## Probability assignment in a quantum statistical model

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### Motivation

# The pdf of the magnetization of a molecular magnet calculated from

$$p(m,\beta) = \sum_{m'} p(m,\beta \mid m',0) p(m',0)$$

is different from the pdf of the magnetization calculated from  $p(m,\beta) = Z^{-1}(\beta) \langle m \mid \exp(-\beta H) \mid m \rangle$ 



#### Magnetization



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### Organization

- Probability assignments
- The mapping of a Quantum model on a Markov chain Example 1
- The mapping of a Markov chain on a Quantum model Example 2
- Model selection using the Maximum Entropy Principle for both models
- Consistency



This probability assignment is frequently used in quantum statistical models



$$\mathbf{O} K_{l\,k} \left(\beta\right) = \frac{g_k}{g_l} \left\langle k \right| \exp\left(-\beta H\right) \left|l\right\rangle$$

Propagator

$$H\left|l\right\rangle = \sum_{k\neq l}\left|k\right\rangle\left\langle k\right|H\left|l\right\rangle + \left|l\right\rangle\left\langle l\right|H\left|l\right\rangle \qquad \text{Hamiltonian}$$

$$\begin{split} \partial_{\beta} K_{l\,k}\left(\beta\right) &= \sum_{p \neq l} q_{l\,p} K_{p\,k}\left(\beta\right) - v_{l} K_{l\,k}\left(\beta\right) - V_{l} K_{l\,k}\left(\beta\right) \\ & \text{Evolution in the parameter} \\ q_{l\,p} &= -\left\langle p\right| H \left|l\right\rangle \frac{g_{p}}{g_{l}} \quad v_{l} = \sum_{p \neq l} q_{l\,p} \quad V_{l} = \left\langle l \mid H \mid l\right\rangle - v_{l} \end{split}$$

Characterization of the evolution

Markov for  $\, q_{l\,p} \,$  not negative and  $\, V_{l} = 0 \,$ 



# Conditions for a Markov representation

$$K_{cl}(\beta) = 0$$

$$K_{cc}(\beta) = 1$$

$$\sum_{k \neq c} K_{lk}(\beta) + K_{lc}(\beta) = 1$$
regularization of the conservation of probability

$$\begin{array}{ll} q_{l\,p} & \mbox{not negative} \\ \langle \phi \mid = \sum_{k} g_{k} \langle k \mid \ \langle \phi \mid H = 0 \\ & \mbox{groundstate} \end{array} \end{array}$$



- Molecular magnets Markov representation
  - Hamiltonian
  - Mapping
  - Transition probability
  - Evolution equation
  - Shannon entropy
- Molecular Magnets Information entropy
  - Partition function
  - Diagonal part of the propagator
  - Information entropy
- Maximum Entropy Principle
  - Model selection

$$\begin{split} & w(m,m+1) &= b(N-m) \quad w(m,m-1) = bm \\ & w(m,m+2) &= E(N-m)(N-m-1) \quad w(m,m-2) = Em(m-1) \\ & e_m = D(\frac{N-2m}{2})^2 + g\mu_B b_z \frac{N-2m}{2} \qquad b = g\mu_B b_x \end{split}$$









$$p_X(m \mid \beta) \propto \sum K(m \beta \mid k 0) p_X(k \mid 0)$$
$$S_X(\beta) = -\sum_m p_X(m \mid \beta) \ln(p_X(m \mid \beta))$$



$$p_{MS}^{IE}(m \mid \beta) \propto K(m, \beta; m).$$
$$p_{MS}^{IE}(m \mid \beta) \propto \binom{N}{m} K(m, \beta; m).$$

Single spin

Many spin





### Example 1 Single Spin

Entropy vs Inverse Temperature - Single Spin Model





### Example 1 Many Spins

Entropy vs Inverse Temperature - Many Spin Model





#### Phase change Many Spins



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### Example 2

#### • $M/M/\infty$ queue using stochastic methods

- Transition probability
- Evolution equation
- Shannon entropy for two initial conditions
- $M/M/\infty$  queue using Quantum methods
  - Mapping on the displaced oscillator
  - Partition function
  - Entropy
  - Diagonal part of the propagator
  - Information entropy
- Maximum Entropy Principle
  - Model selection



$$\frac{\partial K(n,\beta;n',0)}{\partial \beta} = \gamma K(n+1,\beta;n',0) + \lambda n K(n-1,\beta;n',0) - (\gamma+\lambda n) K(n,\beta;n',0)$$

$$H = \lambda A^{\dagger} A - \gamma A - \lambda A^{\dagger} + \gamma,$$



- Methods
  - algebraic methods in the complex plane
  - resemble methods used in coherent states
  - key trick: the following representation of the diracdelta function:

$$n!\delta_{n,k} = \frac{1}{\pi} \int d^2 z (z^*)^n z^k \exp(-zz^*)$$

• Transition probability

 $K(n,\beta;m,0) = \exp\left(-\frac{\gamma}{\lambda}g(\beta)\right)$ 

$$\sum_{k}^{\min(m,n)} {n \choose k} \frac{\left(\frac{\gamma}{\lambda}\right)^{m-k}}{(m-k)!} (1 - g(\beta))^k \left(g(\beta)\right)^{n+m-2k}$$
$$g(\beta) = 1 - \exp\left(-\lambda(\beta)\right)$$



generating function for the moments  

$$M_{gf}(t) = \frac{g(\beta)}{1 - \exp(t) + \exp(t)g(\beta)} \\ * \\ \exp(-\frac{\gamma}{\lambda}g(\beta)\frac{1 - \exp(t)}{1 - \exp(t) + \exp(t)g(\beta)}) \\ \xrightarrow{\text{Poisson-like}}$$



- Quantum approach 1
  - Partition function
  - Free energy
  - Entropy
- Quantum approach 2
  - Information entropy
  - Diagonal element of the propagator





Comparison between initially a Poisson or geometric density Poisson : squares

Comparison between the entropy calculated from the partition function and the diagonal element of the propagator



#### Discussion

#### Example 2 shows that

-  $p(n \mid \beta) \propto K(n,\beta \mid n) \;\; \text{is not an good approximation of}$ 

$$- p(n \mid \beta) \propto \sum K(n, \beta \mid k) p(k \mid 0)$$

• Example 1 shows

 $p(n \mid \beta) \propto \sum_{k} K(n, \beta \mid k) p(k \mid 0)$  ma

makes less

#### assumptions than

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#### Consistency

- The Gibbs postulate has to be correct at least for thermal equilibrium
- Is one of both assignments consistent with this postulate?
- Answer
  - consistent:  $p(n \mid \beta) \propto \sum K(n, \beta \mid k)p(k \mid 0)$
  - consistent only if n are eigenstates of H

 $p(n \mid \beta) \propto K(n, \beta \mid n)$ 



# Proof of consistency heuristic $p(m,\beta) = \sum_{\underline{\nu}} U(m,\nu) \exp(-\beta\epsilon_{\nu}) \sum_{l} U^{-1}(\nu,l) p(l,0)$ Spectral representation of the propagator $w(\nu,\beta) = \sum_{l} U^{-1}(\nu,l)p(l,\beta)$ $w(\nu,\beta) = \exp(-\beta\epsilon_{\nu})w(\nu,0)$

Gibbs postulate