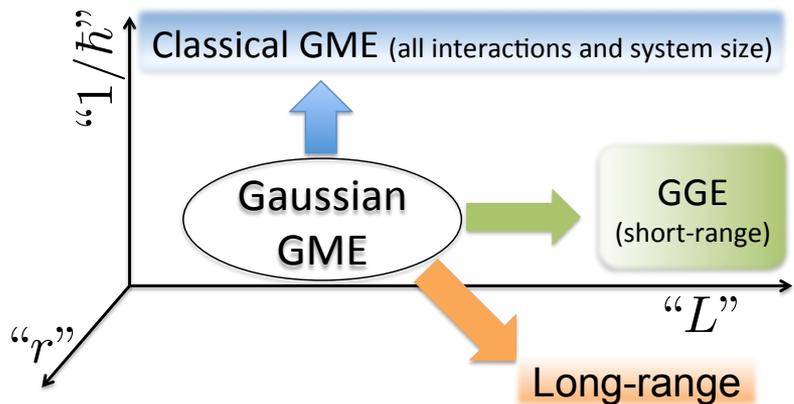
**Example:** 
$$H = - \sum_{j=1}^L (e^{i\phi} c_{j+1}^\dagger c_j + e^{-i\phi} c_j^\dagger c_{j+1}) + \sum_{j=1}^L [V_1 \cos(Qj) + V_2 \cos(2Qj)] n_j$$



GME exact for linear & bilinear combinations of occupation #s for any  $L$ , so consider:

$$D = \frac{\langle \hat{n}_1 \hat{n}_2 \hat{n}_3 \rangle_{\text{GGE}} - \overline{\langle \hat{n}_1 \hat{n}_2 \hat{n}_3 \rangle}_\infty}{\langle \hat{n}_1 \rangle \langle \hat{n}_2 \rangle \langle \hat{n}_3 \rangle}$$

Quench from  $\phi = V_1 = V_2 = 0$  to  $\phi = 0.3, V_1 = 1.5, V_2 = 1.0$



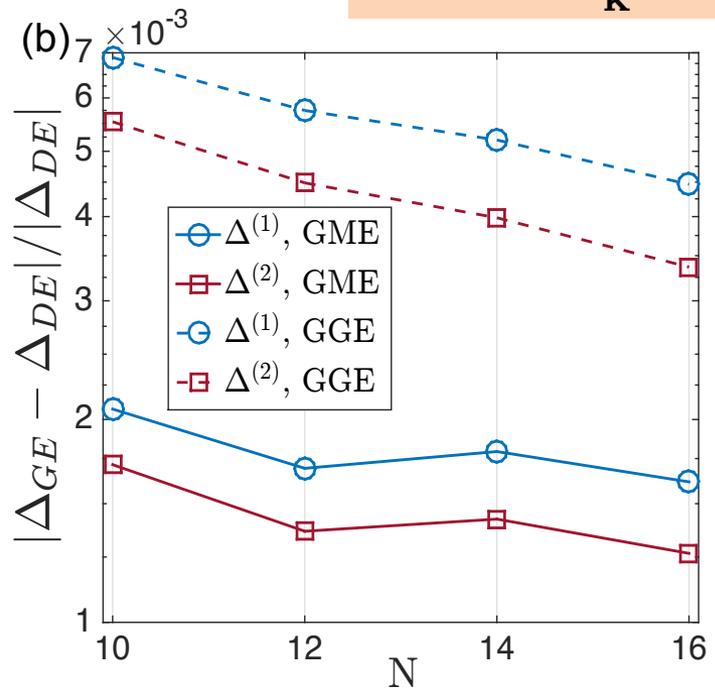
$$\hat{\rho} = C \exp \left[ - \sum_{ik} (\hat{H}_i - \mu_i) M_{ik} (\hat{H}_k - \mu_k) \right]$$

Works well for systems with long-range interactions. Likely exact in  $N \rightarrow \infty$  limit, since dynamics become effectively classical

**Example:**

$$H_{\text{BCS}} = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} s_{\mathbf{k}}^z - g \sum_{\mathbf{k}, \mathbf{p}} s_{\mathbf{k}}^+ s_{\mathbf{p}}^-$$

$$H_{\mathbf{k}} = \sum_{\mathbf{p}} \frac{\vec{s}_{\mathbf{k}} \cdot \vec{s}_{\mathbf{p}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} - \frac{s_{\mathbf{k}}^z}{g}$$



Canonical order parameters:

$$\Delta^{(1)} = g \sqrt{\sum_{\mathbf{k}, \mathbf{p}} \langle s_{\mathbf{k}}^+ s_{\mathbf{p}}^- \rangle - \frac{N}{2}},$$

$$\Delta^{(2)} = g \sum_{\mathbf{k}} \sqrt{\frac{1}{4} - \langle s_{\mathbf{k}}^z \rangle^2}$$

$N$  - # of spins,  $s_{\mathbf{k}} = 1/2$ , total  $S^z = 0$

Quench  $g_i = 0.5\delta \rightarrow g_f = 2.0\delta$ , where  $\delta =$  spacing between  $\epsilon_{\mathbf{k}}$



Anatoli Polkovnikov  
*Boston University*



Hyungwon Kim  
*Rutgers University*

Yuzbashyan, *Ann. Phys.* 367, 288 (2016)

Kim, Polkovnikov, Yuzbashyan, [arXiv:1606.08459](https://arxiv.org/abs/1606.08459)

