Overview of the possibilities of high temperature series expansions

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Centro de Ciencias de Benasque Pedro Pascual
Entanglement in Strongly Correlated Systems,
February 20 to March 5, 2022

Plan

- Introduction
  - ✓ Objectives
  - ✓ Thermodynamical quantities
- The High Temperature Series Expansion (HTSE) coefficients
  - ✓ How they are obtained ?
  - ✓ How to sum the series ?
  - ✓ How to directly extract information from the coefficients ?
- The toolkit of extrapolation methods, with examples
  - ✓ When there is no phase transition: the entropy method
  - ✓ 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

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Objectives

One aspect is purely theoretical: what are the properties of a spin lattice model ?

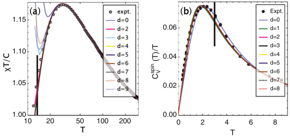
Another is experimental: how to fit experimental measurements with a model ?

The model is then a compromise between:

- accuracy (many parameters),
- simplicity (few parameters).

Magnetic compound

Thermodynamic measurements



Kapellasite, PRB **87**, 155107 (2013)

Model Hamiltonian

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

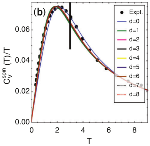
Thermodynamic quantities

Experiments:

- Thermodynamic quantities that are probed experimentally:
  - ✓ Specific heat $C_v = \frac{1}{N}\frac{\partial E}{\partial T}$,
  - ✓ Magnetic susceptibility $\chi = \frac{1}{N}\frac{m}{h}$ $(\neq \frac{1}{N}\frac{\partial m}{\partial h})$.
- Deviations due to:
  - ✓ Phonons at large T in $C_v \to$ subtraction.
  - ✓ Impurities at low T in $\chi \to$ Curie tails.

Theory: what do we know ?

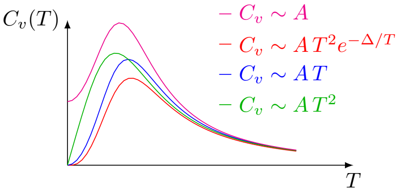
- Low-T behavior: depends on the ground state nature, on low energy excitations (a gap ?)
- High temperatures: accessible via high temperature series expansions (HTSE).
- Can we access the intermediate temperature range ?



Thermodynamic quantities: $C_v = dE/dT$

Low-T behavior of C_v

- A classical long-range order (LRO): $C_v \sim \frac{n}{2}$ (n soft modes).
- A quantum ferromagnetic LRO: $C_v \sim AT^{d/2}$ (d: dimension).
  Spin waves $\longrightarrow$ quadratic bosonic excitations
- A quantum antiferromagnetic LRO: $C_v \sim AT^d$.
  Spin waves $\longrightarrow$ linear bosonic excitations
- A gapped phase: $C_v \sim AT^2 e^{-\Delta/T}$ (Δ: gap).
- A Dirac spin liquid: $C_v \sim AT^d$.
  $\longrightarrow$ conic fermionic dispersion relation
- A Fermi surface spin liquid: $C_v \sim AT^{d-1}$.



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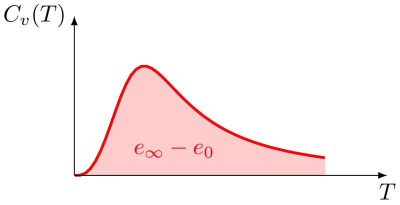

Sum rules:

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

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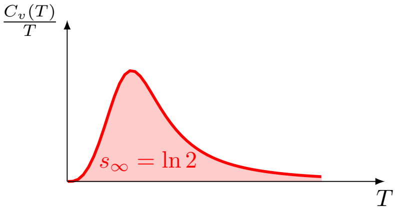

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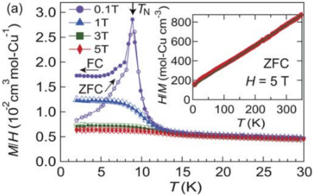
Thermodynamic quantities: $\chi = m/h$

Curie-law:

$$\chi \sim \frac{C}{T-\theta}, \quad \theta = -S(S+1)\sum_{j(i)} J_{ij}$$



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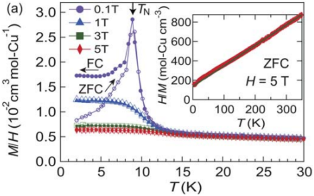
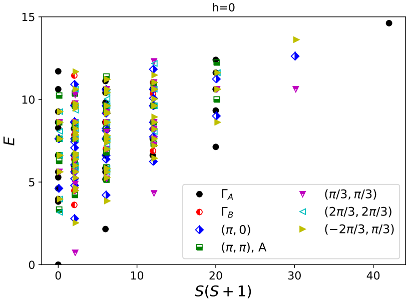


Low-T behavior of χ

Typical exact diagonalization results (figures from Sylvain Capponi):



- For a gapped phase: $\chi(T=0, h=0) = 0$
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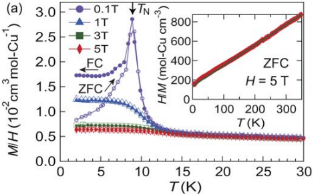

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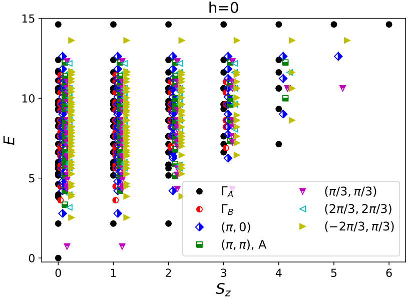

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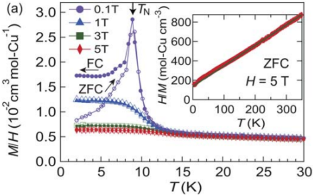

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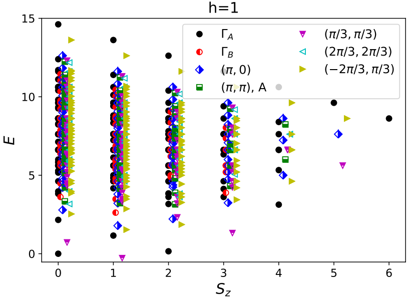

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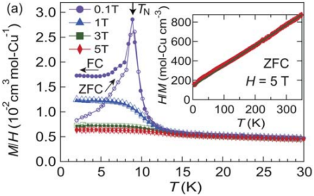

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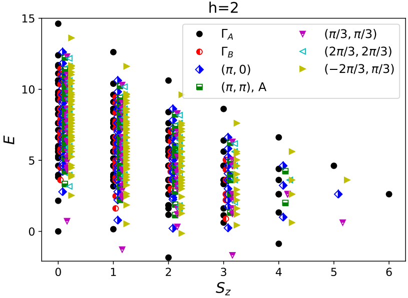

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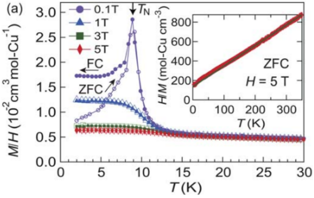

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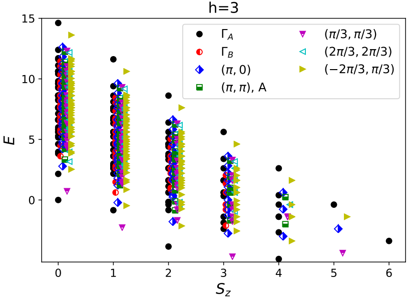

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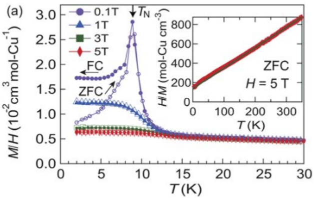

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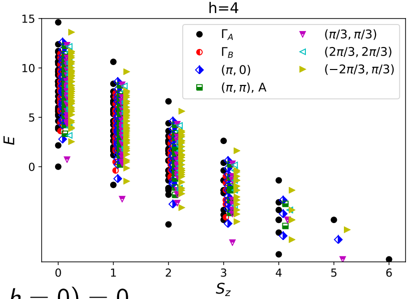

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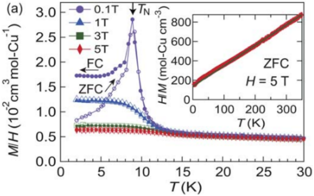

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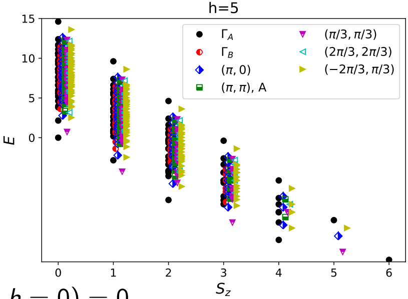

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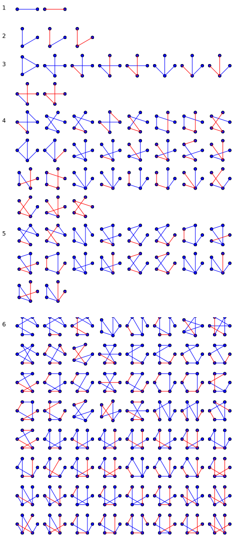
How to obtain the HTSE coefficients ?

kagome, 1st and 3rd neighbors:



- The partition function $Z(\beta, h)$ gives everything:

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

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

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle H^n \rangle_{\beta=0}$$

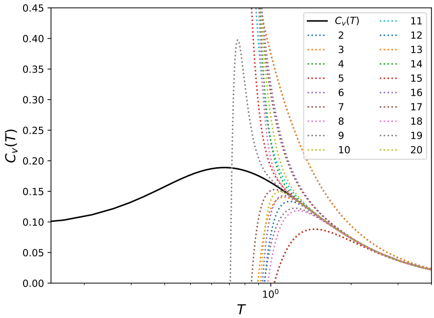
- $\ln Z$ discards disconnected clusters.

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

Summation of HTSE, kagome AF (order 20)

- Truncated series

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



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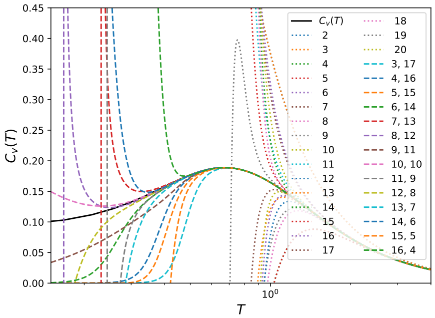

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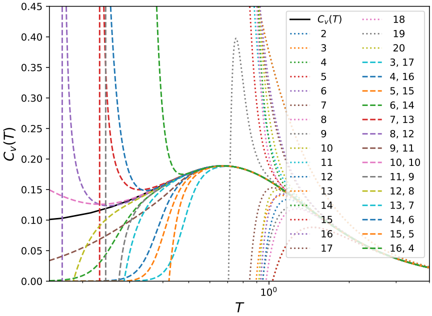
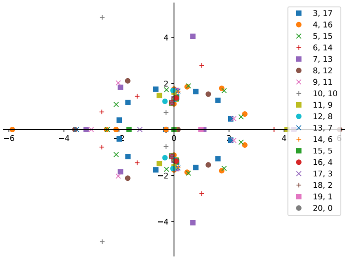
Singularities in the $\mathbb{C}$-plane.





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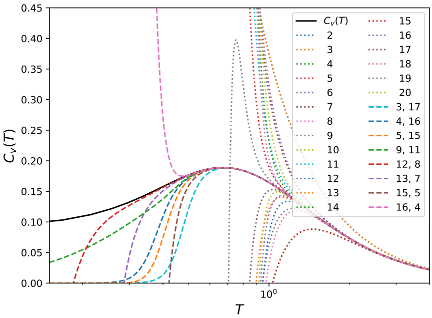

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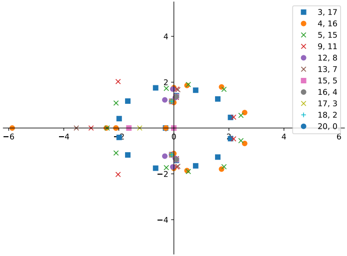

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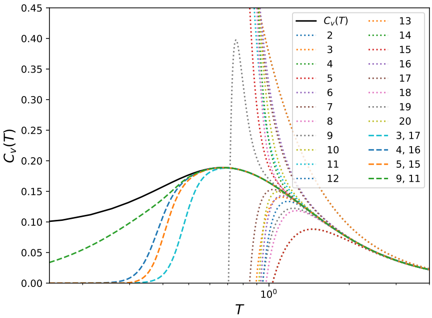

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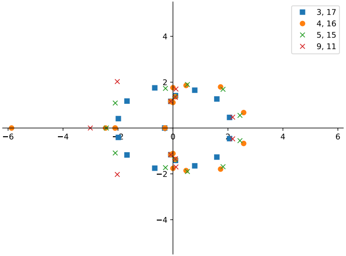

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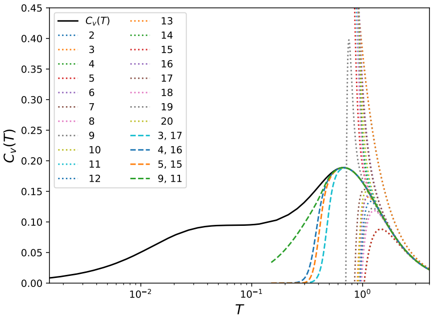
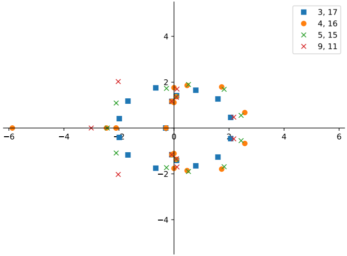




Directly extract informations from HTSE

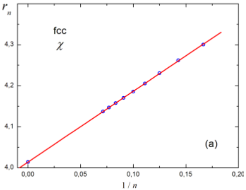
When a finite T phase transition occurs, real singularity at T_c:

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

- The ratio method

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

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



Kuzmin (2019)

- The Dlog-Pade method:

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

$\longrightarrow \alpha$ and T_c obtained from statistics on the poles of Q.

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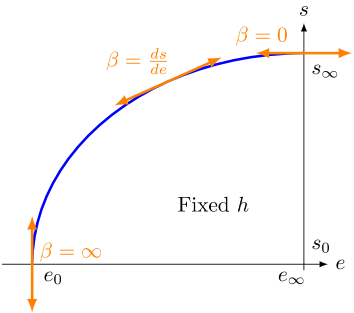
The entropy method (no phase transition)

$$f = -T\frac{\ln Z}{N} = e - Ts, \qquad \frac{\ln Z}{N} = s - \beta e$$

Low temperature behavior is imposed to $s(e)$.

$\rightarrow$ the sum rules are automatically verified.

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



$$\frac{\ln Z^{\mathrm{trunc}}}{N}(\beta) = \sum_i z_i \beta^i$$

↓

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

↓

$$s^{\mathrm{approx}}(e)$$

↓

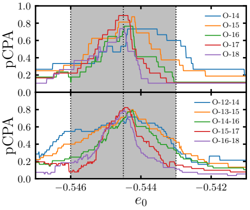
$$\chi(T), c_V(T) \ldots$$

$$c_V(e) = -\frac{s'^2}{s''}$$

The entropy method: difficulties

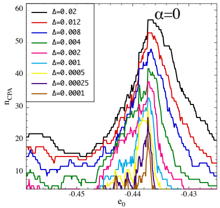
- Unsure step: $s^{\mathrm{trunc}}(e) \rightarrow s^{\mathrm{approx}}(e)$.
  We have to take care of the singularity at e_0, whose type depends on the ground state nature.

- By the way... what is e_0 ?
  Sometimes it is known (ferromagnet), or approximatively known.
  Sometimes not...
  $\longrightarrow n_{\mathrm{CPA}}$: number of coinciding Padé app.: most probable e_0.



Triangular J_1

Gonzalez et al, arXiv:2112.08128 (2021)



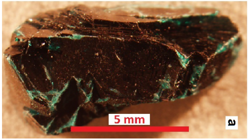
Kagome J_1

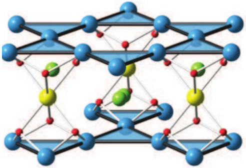
Bernu et al, PRB **101**, 140403 (2021)

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

Application: Herbertsmithite $Cu_3Zn(OH)_6Cl_2$

- Synthesis of Herbertsmithite crystals ($\neq$ powder) $ZnCu_3(OD)_6Cl$.
  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 p of impurities:

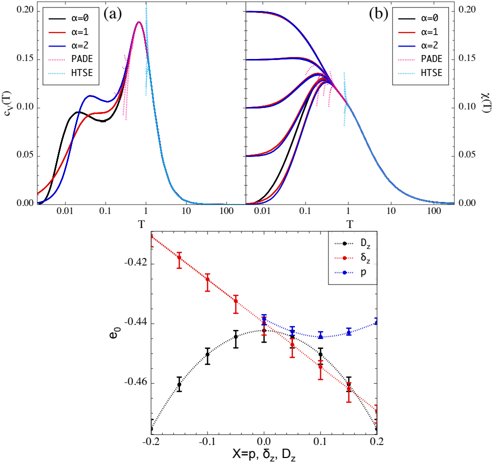
$$H = J_1 \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j + \delta S_i^z S_j^z \right) + D_z \sum_{\langle i,j \rangle} (\mathbf{S}_i \wedge \mathbf{S}_j)_z - h \sum_i S_i^z$$

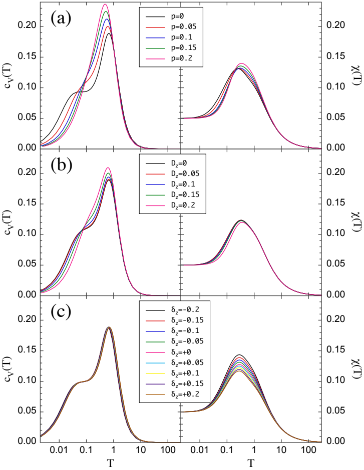
- Highly debated nature of the ground state.

Application: Herbertsmithite $Cu_3Zn(OH)_6Cl_2$

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 $Cu_3Zn(OH)_6Cl_2$

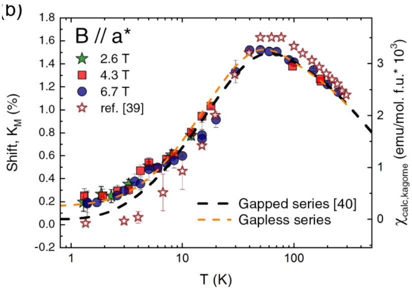
Experimental results

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

$\longrightarrow$ ungapped ground state.

$U(1)$ spin liquid ?

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



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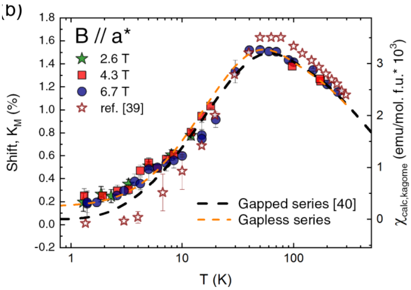
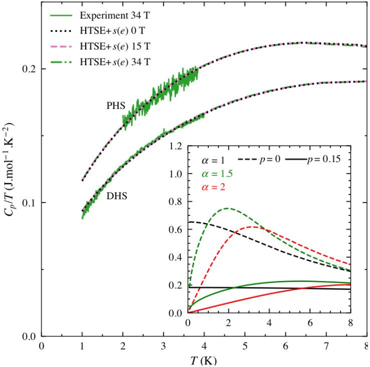




C_v measurements at high h - low T.
$\longrightarrow C_v \sim A\,T^{1.5}$.
No model to explain this...

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

Plan

- Introduction
  - ✓ Objectives
  - ✓ Thermodynamical quantities
- The High Temperature Series Expansion (HTSE) coefficients
  - ✓ How they are obtained ?
  - ✓ How to sum the series ?
  - ✓ How to directly extract information from the coefficients ?
- The toolkit of extrapolation methods, with examples
  - ✓ When there is no phase transition: the entropy method
  - ✓ 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

2d Ising like phase transition

- The *solution* of 2d Ising models is known on many lattices.
  $\longrightarrow T_c$, $C_v(T)$ exact formula.
- Similar models (same universality class) remain unsolved (XXZ),
- Different models share the same universality class (square $J_1 - J_2$), with emergent order parameters.
- Previously: HTSE of $\chi(\beta) \longrightarrow \gamma$ and T_c (ratio, Dlog methods).
- We focus on the HTSE of $C_v(T)$, knowing that

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

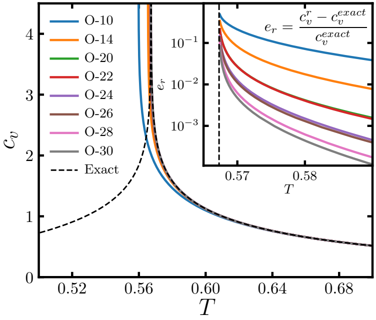
  we will extract T_c, A and reconstruct the $C_v(\beta < \beta_c)$ function.

2d Ising like phase transition, reconstruction method

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

$\beta \sim \beta_c$ behavior is imposed to $C_v(\beta)$.

$\rightarrow$ we extrapolate the regular part $R(\beta)$ only.



$C_v^{\mathrm{trunc}}(\beta) = \sum_i c_i \beta^i$

↓

$R^{\mathrm{trunc}}(\beta) = \sum_i r_i \beta^i$

↓

$R^{\mathrm{approx}}(\beta)$

↓

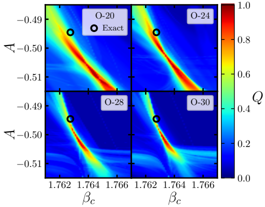
$c_V(T)$

Gonzalez et al, PRB **104** 165113 (2021)

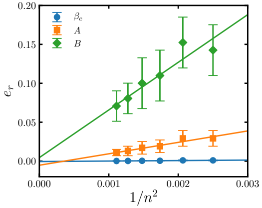
The reconstruction method: difficulties

- Unsure step: $R^{\text{trunc}}(\beta) \rightarrow R^{\text{approx}}(\beta)$.
  We have to take care of the singularity at β_c, whose amplitude A depends on the model.

- By the way... what are A and β_c ?
  Sometimes they are known (Ising models), or approximatively known.
  If not $\longrightarrow$ quality function: most probable A and β_c.



Quality map, square J1 model



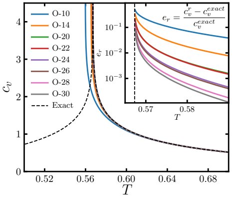
Convergence of A and β_c.

Gonzalez et al, PRB **104**, 165113 (2021)

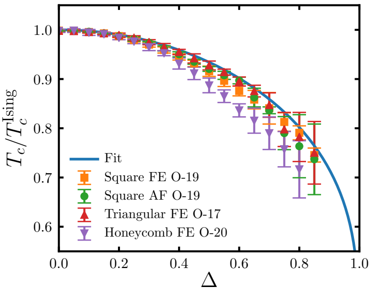
Application: XXZ ferromagnetic models

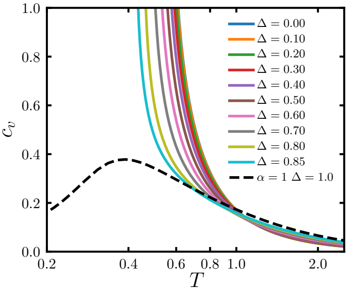
$$H = -\sum_{\langle i,j \rangle} (S_i^z S_j^z + \Delta \mathbf{S}_i^\perp \cdot \mathbf{S}_j^\perp)$$

Novelty: $C_v(T)$ not only near β_c, but for any $\beta < \beta_c$, in the thermodynamic limit.



$\Delta = 0$, square AF lattice.





Gonzalez et al, PRB **104**, 165113 (2021)

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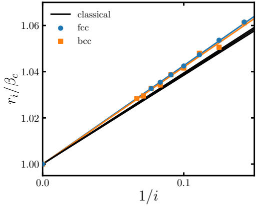
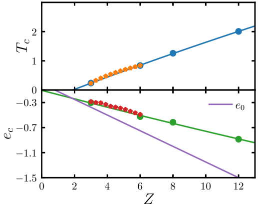
- With a magnetic field: other possible thermodynamic ensembles

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

- No exact solution for 3d ferromagnetic Heisenberg models.
- Previously: HTSE of $\chi(\beta) \longrightarrow \gamma$ and T_c (ratio, Dlog methods).

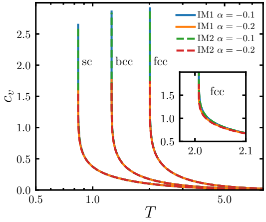




- HTSE of $C_v(T)$, with a cusp ($\alpha < 0$):

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

$\longrightarrow$ extraction of T_c, A, α
$\longrightarrow$ reconstruction of $C_v(\beta < \beta_c)$.



Gonzalez et al, draft

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- With a magnetic field: other possible thermodynamic ensembles

With a magnetic field h

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

$$Z = \mathrm{Tr} e^{-\beta H} = \mathrm{Tr}(e^{-\beta H_0} e^{\beta h S^z}) = \sum_{k=0|\frac{1}{2}}^{N/2} \underbrace{2\cosh(kx)}_{P_k(z_0^2)} \mathrm{Tr}_{(S_z=k)} \left(e^{-\beta H_0}\right)$$

- Expanding in β and in h

$$\frac{\ln Z(\beta, h)}{N} = \ln 2 + \sum_{i=1}^{\infty} \left(\sum_{k=0}^{i} Q_{i,k} h^k \right) \beta^i.$$

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

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

$$\frac{\ln Z(\beta, x)}{N} = \ln z_0 + \sum_{i=1}^{\infty} \left(\sum_{k=0}^{i} P_{i,k} {z_0}^{-2k} \right) \beta^i.$$

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

$$x = \beta h$$

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

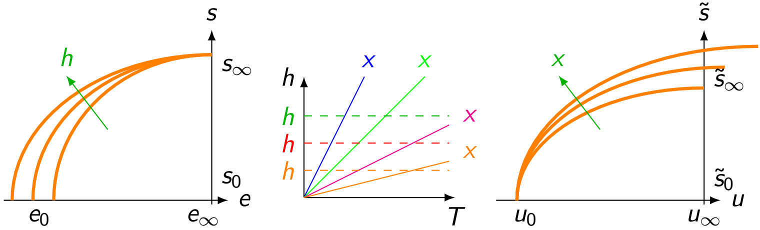
Consequences on the entropy method

- A bit of thermodynamics: Legendre transformations.

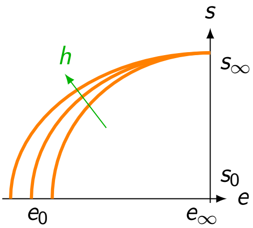
$$\ln Z(\beta, h) = s(e, h) - \beta e, \qquad \beta = \left.\frac{\partial s}{\partial e}\right|_h, \qquad e = \left.\frac{\partial \ln Z}{\partial \beta}\right|_h$$

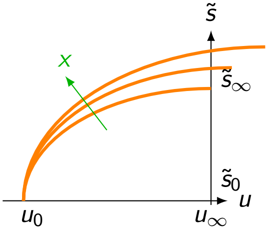
$$\ln Z(\beta, x) = \tilde{s}(u, x) - \beta u, \qquad \beta = \left.\frac{\partial \tilde{s}}{\partial u}\right|_x, \qquad u = \left.\frac{\partial \ln Z}{\partial \beta}\right|_x$$

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



Thermodynamic quantities in practice





	With $s(e,h)$	With $\tilde{s}(u,x)$
c_V	$-\frac{s'^2}{s''}$	$-\frac{1}{\tilde{s}''}\left(\tilde{s}' - x\left.\frac{\partial \tilde{s}'}{\partial x}\right\|_u\right)^2 + x^2\left.\frac{\partial^2 \tilde{s}}{\partial x^2}\right\|_u$
m	$\frac{1}{s'}\left.\frac{\partial s}{\partial h}\right\|_e$	$\left.\frac{\partial \tilde{s}}{\partial x}\right\|_u$
$\chi(T=0)$	$-\frac{d^2 e_\infty}{dh^2}$	$\frac{\tilde{s}'}{x}\left.\frac{\partial \tilde{s}}{\partial x}\right\|_{u_\infty}$

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  - ✓ a pseudo-energy: $u = e + mh$
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$$\ln Z(\beta, x) = s(u, m) + xm - \beta u, \qquad \beta = \left.\frac{\partial s}{\partial u}\right|_m, \qquad u = \left.\frac{\partial \ln Z}{\partial \beta}\right|_x$$

$$x = \left.\frac{\partial s}{\partial m}\right|_u, \qquad m = \left.\frac{\partial \ln Z}{\partial x}\right|_\beta$$

- Definition of
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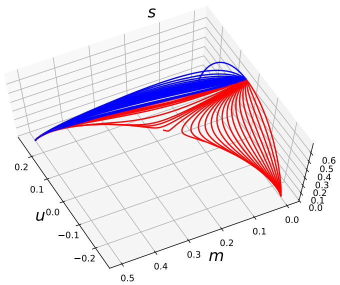
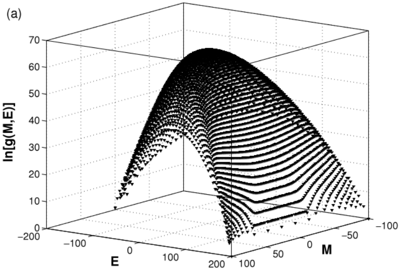
New thermodynamic ensemble with (u, m) fixed.
$s(u, m) = \ln g(u, m)$.



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



Wang-Landau simulations.

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

Conclusion

- Sum rules are implicitly taken into account via the entropy method, with self-consistent determination of e_0.
- Methods to reconstruct C_v for phase transitions with log or cusp singularities.
- Current state of the art:
  - ✓ Any lattice (1D, 2D, 3D)
  - ✓ $S = 1/2$ only
  - ✓ 1st, 2nd... neighbor Heisenberg interactions
  - ✓ Magnetic random vacancies,
  - ✓ Ising anisotropy.
  - ✓ DM interaction.
- Change of thermodynamic ensembles open new possibilities: information obtained from HTSE on $g(u, m)$.
- Relation with SSE: sampling of all clusters, versus enumeration of connected clusters for HTSE... In fact, really less informations in SSE ???

THANK YOU !

and (experiments on Herbertsmithite)

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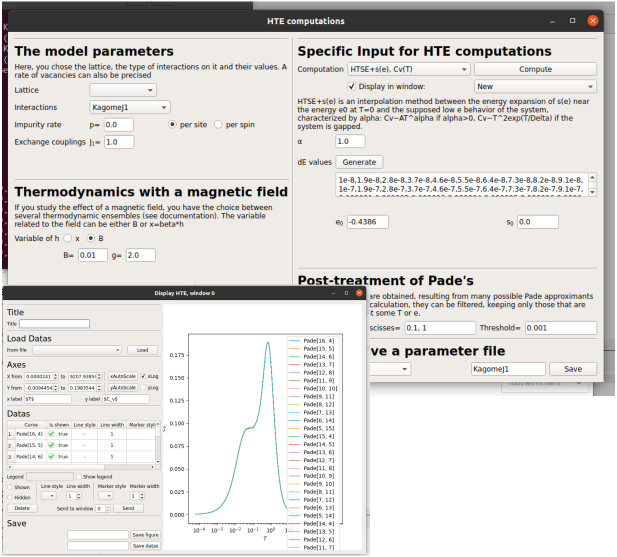
C. Marcenat, A. Demuer, T. Klein, M. Velázquez (Grenoble),
A. Zorko (Slovenia)

The interface



Entropy method

Derivation of the series $e^{tr}(T)$ and $s^{tr}(T)$.
$e(T) = -\frac{d \ln Z}{d\beta}$, $S(T) = \beta e + \ln Z$
Elimination of T in $e^{tr}(T)$ and $s^{tr}(T)$ to get $s^{tr}(e)$

$$\frac{\ln Z^{\rm trunc}}{N}(\beta) = \sum_i z_i \beta^i$$

$$\downarrow$$

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

Choice of a G function regular at e_∞.
For non gapped systems $s(e_\infty) \sim (e - e_\infty)^{\frac{\alpha}{1+\alpha}}$
$G(e) = s(e)^{1+1/\alpha}/(e - e_\infty)$.

$$\downarrow$$

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

Pade approximant

$$\downarrow$$

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

Inverse transformation $G \to s$

$$\downarrow$$

$$s^{\rm approx}(e)$$

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

$$\downarrow$$

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