Symmetry shapes thermodynamics in macroscopic quantum systems

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V. Cavina, A. Soret, T. Aslyamov, K. Ptaszyński, M. Esposito, Phys. Rev. Lett. 133, 130401 (2024)

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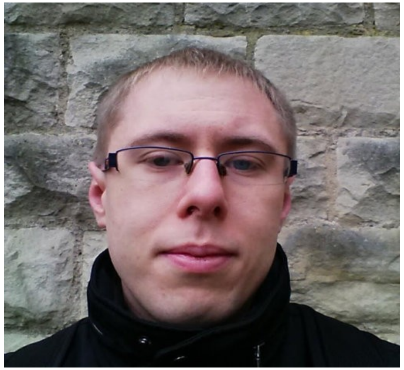

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Outline

- Introduction
- Symmetries in quantum systems
- Entropy decomposition
- Permutation group
- Quantum phase transition in the transverse Curie-Weiss model

Symmetries in physics...

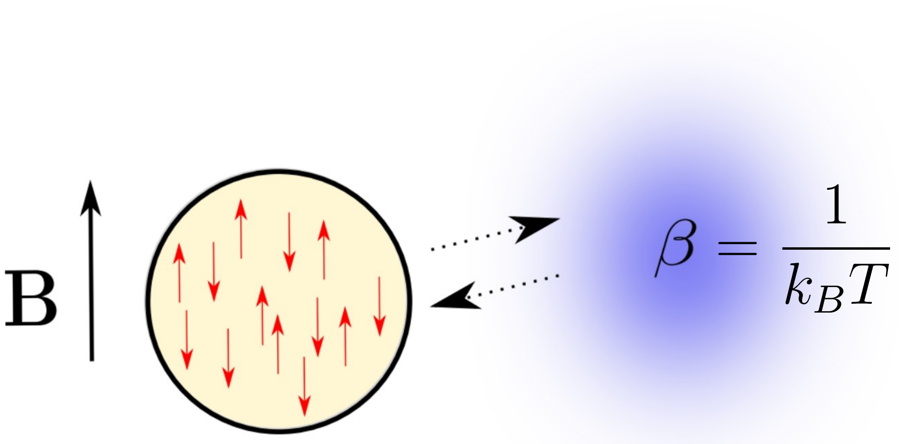
- Out of equilibrium: stochastic energetics, dynamical phase transitions,…
- At equilibrium: entropy scalings, ground state properties…
- Influences thermalization
- Can be exploited to optimize quantum computing, numerics…
- ...

Symmetry and thermodynamics in quantum systems? Quantum phase transitions?

Classical Curie-Weiss model

N interacting spins in magnetic field

$$H = -\frac{J}{N}\sum_{i<j} m_i m_j - \mu B \sum_i m_i$$



$(\hbar = k_B = 1)$

Invariant under permutation of particles:

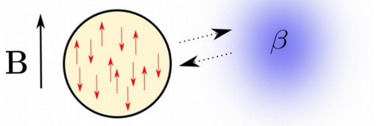
$$\pi[H(m_1, m_2, ...m_N)] = H(m_{\pi(1)}, m_{\pi(2)}, ...m_{\pi(N)}) = H(m_1, m_2, ...m_N)$$

$$H(\vec{m}) = H(\vec{m}(\mu_1, \mu_2)) = \omega(\mu_1 - \mu_2) + \frac{t}{N}(\mu_1 - \mu_2)^2$$

Occupation numbers

Rate function and phase transition

Equilibrium partition function: $Z_{\text{eq}} = \sum_{\vec{m}} e^{-\beta H(\vec{m})} = \sum_{\mu_1} \underline{\mathcal{N}(\mu_1)} e^{-\beta \underline{H(\mu_1)}}$



$$\mathcal{N}(\mu_1) = \frac{N!}{\mu_1!(N-\mu_1)!} \approx e^{\underline{-\mu_1 \log(\mu_1) - (N-\mu_1)\log(N-\mu_1)}}$$

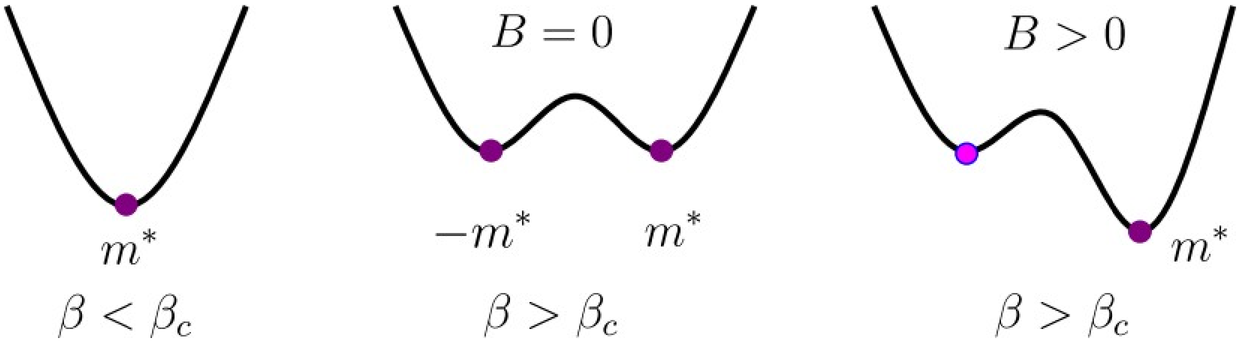
Density $x = \mu_1/N$

Macroscopic limit: $Z_{\text{eq}} \asymp N \int dx\, e^{-N\beta^{-1}(\underline{e(x)} - \beta^{-1}\underline{s(x)})}$

Energetic contribution

Entropic contribution

Phase transition:



Quantum case ?

$$\hat{H} = -\frac{J}{N}\sum_{i<j}\hat{\sigma}_x^{(i)}\hat{\sigma}_x^{(j)} - \mu B\sum_i \hat{\sigma}_z^{(i)}$$

- Choice of basis: $|v\rangle = |v_1\rangle \otimes |v_2\rangle \ldots \otimes |v_N\rangle$ with $|v_j\rangle = |0\rangle, |1\rangle$
- Permutation: $\pi|v\rangle = |v_{\pi(1)}\rangle \otimes |v_{\pi(2)}\rangle \ldots \otimes |v_{\pi(N)}\rangle$

Label states with occupation number?

Phase transition?

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Symmetry group

- Quantum system : defined in Hilbert space $\mathcal{H}$
- Characterised by density matrix ρ
- Symmetry : associated with a unitary transformation $\in U(N)$
- ρ satisfies a symmetry $g \in U(N)$ if $g\rho g^{-1} = \rho$

The set of symmetries of ρ is a group (*g*,*g'* symmetries → *gg'* symmetry, …) called the **symmetry group** G:

$$G \subseteq U(N) \; ; \; \forall g \in G \quad g\rho g^{-1} = \rho$$

Group representations

In general: no common eigenbasis for all the $g \in G$

BUT: There are subspaces of the Hilbert $\mathcal{H}$ space invariant under the action of G:

$$\mathcal{H} = \bigoplus_{\lambda} \bigoplus_{k=1}^{\deg\lambda} V_k^{\lambda} \qquad |v\rangle \in V_l^{\lambda} \Rightarrow g|v\rangle \in V_l^{\lambda}$$

REPRESENTATIONS

If the representations cannot be decomposed further, they are called **irreducible.**

Form of the density matrix of a system symmetric under G

$$[A, \rho] = 0 \quad \Rightarrow \quad \text{Common eigenbasis}$$

What happens if ρ commutes with a full group?

$$\forall g \in G \qquad g\rho g^{-1} = \rho \qquad [g, \rho] = 0$$

Form of the density matrix of a system symmetric under G

$$\forall g \in G \quad [g, \rho] = 0 \quad \Longrightarrow$$

Common invariant subspaces

$$\rho V_k^\lambda \subseteq V_k^\lambda$$

$$g V_k^\lambda \subseteq V_k^\lambda$$

ρ block diagonal and proportional to the identity in every block (Schur's lemma):

$$\rho = \begin{array}{c} \begin{array}{ccc} \overbrace{\qquad\qquad}^{V_1^\lambda} & \overbrace{\qquad\qquad}^{V_2^\lambda} & \overbrace{\qquad\qquad\qquad}^{V_1^{\lambda'}} \end{array} \\ \left(\begin{array}{cc|cc|ccc} d_{1,1} & 0 & c & 0 & 0 & 0 & 0 \\ 0 & d_{1,1} & 0 & c & 0 & 0 & 0 \\ \hline c^* & 0 & d_{1,2} & 0 & 0 & 0 & 0 \\ 0 & c^* & 0 & d_{1,2} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & d_{2,1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{2,1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & d_{2,1} \end{array}\right) \end{array}$$

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Von Neumann entropy

$$\rho = \begin{array}{c} \begin{array}{ccc} \overbrace{\qquad\qquad}^{V_1^{\lambda}} & \overbrace{\qquad\qquad}^{V_2^{\lambda}} & \overbrace{\qquad\qquad\qquad}^{V_1^{\lambda'}} \end{array} \\ \left(\begin{array}{cc|cc|ccc} d_{1,1} & 0 & c & 0 & 0 & 0 & 0 \\ 0 & d_{1,1} & 0 & c & 0 & 0 & 0 \\ \hline c^* & 0 & d_{1,2} & 0 & 0 & 0 & 0 \\ 0 & c^* & 0 & d_{1,2} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & d_{2,1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{2,1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & d_{2,1} \end{array}\right) \end{array}$$

$$\rho = \sum_{\lambda} p_\lambda \rho_\lambda$$

$$\rho_\lambda = \frac{1}{\dim\lambda} \tilde{\rho}_\lambda \otimes \mathbf{I}_\lambda$$

$$\begin{pmatrix} d_{11} & c \\ c^* & d_{12} \end{pmatrix}$$

$$S(\rho) \equiv -\mathrm{Tr}(\rho \log \rho)$$

$$= \sum_{\lambda} p_\lambda [\log \dim \lambda + S(\tilde{\rho}_\lambda)] + H(p)$$

Shannon entropy

$$H(p) = -\sum_{\lambda} p_\lambda \log p_\lambda$$

Depends on group

bounded

Summary

- Group representation theory gives natural basis to study a symmetric system
- Universal decomposition of Von Neumann entropy

Wich entropic term dominates? Phase transitions?

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Permutation group S_N

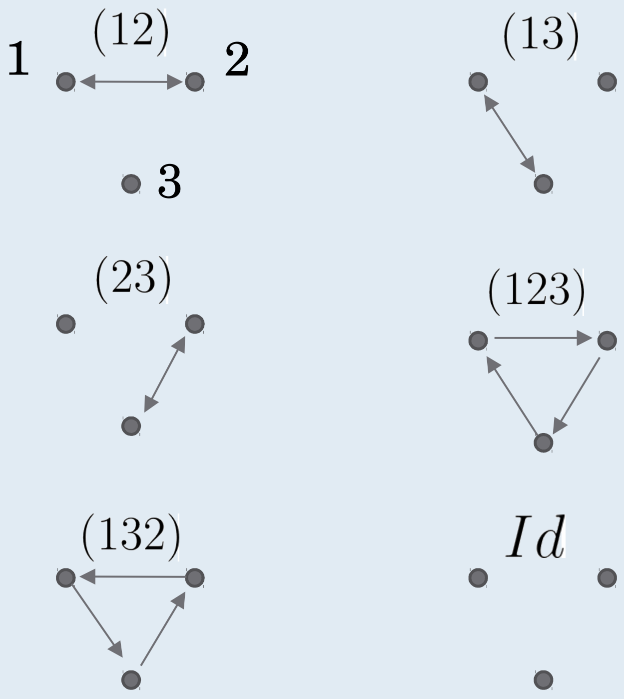
- Acts on *N* ordered objects by permuting them

- $N!$ elements in the group

- Acts on the tensor product of Hilbert spaces:

$$\pi\left[|v_1\rangle \otimes |v_2\rangle ... \otimes |v_N\rangle\right] = |v_{\pi(1)}\rangle \otimes |v_{\pi(2)}\rangle ... \otimes |v_{\pi(N)}\rangle$$

Example $N = 3$



In what follows: consider a system of N particles of d levels

Irreducible representations of the permutation group?

Example: 3 identical 2 level systems; dim $\mathcal{H}$ = 8 $\boxed{\mathcal{H} = M_{(3,0)} \oplus M_{(2,1)} \oplus M_{(1,2)} \oplus M_{(0,3)}}$

INVARIANT SUBSPACE	DIM	OCCUPATION NUMBERS
$\|000\rangle$	1	(3,0)
$\frac{\|100\rangle + \|010\rangle + \|001\rangle}{\sqrt{3}}$	1	(2,1)
$a\frac{\|001\rangle - \|100\rangle}{\sqrt{2}} + b\frac{\|001\rangle - \|010\rangle}{\sqrt{2}}$	2	(2,1)
$\frac{\|110\rangle + \|101\rangle + \|011\rangle}{\sqrt{3}}$	1	(1,2)
$a\frac{\|110\rangle - \|011\rangle}{\sqrt{2}} + b\frac{\|110\rangle - \|101\rangle}{\sqrt{2}}$	2	(1,2)
$\|111\rangle$	1	(0,3)

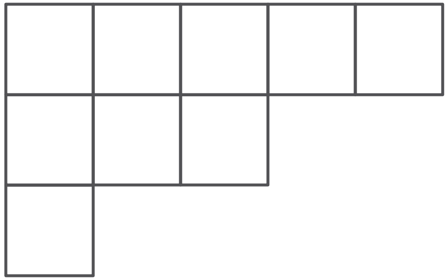
(You may ignore the next three slides...)

Irreducible representations of the permutation group

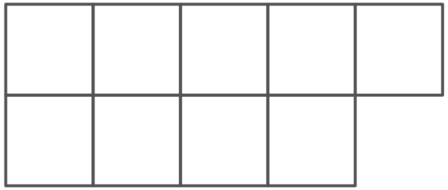
General case: *N* particles of *d* levels

- The irreducibles of S_N are labelled by **Young tableaux:** tables of *N* boxes with decreasing number of rows.
- Number of rows = number of levels *d*
- $\boldsymbol{\lambda}$ = **partition of *N*** $\rightarrow$ shape

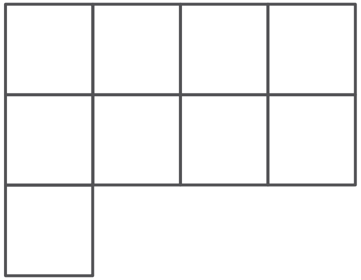
EXAMPLE: some irreducibles appearing in 9 3-level systems



$\boldsymbol{\lambda}$ = (5,3,1)



$\boldsymbol{\lambda}$ = (5,4,0)



$\boldsymbol{\lambda}$ = (4,4,1)

Connection between tableaux and the Hilbert space

Back to 3 2-level systems

Fill the tableaux:

$$t = \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & \multicolumn{1}{c}{} \\ \cline{1-1}\end{array}$$

Vector (tabloid):

$$\{t\} \equiv \begin{array}{cc}\hline 1 & 2 \\ \hline 3 & \\ \cline{1-1}\end{array} \equiv \left\{ \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & \multicolumn{1}{c}{} \\ \cline{1-1}\end{array}, \begin{array}{|c|c|}\hline 2 & 1 \\ \hline 3 & \multicolumn{1}{c}{} \\ \cline{1-1}\end{array} \right\}$$

Vector space (permutation module) generated by:

$$\begin{array}{cc}\hline 1 & 2 \\ \hline 3 & \\ \cline{1-1}\end{array}, \begin{array}{cc}\hline 1 & 3 \\ \hline 2 & \\ \cline{1-1}\end{array}, \begin{array}{cc}\hline 2 & 3 \\ \hline 1 & \\ \cline{1-1}\end{array}$$

isomorphism

$$|e_1\rangle \otimes |e_2\rangle \ldots \otimes |e_n\rangle \longrightarrow \begin{array}{c}\hline i \quad s.t. \quad e_i = 1 \\ \hline i \quad s.t. \quad e_i = 2 \\ \hline \ldots. \quad \ldots. \\ \hline i \quad s.t. \quad e_i = d \\ \hline \end{array}$$

Subspace of fixed occupation number

$$M_{\boldsymbol{\mu}}$$

$$\mathcal{H} = \bigoplus_{\boldsymbol{\mu}} M_{\boldsymbol{\mu}}$$

Young's rule: $$M_{\boldsymbol{\mu}} = \bigoplus_{\boldsymbol{\lambda}} \bigoplus_{h=1}^{K_{\boldsymbol{\lambda},\boldsymbol{\mu}}} \mathcal{S}^{\boldsymbol{\lambda}}_{h,\boldsymbol{\mu}}$$

Back to 3 identical 2 level systems

$$\mathcal{H} = M_{(3,0)} \oplus M_{(2,1)} \oplus M_{(1,2)} \oplus M_{(0,3)}$$

Irreducibles

λ_1 $\begin{array}{|c|c|c|}\hline & & \\ \hline \end{array}$ $\quad \dim \lambda_1 = 1$

λ_2 $\begin{array}{|c|c|}\hline & \\ \hline \\ \cline{1-1} \end{array}$ $\quad \dim \lambda_2 = 2$

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$\frac{\|110\rangle + \|101\rangle + \|011\rangle}{\sqrt{3}}$	1	(1,2)
$a\frac{\|110\rangle - \|011\rangle}{\sqrt{2}} + b\frac{\|110\rangle - \|101\rangle}{\sqrt{2}}$	2	(1,2)
$\|111\rangle$	1	(0,3)

Young's rule

$$M_{(3,0)} = S^{\lambda_1}_{(3,0)} \longrightarrow \begin{array}{|c|c|c|}\hline 0 & 0 & 0 \\ \hline \end{array}$$

$$M_{(2,1)} = S^{\lambda_1}_{(2,1)} \oplus S^{\lambda_2}_{(2,1)}, \qquad S^{\lambda_1}_{(2,1)} \longrightarrow \begin{array}{|c|c|c|}\hline 0 & 0 & 1 \\ \hline \end{array}, \qquad S^{\lambda_2}_{(2,1)} \longrightarrow \begin{array}{|c|c|}\hline 0 & 0 \\ \hline 1 \\ \cline{1-1} \end{array}$$

$$M_{(1,2)} = S^{\lambda_1}_{(1,2)} \oplus S^{\lambda_2}_{(1,2)}, \qquad S^{\lambda_1}_{(1,2)} \longrightarrow \begin{array}{|c|c|c|}\hline 0 & 1 & 1 \\ \hline \end{array}, \qquad S^{\lambda_2}_{(1,2)} \longrightarrow \begin{array}{|c|c|}\hline 0 & 1 \\ \hline 1 \\ \cline{1-1} \end{array}$$

$$M_{(0,3)} = S^{\lambda_1}_{(0,3)} \longrightarrow \begin{array}{|c|c|c|}\hline 1 & 1 & 1 \\ \hline \end{array}$$

Take home message

- We can map the product basis to the basis of the irreducibles
- We actually don't need to know the details of the mapping
- Importantly:

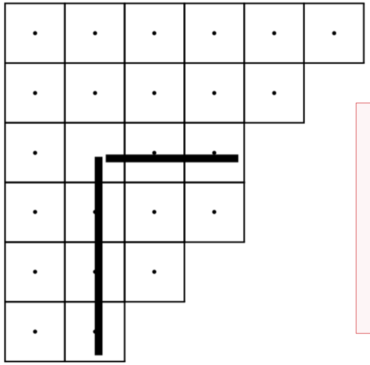
Kotska number

$$\mathcal{H} = \bigoplus_{\boldsymbol{\lambda},\boldsymbol{\mu}} \bigoplus_{h=1}^{K_{\boldsymbol{\lambda},\boldsymbol{\mu}}} \mathcal{S}^{\boldsymbol{\lambda}}_{h,\boldsymbol{\mu}}$$

Occupation numbers

Von Neumann entropy: large *N* limit

$$S(\rho) = \sum_{\boldsymbol{\lambda}} p_{\boldsymbol{\lambda}} \Big[\underbrace{\log \dim \boldsymbol{\lambda}}_{\sim N} + \underbrace{S(\tilde{\rho}_{\boldsymbol{\lambda}})}_{\leq \frac{d(d-1)}{2} \log N} \Big] + \underbrace{H(p)}_{\leq d \log N}$$



Hook length formula:

$$\dim \boldsymbol{\lambda} = \frac{N!}{\prod_{(i,j)} h_{\boldsymbol{\lambda}}(i,j)}$$

Large *N* limit

$$\boldsymbol{x} \equiv \frac{\boldsymbol{\lambda}}{N} \qquad \dim(N\boldsymbol{x}) \asymp e^{N s(\boldsymbol{x})}$$

$$\Rightarrow \quad \lim_{N\to\infty} \frac{S(\rho)}{N} = \lim_{N\to\infty} \sum_{\boldsymbol{\lambda}} \frac{p_{\boldsymbol{\lambda}}}{N} \log \dim \boldsymbol{\lambda} = \int p(\boldsymbol{x}) s(\boldsymbol{x}) d\boldsymbol{x}$$

$$p(\boldsymbol{x}) \equiv N p_{\boldsymbol{\lambda}=N\boldsymbol{x}}$$

$$s(\boldsymbol{x}) = -\sum_{j=1}^{d} x_j \log x_j$$ entropy rate function depending **only** on group properties

Equilibrium free energy

$$e^{-\beta\hat{H}} = \sum_{\boldsymbol{\lambda}} e^{-\beta\tilde{H}_{\boldsymbol{\lambda}}\otimes\mathbf{I}_{\boldsymbol{\lambda}}} \Rightarrow F \equiv -\frac{1}{\beta}\log \mathrm{Tr}[e^{-\beta\hat{H}}] = -\frac{1}{\beta}\log\left\{\sum_{\boldsymbol{\lambda}} \dim\boldsymbol{\lambda}\,\mathrm{Tr}\left[e^{-\beta\tilde{H}_{\boldsymbol{\lambda}}}\right]\right\}$$

Intensive free energy in subspace $\boldsymbol{x} \equiv \frac{\boldsymbol{\lambda}}{N}$:

$$e(\boldsymbol{x}) \equiv -\lim_{N\to\infty}\frac{1}{\beta N}\log\left\{\mathrm{Tr}[e^{-\beta\tilde{H}(\boldsymbol{x})}]\right\} = \lim_{N\to\infty}\frac{E^0_{\boldsymbol{x}}}{N}$$

ground state energy in block

Large *N* limit

$$\boldsymbol{x} \equiv \frac{\boldsymbol{\lambda}}{N} \qquad \lim_{N\to\infty}\frac{F}{N} = -\lim_{N\to\infty}\frac{1}{\beta N}\ln\int e^{-N\beta f(\boldsymbol{x})}d\boldsymbol{x}$$

$$f(\boldsymbol{x}) \equiv e(\boldsymbol{x}) - \beta^{-1}s(\boldsymbol{x})$$

Energy rate function, given by ground state energy in the irreducible subspaces

Minimization

Free energy rate function:

$$\lim_{N\to\infty} \frac{F}{N} = -\lim_{N\to\infty} \frac{1}{\beta N} \ln \int e^{-N\beta f(\boldsymbol{x})} d\boldsymbol{x} = f(\boldsymbol{x}^*)$$

$$\boldsymbol{x}^* = \arg\min_{\boldsymbol{x}} f(\boldsymbol{x})$$

$$p_{\boldsymbol{\lambda}} = \dim \boldsymbol{\lambda} \mathrm{Tr}\left[e^{-\beta(\tilde{H}_\lambda - F)}\right] \Rightarrow \lim_{N\to\infty} \frac{1}{N} \log p_{\boldsymbol{\lambda}} = -\beta\left[f(\boldsymbol{x}) - f(\boldsymbol{x}^*)\right]$$

Entropy:

$$\lim_{N\to\infty} \frac{S}{N} = s(\boldsymbol{x}^*)$$

Energy:

$$\lim_{N\to\infty} \frac{E}{N} = \lim_{N\to\infty} \frac{\mathrm{Tr}\left[\hat{H} e^{-\beta(\hat{H} - F)}\right]}{N} = e(\boldsymbol{x}^*)$$

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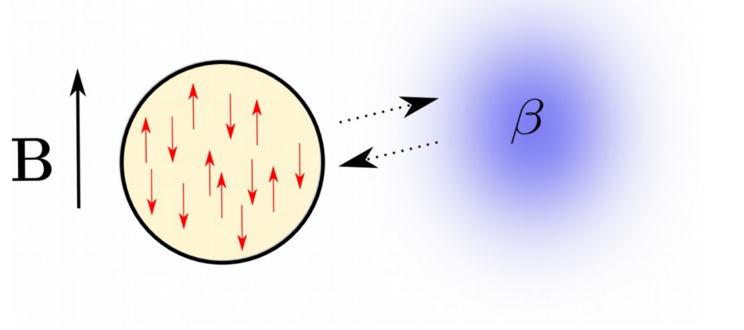
Quantum transverse Curie-Weiss model

T. Jorg et al, EPL 89, 40004 (2010)
L. Chayes et al, J. Stat. Phys. 133, 131 (2008).

$$\hat{H} = -\frac{J}{N}\sum_{i<j}\hat{\sigma}_x^{(i)}\hat{\sigma}_x^{(j)} - \mu B \sum_i \hat{\sigma}_z^{(i)}$$

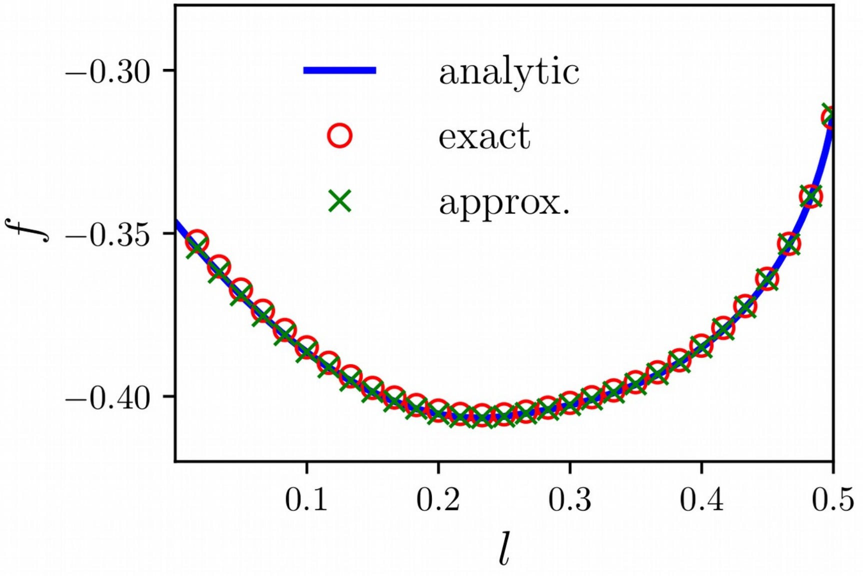


Irreducibles labelled by $\boldsymbol{\lambda} = (\lambda_1, \lambda_2)$

Rescaled total angular momentum (or magnetization): $l = \frac{\lambda_1 - \lambda_2}{2N}$

$$s(l) = -\left(\tfrac{1}{2} - l\right)\log\left(\tfrac{1}{2} - l\right) - \left(\tfrac{1}{2} + l\right)\log\left(\tfrac{1}{2} + l\right)$$

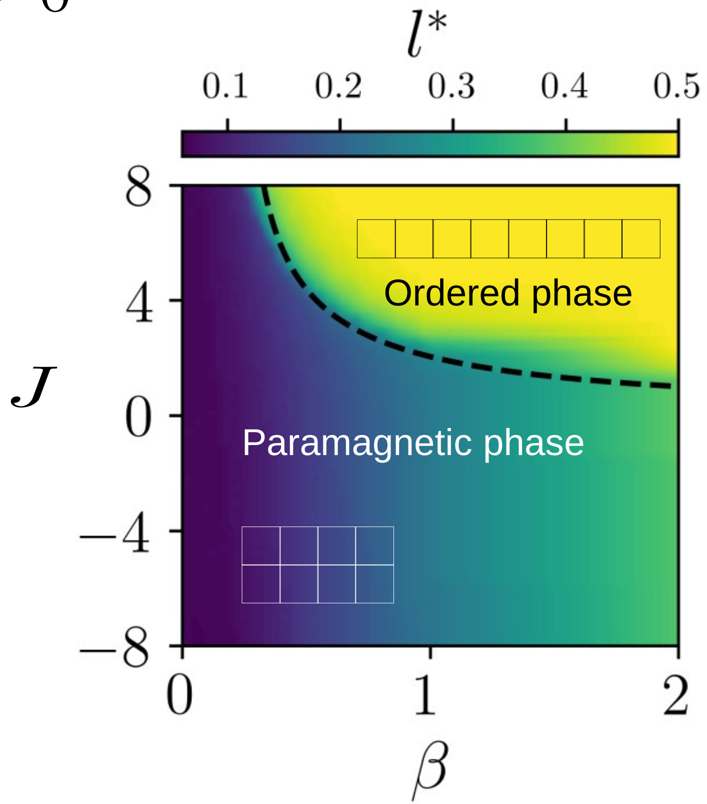
$$e(l) = \begin{cases} -\omega l & \text{for} \quad l \leq \frac{\omega}{2\alpha}\,, \\ -l^2 J - \frac{\omega^2}{2J} & \text{for} \quad l > \frac{\omega}{2\alpha}\,. \end{cases}$$

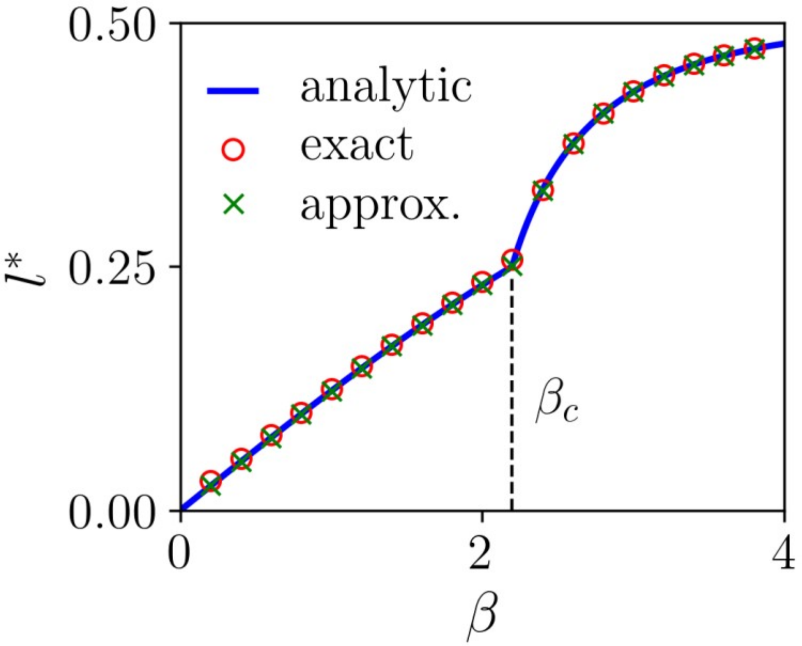


$$l = \frac{\lambda_1 - \lambda_2}{2N}$$

Quantum phase transition

$$B > 0$$





Conclusions

- Group representation theory provides the natural basis for the Hilbert space
- Universal decomposition of entropy
- For the permutation group: entropy and free energy satisfy large deviation principles
- The free energy rate function shows a competition between entropic (group theory) and energetic rate functions
- Powerful tool for the study of quantum phase transitions

Perspectives

- Physical meaning of the labelling λ for $d > 2$?
- Phase transitions with other groups than permutation group?
- Open systems?
- Out of equilibrium?

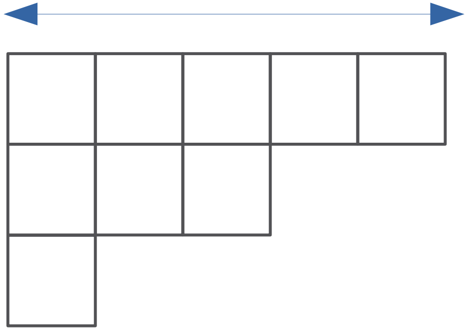
Appendices

Limit shape (simple version of Vershik-Kerov theorem)

S. V. Kerov, A. M. Vershik, SIAM J. on Algebraic Discrete Methods 7, 116 (1986)

$$s(\boldsymbol{x}) = -\sum_{j=1}^{d} x_j \log x_j$$

$$\lambda_1 = N x_1$$



Vershik-Kerov (finite *d* case)

$$\lim_{N\to+\infty} \dim\{N\boldsymbol{x} : \left|x_j - \frac{1}{d}\right| \geq \epsilon\}/\dim(N\bar{\boldsymbol{x}}\ ) = 0$$

Limit shape: