

Overview of the possibilities of high temperature series expansions

Laura MESSIO

Benard Bernu (LPTMC, Paris), Laurent Pierre (Université de Nanterre),

Karim Essafi, Matias Gonzalez, Clément Supiot

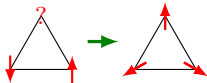
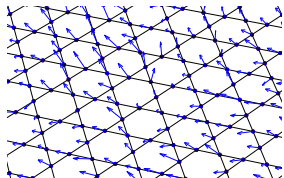
Quentin Barthélemy, Panchanan Khuntia, Edwin Kermarrec, Fabrice Bert, Philippe Mendels



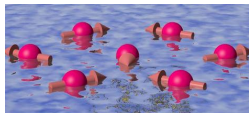
The domain of frustrated magnetism

In Mott insulators, the low- T behavior only depends from the electronic spin on crystal sites:

$$\hat{H} = \sum_{\langle ij \rangle} J_1 \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j.$$

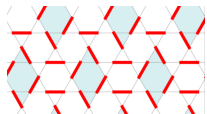


Frustration arises from the lattice geometry or from competing interactions and gives rise to exotic phases.



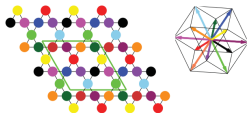
spin liquids
(topological or gapless)

Oxford University



valence bond solids

Hwang et al., PRB 92, 205131 (2015)



or simply **non-collinear long-range orders**

Messio et al, PRB.83, 184401 (2011)

The experimental realizations of Mott insulators



Herbertsmithite ©Steve Rust



Kapellasite ©Chris Auer



Vesignieite ©JM2011

- What is the most faithful Hamiltonian for a given compound ? What are the effect of unexpected/uncontrolled terms (impurities) ?

$$H = J_1 \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j + \delta S_i^z S_j^z) + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\ + K \sum_{\diamond} (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + D_z \sum_{\langle i,j \rangle} (\mathbf{S}_i \wedge \mathbf{S}_j)_z - h \sum_i S_i^z$$

- How to exploit measurements ? What are the phase transitions ?
→ Need for finite T calculations (specific heat $c_V(T)$, magnetic susceptibility $\chi(T)$).

Numerical tools for quantum models

Unbiased

Biased

Series expansions

Non stochastic

HTSE

NLC

Linked Cluster
Expansions

Tensor network
methods

MPS

MERA

PEPS

ED

Stochastic

Diagrammatic
Monte Carlo

WLQMC

SSE

DMC

VMC

VMC: Variational Monte Carlo
ED: Exact Diagonalization
HTSE: High Temperature Series
Expansion
NLC: Numerical Linked Cluster
(expansion)
WLQMC: World Line Quantum Monte
Carlo
SSE: Stochastic Series Expansions
MPS: Matrix Product States
PEPS: Projected Entangled Pair States
MERA: Multiscale Entanglement
Renormalisation Ansatz
DMC: Determinantal Monte Carlo

Plan

- **Introduction to High Temperature Series Expansions (HTSE)**
 - ✓ Definition of HTSE
 - ✓ The HTSE coefficients
- Extrapolation when there is no phase transition
- Extrapolation methods and examples when there is a phase transition
- With a magnetic field: other possible thermodynamic ensembles
- Conclusion and perspectives

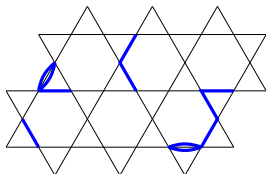
Short introduction to HTSE

- The partition function $Z(\beta, h)$ gives access to many thermodynamic quantities:

$$c_V = \frac{\partial e}{\partial T} = \beta^2 \frac{\partial^2 \frac{\ln Z}{N}}{\partial \beta^2}, \quad \chi = \frac{1}{\beta h} \frac{\partial \frac{\ln Z}{N}}{\partial h}.$$

- We expand Z at $\beta = 0$ (\rightarrow SSE):

$$Z = \text{Tr} e^{-\beta \hat{H}} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \underbrace{\langle \hat{H}^n \rangle_{\beta=0}}_{\text{Moment, } \propto N^n}$$



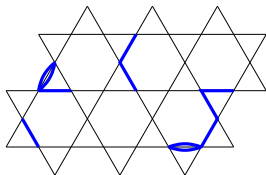
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- $\ln Z$ discards disconnected clusters.

$$\frac{\ln Z}{N} = \ln z_0 + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \frac{1}{N} \underbrace{[\hat{H}^{(n)}]}_{\text{Cumulant, } \propto N}$$



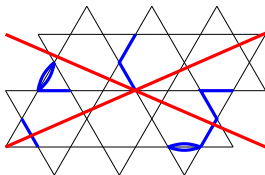
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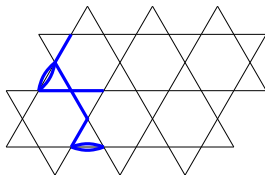
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How to get coefficients up to order n

$$\hat{H} = J_1 \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + h \sum_i \hat{S}_i^z$$

- Coefficients are polynomials in J_1 , J_2 , h ...
- Most HTSE expansions only calculate the 0th and 1st order in h .
- h has a special role as
 - ✓ it is a one-site term,
 - ✓ $[\hat{H}, \hat{S}_{\text{tot}}^z] = 0$,
 - ✓ it is tunable and gives information on the model (magnetic susceptibility, magnetization plateaus)

We developed an expansion at fixed $x = \beta h$:

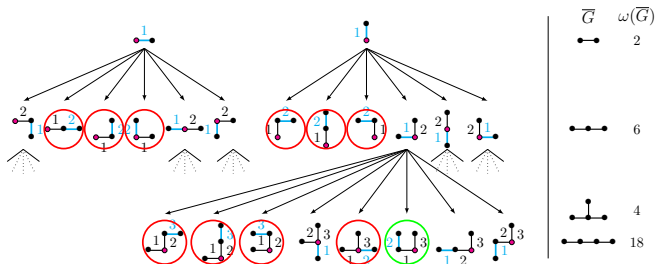
$$\frac{\ln Z}{N}(\beta, J_1, J_2, h) = \ln \left(\frac{\text{Tr} e^{-\beta \hat{H}}}{\text{Tr}(I)} 2^{N_s} \right) = \ln 2 + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{N n!} [\hat{H}^{(n)}]$$

$$\rightarrow \frac{\ln Z}{N}(\beta, J_1, J_2, x) = \ln \left(\frac{\text{Tr} \left(e^{-\beta \hat{H}_J} e^{x \hat{S}_{\text{tot}}^z} \right)}{\text{Tr} \left(e^{x \hat{S}_{\text{tot}}^z} \right)} \gamma^{N_s} \right) = \ln z_0(x) + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{N n!} \left[\hat{H}^{(n)} \right].$$

How to get coefficients up to order n

$$\frac{\ln Z}{N} = \ln z_0 + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \frac{1}{N} [\hat{H}^{(n)}]$$

- First, the **connected simple graphs** up to n links are enumerated,



- For each of them G , the contribution to orders $\leq n$, $F(G)$ is determined through trace calculations: $\langle \hat{H}_G \rangle, \langle \hat{H}_G^2 \rangle, \dots, \langle \hat{H}_G^n \rangle$ using the linked cluster expansion:

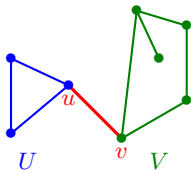
$$F(G) = \sum_{U \in \mathbb{N}_{>0}^G} \frac{J^U[U]}{U!}$$

How to get coefficients up to order n

Two useful formulas limit the time of trace calculations ($t \sim 4^{N_s} n N_I / \sqrt{N_s}$) using $\theta = \tanh \frac{x}{2}$:

- For a simple graph G with a bridge:

$$\llbracket G \rrbracket = \llbracket U, u \leftrightarrow v, V \rrbracket = \frac{2}{\theta^2} \llbracket U, u \leftrightarrow v \rrbracket \llbracket u \leftrightarrow v, V \rrbracket,$$

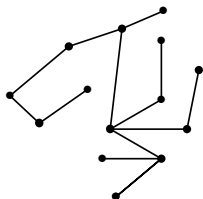


- For a tree T with $N_l \geq 2$:

$$\llbracket T \rrbracket = \frac{1}{2} \prod_{s \in \text{sites of } T} 2C_{d^{\circ}s},$$

where $d^{\circ}s$ is the degree of site s , and:

$$C_1 = \frac{\theta}{2}, \quad C_{k+1} = \frac{dC_k}{dh} = \frac{1-\theta^2}{2} \frac{dC_k}{d\theta}.$$



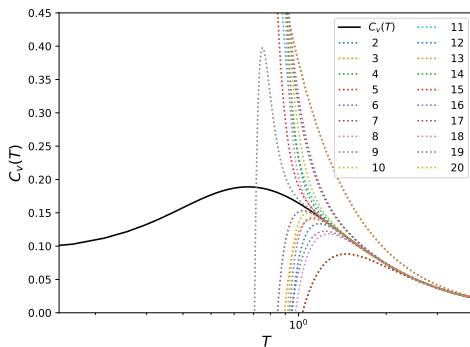
Plan

- Introduction to HTSE
- **Extrapolation when there is no phase transition**
 - ✓ How to sum the series ?
 - ✓ The entropy method
 - ✓ Herbertsmithite
- Extrapolation methods and examples when there is a phase transition
- With a magnetic field: other possible thermodynamic ensembles
- Conclusion and perspectives

The entropy method, example of kagome AF ($n = 20$)

- Truncated series

$$c_V = \underbrace{\sum_{i=0}^n c_i \beta^i}_{c_V^{trunc}} + \mathcal{O}(x^n)$$



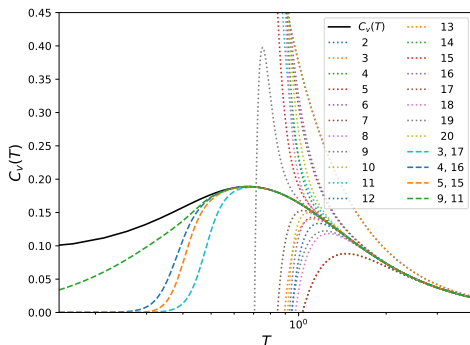
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- Pade approximants:

$$c_V = \underbrace{\frac{P_p(\beta)}{Q_q(\beta)}}_{c_V^{[p,q]}} + \mathcal{O}(x^n)$$



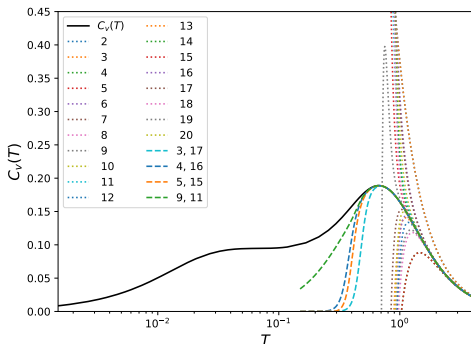
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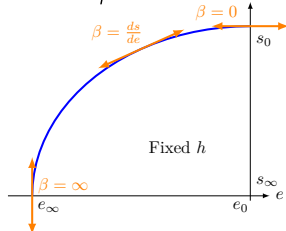
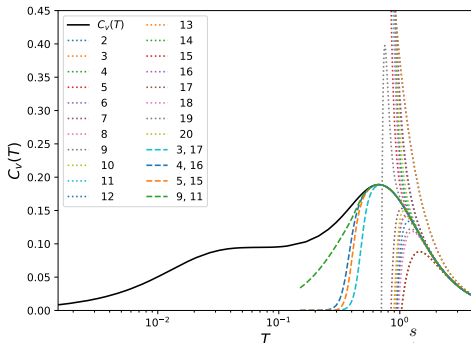
- Pade approximants:

$$c_V = \underbrace{\frac{P_p(\beta)}{Q_q(\beta)}}_{c_V^{[p,q]}} + \mathcal{O}(x^n)$$

- The entropy method verifies sum rules:

$$\int_0^\infty \frac{c_V}{T} dT = \int_{T=0}^{T=\infty} ds$$

$$\int_0^\infty c_V dT = \int_{T=0}^{T=\infty} de$$



Bernu et al, PRB **63**, 134409 (2001)

Bernu et al, PRL **114**, 057201 (2015)

The entropy method

Derivation of the truncated series $e^{trunc}(\beta)$ and $s^{trunc}(\beta)$.

Combination of $e^{trunc}(\beta)$ and $s^{trunc}(\beta)$ to get $s^{trunc}(e)$

Choice of a G function non singular at e_0 .

For non gapped systems $s(e) \sim_{e_0} (e - e_0)^{\frac{\alpha}{1+\alpha}}$

$$G(e) = s(e)^{1+\frac{1}{\alpha}} / (e - e_0).$$

Pade approximant

Inverse transformation $G \rightarrow s$

Free energy: $s \rightarrow f$

$$\frac{1}{T} = \frac{ds}{de}, \quad c_V(e) = \frac{s'(e)^2}{s''(e)}$$

$$\ln z^{trunc}(\beta) = \sum_i z_i \beta^i$$



$$s^{trunc}(e) = \sum_i s_i e^i$$



$$G^{trunc}(e) = \sum_i g_i e^i$$



$$G^{[p,q]}(e) = \frac{P_p(e)}{Q_q(e)}$$



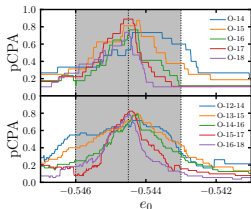
$$s^{extra}(e)$$



$$e(T), c_V(T) \dots$$

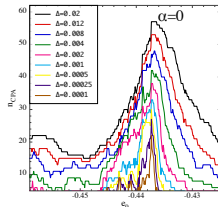
The entropy method: hypotheses

1. The **singularity at e_0** depends on the ground state nature.
2. e_0 is either known (ferromagnet), or approximately known, or not known at all...
 → n_{CPA} : number of coinciding Padé app.: most probable e_0 .



Triangular J_1

Gonzalez et al, arXiv:2112.08128 (2021)



Kagome J_1

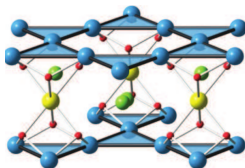
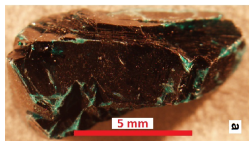
Bernu et al, PRB **101**, 140403 (2021)

$$e_{\text{DMRG}} = -0.4386(5)$$

3. $e_0(h) = e_0 - \chi_0 \frac{h^2}{2} + o(h^2)$, and χ_0 is another hypothesis to get $\chi(T) = \frac{s'_h}{hs'_e}$.

Application: Herbertsmithite $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$

- Synthesis of Herbertsmithite crystals (\neq powder) $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$.
Han et al, Nature 492, 406 (2012), Zorko et al., PRL 118, 017202 (2017)



- Mainly a kagome lattice with 1st neighbor Heisenberg interactions, with a rate ρ of impurities:

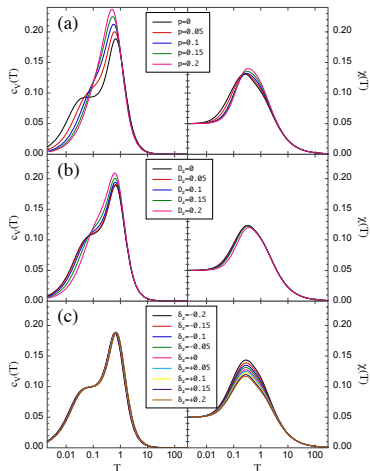
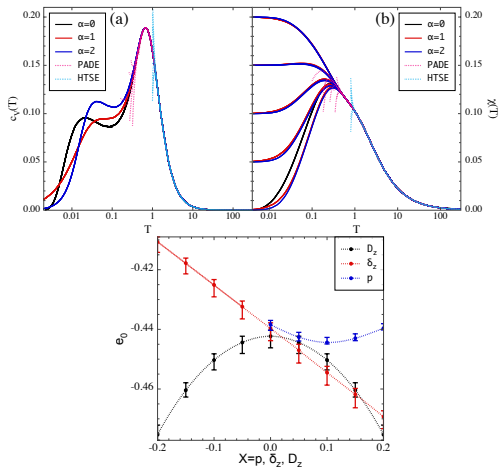
$$H = J_1 \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j + \delta S_i^z S_j^z) + D_z \sum_{\langle i,j \rangle} (\mathbf{S}_i \wedge \mathbf{S}_j)_z - h \sum_i S_i^z$$

- Highly debated nature of the ground state.

Application: Herbertsmithite $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$

Studied perturbations: magnetic vacancies (p), DM (D_z), Ising anisotropy (δ_z), J_2 , J_3 , J_{3h} .

Bernu et al, PRB **101**, 140403 (2020)



Application: Herbertsmithite $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$

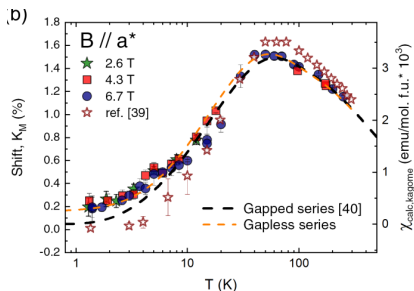
Experimental results

$\chi_0 \neq 0$ (observed by NMR)

→ ungapped ground state.

$U(1)$ spin liquid ?

Khuntia et al, Nat. Phys. **16**, 469 (2020)



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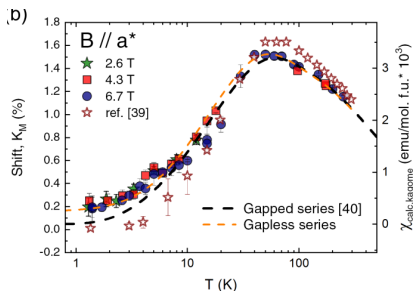
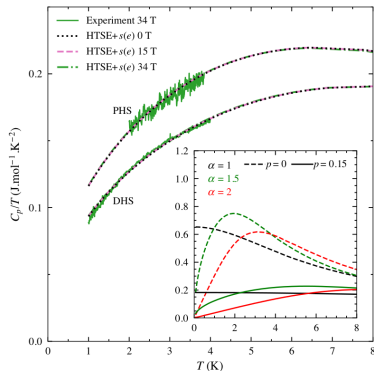
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Khuntia et al, Nat. Phys. **16**, 469 (2020)



C_V measurements at high h - low T .

→ $C_V \sim AT^{1.5}$.

No model to explain this...

Barthelemy et al, PRX **12**, 011014 (2022)

Plan

- Introduction to HTSE
- Extrapolation when there is no phase transition
- **Extrapolation when there is a phase transition**
 - ✓ How to directly extract information from the coefficients ?
 - ✓ When $c_v \sim A \ln(1 - \beta/\beta_c)$ (2d-Ising like phase transition)
 - ✓ When $c_v \sim B - \frac{A}{(\beta_c - \beta)^\alpha}$ (3d-Heisenberg like phase transition)
- With a magnetic field: other possible thermodynamic ensembles
- Conclusion and perspectives

Directly extract informations from HTSE

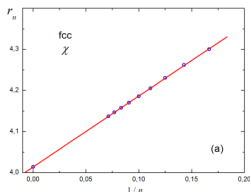
When a finite T phase transition occurs, real singularity at T_c :

$$f(\beta) \sim A(\beta - \beta_c)^\alpha, \quad f(\beta) = \sum_i f_i \beta^i$$

- The ratio method

$$\frac{f_i}{f_{i-1}} = T_c \frac{i - \alpha}{i + 1} \simeq T_c - \frac{\alpha T_c}{i}$$

→ α and T_c obtained from $\frac{f_i}{f_{i-1}}$ vs $1/i$.



Kuzmin (2019)

- The Dlog-Pade method:

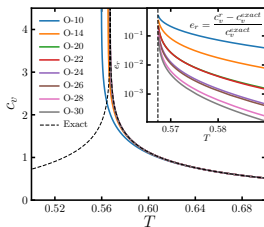
$$\frac{d}{d\beta} \ln f(\beta) = \sum_i c_i \beta^i = \frac{P(\beta)}{Q(\beta)} + \mathcal{O}(\beta^n) \sim \frac{\alpha}{\beta - \beta_c}$$

→ α and T_c obtained from statistics on the poles of Q .

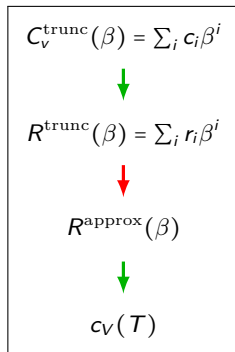
The 2d-Ising class: extrapolation method

- Exact *solution* known for many 2d Ising models, but others remain unsolved, either similar (XXZ) or very different ones (square $J_1 - J_2$).
- Previously: HTSE of $\chi(\beta) \rightarrow \gamma$ and T_c (ratio, Dlog methods).
- Only the regular part $R(\beta)$ of $c_V(\beta)$ is extrapolated:

$$c_V(\beta < \beta_c) = R(\beta) + A \ln \left(1 - \frac{\beta}{\beta_c} \right),$$

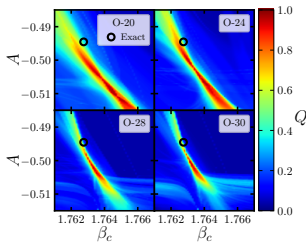


Gonzalez, Bernu, Pierre, LM, PRB **104** 165113 (2021)



The 2d-Ising class: hypotheses, application

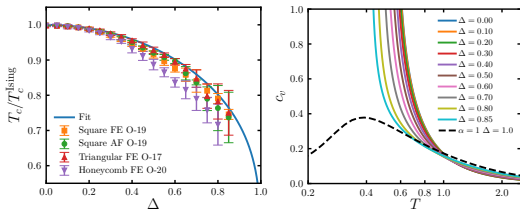
- $R^{\text{trunc}}(\beta) \rightarrow R^{\text{approx}}(\beta)$
The amplitude A of the singularity and the critical temperature $1/\beta_c$ depends on the model.
- ... what are A and β_c ?
They are known (Ising models), or not.
→ quality function $Q(A, \beta_c)$, as previously for e_0 .



Quality, F-square.

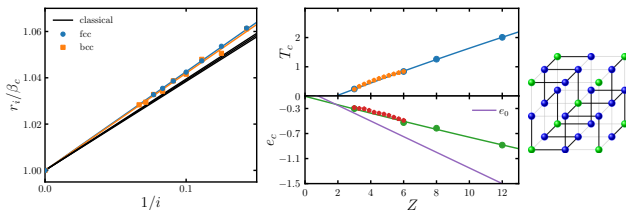
Application to the XXZ model: $H = -\sum_{\langle i,j \rangle} (S_i^z S_j^z + \Delta S_i^{\pm} \cdot S_j^{\pm})$

Gonzalez, Bernu, Pierre, LM, PRB 104, 165113 (2021)



3d Heisenberg like phase transition (fcc, bcc, sc...)

- No exact solution for 3d ferromagnetic Heisenberg models.
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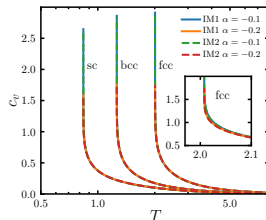


- HTSE of $C_v(T)$, with a cusp ($\alpha < 0$):

$$C_v(\beta < \beta_c) = R(\beta) + A(\beta_c - \beta)^{-\alpha},$$

→ extraction of T_c , A , α

→ reconstruction of $C_v(\beta < \beta_c)$.



Gonzalez et al, draft

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We developed an expansion at fixed $x = \beta h$:

$$\frac{\ln Z}{N}(\beta, J_1, J_2, h) = \ln \left(\frac{\text{Tr} e^{-\beta \hat{H}}}{\text{Tr}(I)} 2^{N_s} \right) = \ln 2 + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{N n!} [\hat{H}^{(n)}]$$

$$\rightarrow \frac{\ln Z}{N}(\beta, J_1, J_2, x) = \ln \left(\frac{\text{Tr} \left(e^{-\beta \hat{H}_J} e^{x \hat{S}_{\text{tot}}^z} \right)}{\text{Tr} \left(e^{x \hat{S}_{\text{tot}}^z} \right)} \gamma^{N_s} \right) = \ln z_0(x) + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{N n!} \left[\hat{H}^{(n)} \right].$$

How to get coefficients up to order n

$$H = H_0 - h \sum_i S_i^z,$$

$$z_0 = e^{-\frac{x}{2}} + e^{\beta \frac{x}{2}} = 2 \cosh\left(\frac{x}{2}\right)$$

Expanding in β and in h

$$\begin{aligned} & \frac{\ln Z}{N}(\beta, J_1, J_2, h) \\ &= \ln \left(\frac{\text{Tr} e^{-\beta \hat{H}}}{\text{Tr}(I)} 2^{N_s} \right) \\ &= \ln 2 + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{Nn!} \left[\hat{H}^{(n)} \right] \end{aligned}$$

$\beta \rightarrow \infty$: free spins, $Z = 2^N$.

Considering $x = \beta h$ as an independent variable

$$\begin{aligned} & \frac{\ln Z}{N}(\beta, J_1, J_2, x) \\ &= \ln \left(\frac{\text{Tr} \left(e^{-\beta \hat{H}_J} e^{x \hat{S}_{\text{tot}}^z} \right)}{\text{Tr} \left(e^{x \hat{S}_{\text{tot}}^z} \right)} \gamma^{N_s} \right) \\ &= \ln z_0(x) + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{Nn!} \left[\hat{H}^{(n)} \right]. \end{aligned}$$

$\beta \rightarrow \infty$: non interacting spins under a magnetic field, $Z = z_0^N$.

Consequences on the entropy method

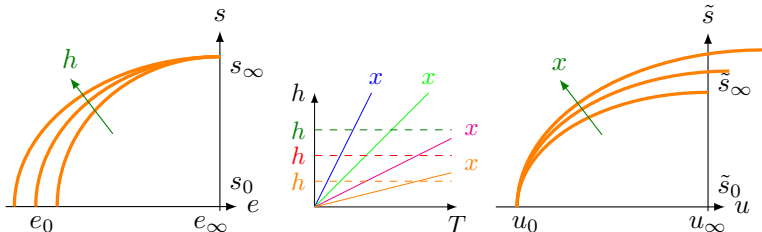
- A bit of thermodynamics: Legendre transformations.

$$\ln Z(\beta, h) = s(e, h) - \beta e, \quad \beta = \left. \frac{\partial s}{\partial e} \right|_h, \quad e = \left. \frac{\partial \ln Z}{\partial \beta} \right|_h$$

$$\ln Z(\beta, x) = \tilde{s}(u, x) - \beta u, \quad \beta = \left. \frac{\partial \tilde{s}}{\partial u} \right|_x, \quad u = \left. \frac{\partial \ln Z}{\partial \beta} \right|_x$$

- Definition of

- ✓ an internal energy: $u = e + mh$
- ✓ a pseudo-entropy: $\tilde{s} = s + mx$.



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$$\ln Z(\beta, x) = s(u, m) + xm - \beta u, \quad \beta = \left. \frac{\partial s}{\partial u} \right|_m, \quad u = \left. \frac{\partial \ln Z}{\partial \beta} \right|_x$$
$$x = \left. \frac{\partial s}{\partial m} \right|_u, \quad m = \left. \frac{\partial \ln Z}{\partial x} \right|_\beta$$

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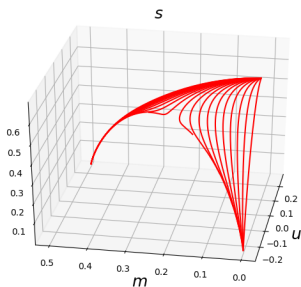
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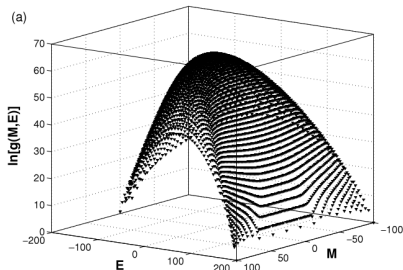
$$\ln Z(\beta, x) = s(u, m) + xm - \beta u, \quad \beta = \left. \frac{\partial s}{\partial u} \right|_m, \quad u = \left. \frac{\partial \ln Z}{\partial \beta} \right|_x$$

New thermodynamic ensemble with (u, m) fixed.

$$s(u, m) = \ln g(u, m).$$



$\beta = 0$ to ∞ trajectories (h fixed)



Wang-Landau simulations.

Wang et al, J. Stat. Mech., L05001 (2007)

Conclusion

- HTSE up to ~ 20 orders, for many lattices and interactions:
 - ✓ Any lattice (1D, 2D, 3D)
 - ✓ $S = 1/2$ only
 - ✓ 1st, 2nd... neighbor Heisenberg interactions
 - ✓ Magnetic random vacancies,
 - ✓ Ising anisotropy.
 - ✓ DM interaction.
- Entropy method with self-consistent determination of e_0 (Sum rules are implicitly taken into) or C_v extrapolation for phase transitions (log/cusp singularities).
- Several thermodynamic ensembles are possible ($\{e, h\}$, $\{u, x\}$, $\{u, m\}$).
- Perspectives
 - Extension to other models ($S > 1/2$, $\mathbf{h} \perp \mathbf{e}_z \dots$),
 - Mathematical study of the singularities in the complex plane, as the Fisher and Yang-Lee zeros,
 - Stochastic evaluation of large order terms ?

Thank you !