Spin models in complex magnetic fields:
a hard sign problem

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Motivation

Potts model coupled to complex external fields:

1. Toy model for heavy-dense QCD ($N = 3$ & particular choice of interaction with external field).
2. Analytically solvable in 1D.
3. Sign-problem:
   - ordinary sign-problem: complex & negative weights (representation dependent),
   - irreduzible sign-problem: zeroes of partition function (representation-independent).
4. Alternative representations:
   - flux-variable representation (only for $N = 2,3$ due to equivalence to "clock model"),
   - cluster representation.
5. Edge singularities:
   - benchmark for sign-problem in different representations,
   - related to non-monotonic/oscillatory two-point functions.

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1. Parameters of the Potts partition function

- Partition function for N-state Potts model in d-dimensions:

$$Z_N(\beta, h_0, \ldots, h_{N-1}) = \sum_{\{s\}} \exp\bigg(\sum_x \Big(\beta \sum_{\nu=1}^{d} \big(2\,\delta_{s_x, s_{x+\hat{\nu}}} - 1\big) + \sum_{n=0}^{N-1} h_n\, \delta_{n, s_x}\Big)\bigg)$$

with:

- Potts spin $s_x \in \{0, \ldots, N-1\}$ on each site x,
- inverse temperature $\beta \in \mathbb{R}_+$,
- and N external fields $h_n \in \mathbb{C}$, $n \in \{0, \ldots, N-1\}$ (only $(N-1)$ independent as $\sum_{n=0}^{N-1} \delta_{n,s_x} = 1\ \forall x$).

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- Consider subset of possible external fields:

$$h_n = h\, e^{\frac{2\pi i n}{N}} + h'\, e^{-\frac{2\pi i n}{N}} \quad \text{with} \quad h, h' \in \mathbb{C} \quad .$$

$\rightarrow$ For $N = 3$: toy-model for heavy-dense QCD with $h = e^{-(M-\mu)/T}$ and $h' = e^{-(M+\mu)/T}$.

$\rightarrow$ Will focus on two special cases:

1. $h' = 0$, $h \in \mathbb{C}$,
2. $h + h' = h_R$, $h - h' = h_I$, where $h_R, h_I \in \mathbb{R}$.

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- Partition function in 1D can be written as:

$$Z_{N,L}\left(\beta, h, h'\right) = \mathrm{Tr}\left(T^{L}\left(\beta,h,h'\right)\right)\,,$$

with:

- transfer-matrix $T_{s_x,s_{x+1}}\left(\beta,h,h'\right) = \exp\left(\beta\left(2\delta_{s_x,s_{x+1}} - 1\right) + h\,\frac{P_x + P_{x+1}}{2} + h'\,\frac{P^*_x + P^*_{x+1}}{2}\right)$,
- system size L (periodic),
- and $P_x = \mathrm{e}^{\frac{2\pi\mathrm{i}s_x}{N}}$, $P^*_x = \mathrm{e}^{-\frac{2\pi\mathrm{i}s_x}{N}}$.

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- Eigenvalue decomposition:

$$T(\beta,h,h') = U^{-1}(\beta,h,h')\,\Lambda(\beta,h,h')\,U(\beta,h,h')$$

with:

  - $U(\beta,h,h') \in \mathrm{L}(N,\mathbb{C})$,
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2. Exact solution in 1D: sign problem

- Consider e.g. case 1 ($h' = 0$ and $h \in \mathbb{C}$) :

$$Z_N(\beta,h) = \sum_{\{s\}} \exp\bigg(\sum_x \bigg(\beta \sum_{\nu=1}^{d} \big(2\,\delta_{s_x,s_{x+\hat{\nu}}} - 1\big) + h\,\mathrm{e}^{\frac{2\pi\mathrm{i}s_x}{N}}\bigg)\bigg)$$

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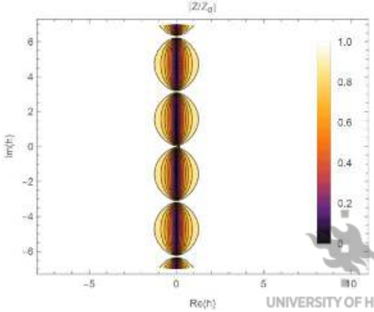

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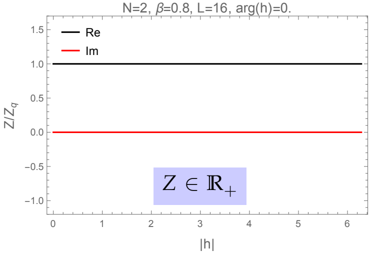

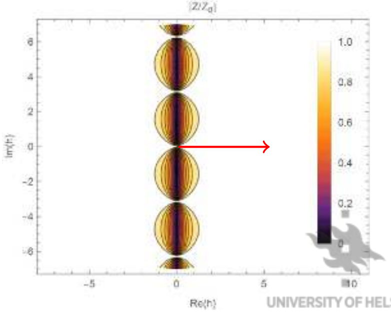

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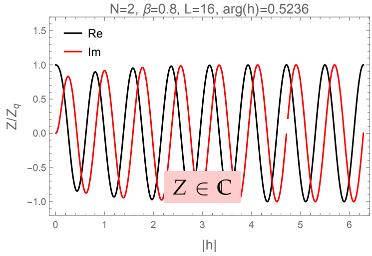

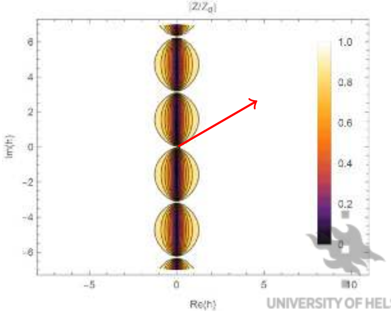

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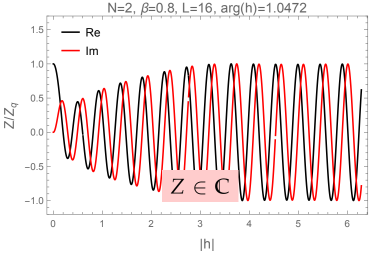

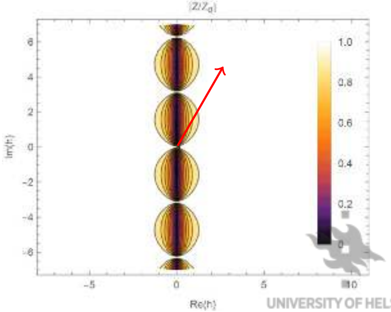

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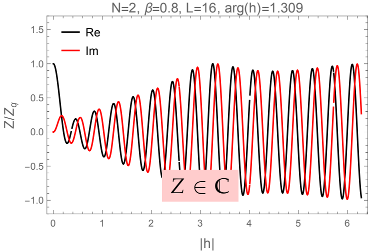

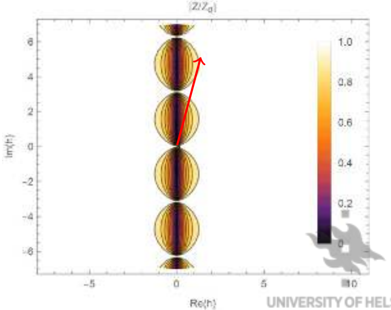

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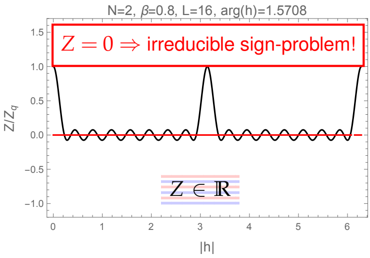

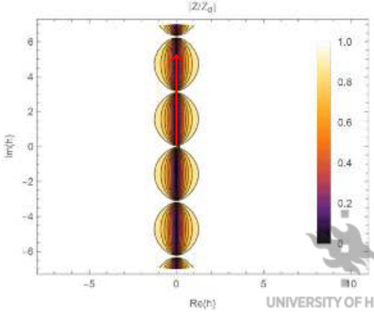

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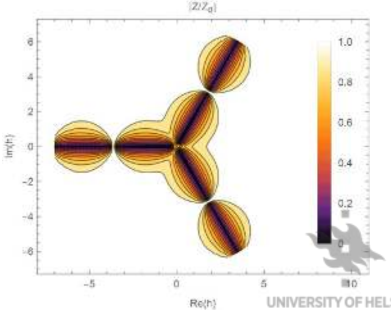

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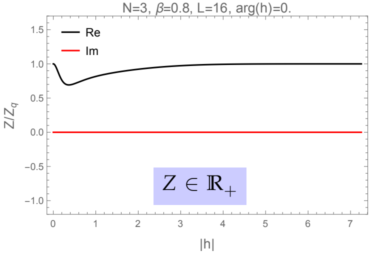

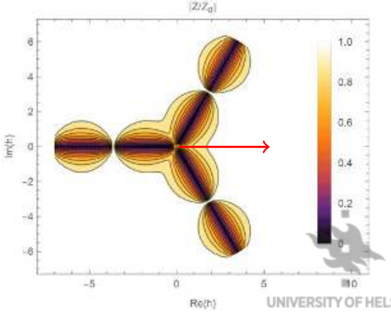

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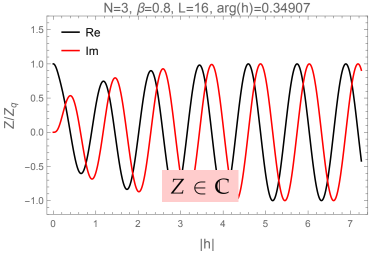

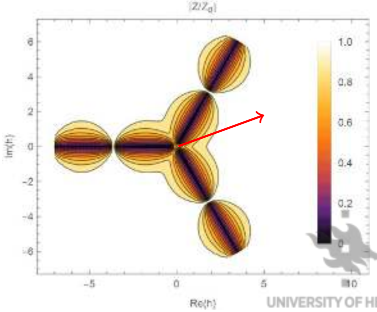

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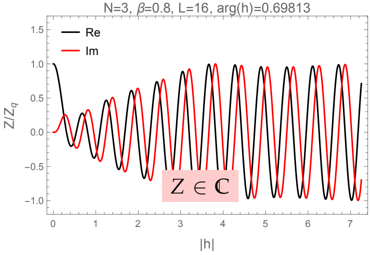

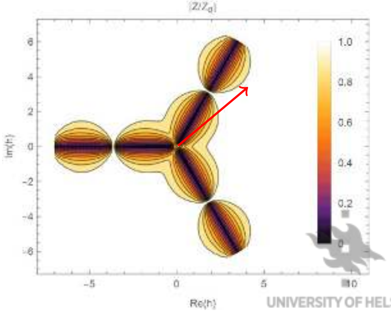

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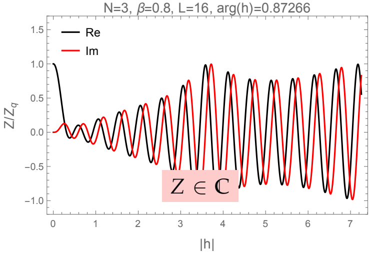

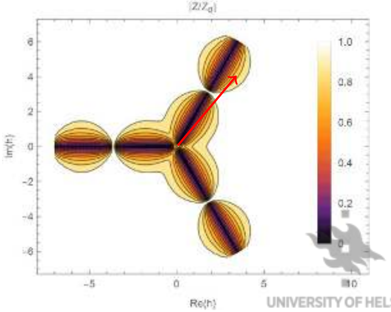

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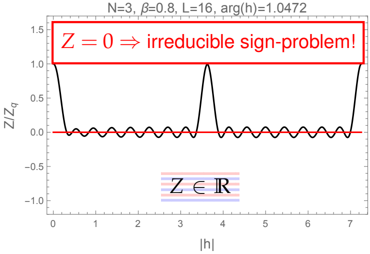
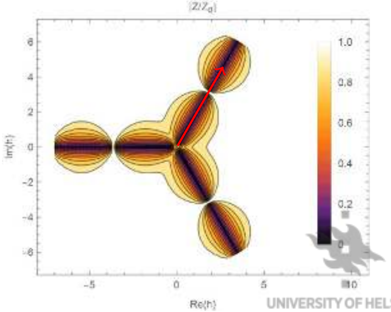
1D system, $L = 16$, $\beta = 0.8$, $N = 3$





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$$Z_N(\beta,h) = \sum_{\{s\}} \exp\left(\sum_x \left(\beta \sum_{\nu=1}^{d} (2\,\delta_{s_x,s_{x+\hat{\nu}}} - 1) + h\,\mathrm{e}^{\frac{2\pi\mathrm{i}s_x}{N}}\right)\right)$$

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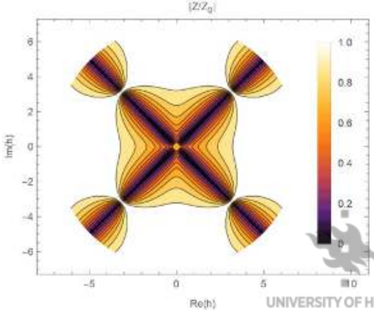

2. Exact solution in 1D: sign problem

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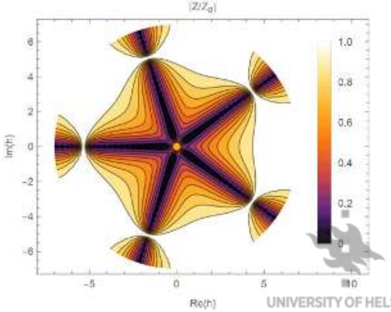
1D system, $L = 16$, $\beta = 0.8$, $N = 5$



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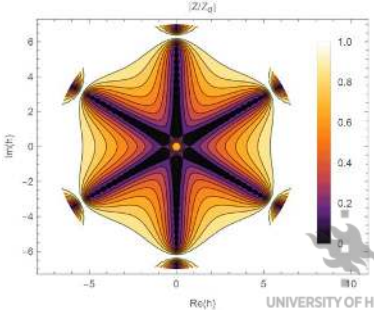

2. Exact solution in 1D: non-Hermitian transfer matrix

- Transfer matrix:

$$T_{s_x,s_{x+1}}(\beta,h,h') = \exp\left(\beta\,(2\,\delta_{s_x,s_{x+1}} - 1) + h\,\frac{P_x + P_{x+1}}{2} + h'\,\frac{P_x^* + P_{x+1}^*}{2}\right)$$

- If transfer matrix non-Hermitian $\rightarrow$ eigenvalues in general complex:

$$T(\beta,h,h') \neq T^\dagger(\beta,h,h') \quad \Rightarrow \quad \lambda_1(\beta,h,h'),\ldots,\lambda_N(\beta,h,h') \in \mathbb{C}\,!$$

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- But if Hamiltonian $\mathcal{CT}$-symmetric: [Ogilvie, 2010, arXiv:1009.0745]

$$H\,|\psi\rangle = E\,|\psi\rangle \Rightarrow H\,\mathcal{CT}\,|\psi\rangle = \mathcal{CT}\,H\,|\psi\rangle = \mathcal{CT}\,E\,|\psi\rangle = E^*\,\mathcal{CT}\,|\psi\rangle\ ,$$

$\rightarrow$ Eigenvalues are either real or appear in complex-conjugate pairs.

$$\forall n \in \{1,\ldots,N\}\,\exists m \in \{1,\ldots,N\} : \lambda_m(\beta,h,h') = \lambda_n^*(\beta,h,h')\ .$$

$\Longrightarrow \quad Z \in \mathbb{R}$ (can be negative or even zero).

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$\rightarrow$ Satisfied if for example:

1. $h' = 0\,, h \in \mathbb{C}$ with $\arg(h) \in \{\,\frac{\pi k}{N}\,|\,k \in \mathbb{Z}\,\}$
   $\rightarrow$ using $\mathcal{SCT}$ instead of $\mathcal{CT}$, $\mathcal{S} \in S_N$ (symmetric group) ,
2. $h + h' = h_R\,, h - h' = h_I$ with $h_R, h_I \in \mathbb{R}$. [Ogilvie, 2010, arXiv:1009.0745]

- Partition function and two-point correlation function:

$$Z_{N,L} = \mathrm{Tr}\left(T^L\right) = \mathrm{Tr}\left(\Lambda^L\right) \quad , \quad \langle P_0\, P_x^* \rangle = \frac{\mathrm{Tr}\left(\phi\, T^x\, \phi^*\, T^{L-x}\right)}{\mathrm{Tr}\left(T^L\right)} = \frac{\mathrm{Tr}\left(\tilde{\phi}\, \Lambda^x\, \tilde{\phi}^*\, \Lambda^{L-x}\right)}{\mathrm{Tr}\left(\Lambda^L\right)},$$

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- Consider limit $L \to \infty$ and assume that:
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→ 3 possible cases (simplified) : [Ogilvie, 2010, arXiv:1009.0745]

2. Exact solution in 1D: edge singularities and disorder lines

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1. $\lambda_n \in \mathbb{R}_+\, \forall n \in \{1, \ldots, N\}$:

$$\to \left\langle P_0\, P_x^* \right\rangle = \sum_{n=1}^{N} |\tilde{\phi}_{1n}|^2 \left(\frac{\lambda_n}{\lambda_1}\right)^x = |\tilde{\phi}_{11}|^2 + |\tilde{\phi}_{12}|^2\, \mathrm{e}^{-m_1 x} + \mathcal{O}\left(\mathrm{e}^{-m_2 x}\right)$$

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   $\to \left\langle P_0\, P_x^* \right\rangle \approx |\tilde{\phi}_{00}|^2 + |\tilde{\phi}_{01}|^2 \left(\left(\frac{\lambda_2}{\lambda_1}\right)^x + \left(\frac{\lambda_2^*}{\lambda_1}\right)^x\right) = |\tilde{\phi}_{00}|^2 + 2\,|\tilde{\phi}_{01}|^2\, \mathrm{e}^{-m_R\, x} \cos(m_I\, x)$,

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   $\to Z_{N,L} \approx \lambda_1^L$.

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$\to$ 3 possible cases (simplified) : [Ogilvie, 2010, arXiv:1009.0745]

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$$\to \langle P_0\, P_x^* \rangle \approx \frac{\lambda_1^{L-x} \sum_{n=1}^{N} |\tilde{\phi}_{1n}|^2 \lambda_n^x + (\lambda_1^*)^{L-x} \sum_{n=1}^{N} |\tilde{\phi}_{2n}|^2 \lambda_n^x}{\lambda_1^L + (\lambda_1^*)^L} \approx |\tilde{\phi}_{11}|^2 + \frac{\cos\left(m_I\,(x-L/2)\right)}{\cos\left(m_I\, L/2\right)}\, |\tilde{\phi}_{12}|^2 ,$$

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2. Exact solution in 1D: edge singularities and disorder lines

- Example: case 2 ($h + h' = h_R$ and $h - h' = h_I \mid h_R, h_I \in \mathbb{R}$) :

[Ogilvie, 2010, arXiv:1009.0745]
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$$\rightarrow h_n = 2\left(h_R \cos\left(\tfrac{2\pi n}{N}\right) + \mathrm{i} h_I \sin\left(\tfrac{2\pi n}{N}\right)\right) .$$

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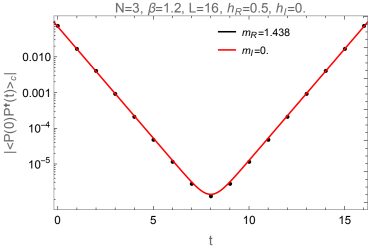
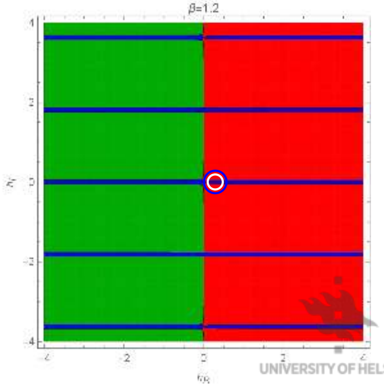
- "Phase diagram":

$\rightarrow$ purely exponential correlation functions ("gaseous" phase) ,

Two-point function:





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- "Phase diagram":

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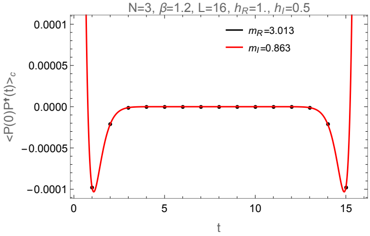
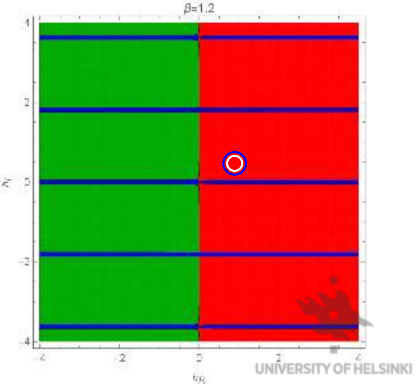
Two-point function:





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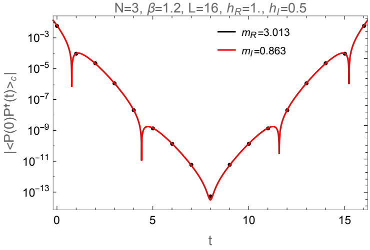

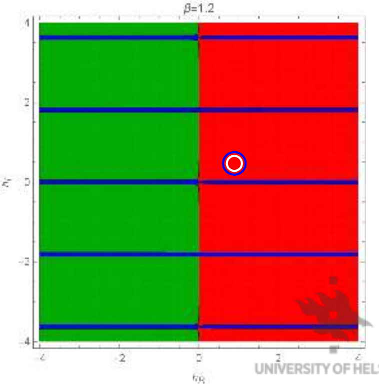

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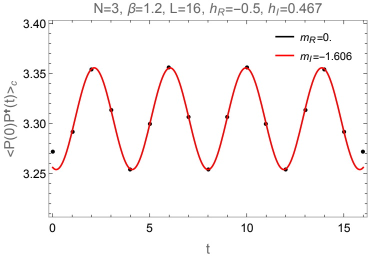

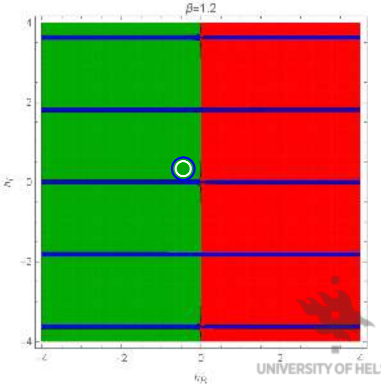

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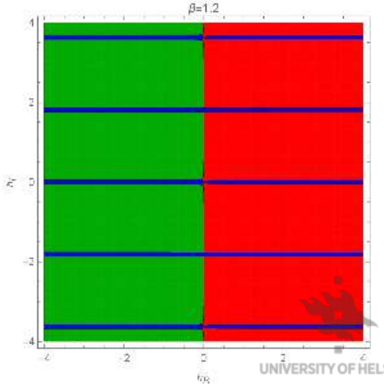
- Transition gas $\leftrightarrow$ liquid : **disorder line**

(no true phase transition; free energy smooth)



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- Transition gas ↔ liquid : **disorder line**

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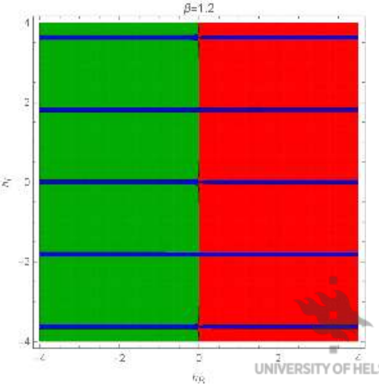
- Transition gas,liquid ↔ crystal : **edge singularity**

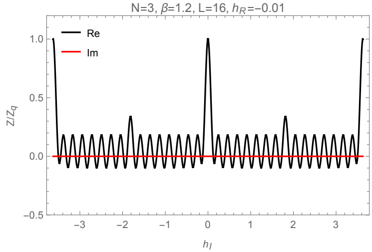
  ($Z = 0$, sign change; free energy discontinuous)

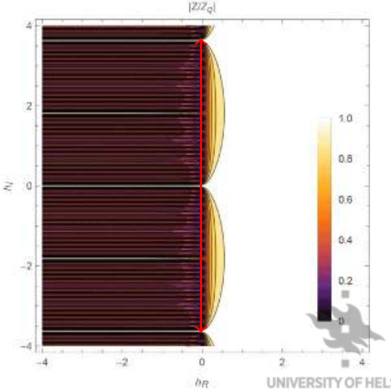


- Average sign $\langle \text{sign} \rangle = Z_N / Z_{N,q}$ as function of h_R and h_I .

→ Again, phase quenched partition function $Z_{N,q} \rightarrow$ Hamiltonian $H_q = \mathrm{Re}(H)$.

1D system, $L = 16$, $\beta = 1.2$, $N = 3$





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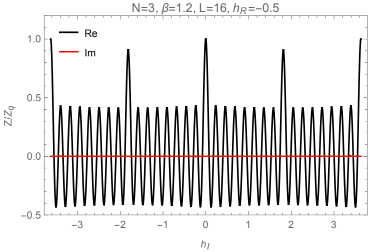

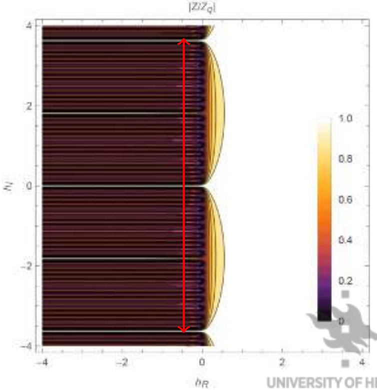

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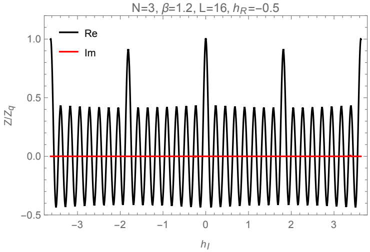

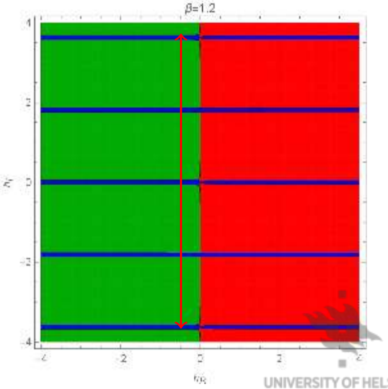

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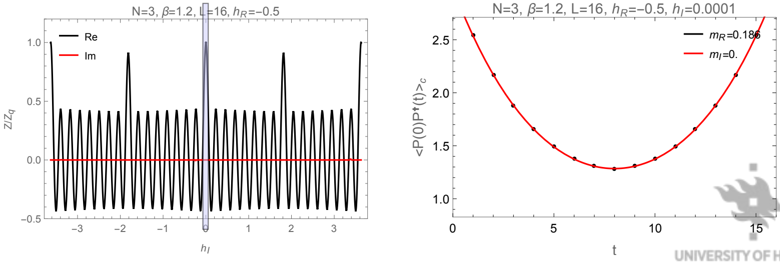

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- Average sign $\langle \text{sign} \rangle = Z_N / Z_{N,q}$ as function of h_R and h_I .
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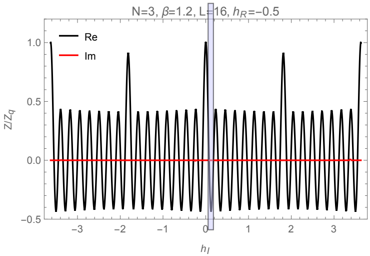

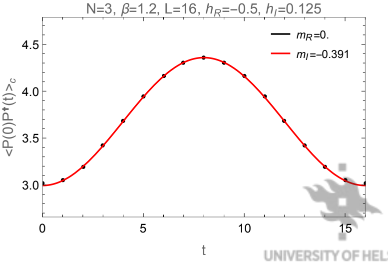

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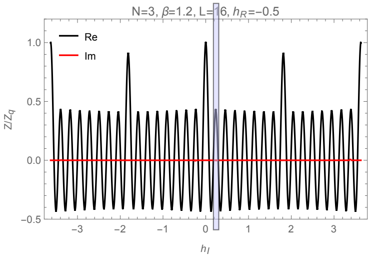

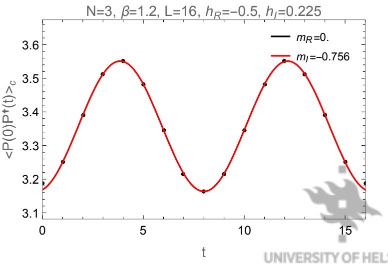

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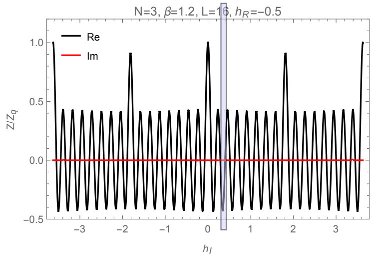

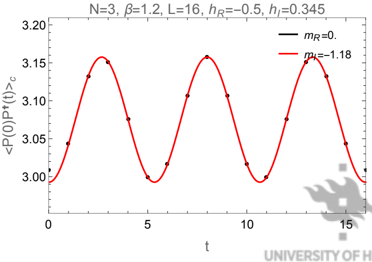

2. Exact solution in 1D: edge singularities and two-point function

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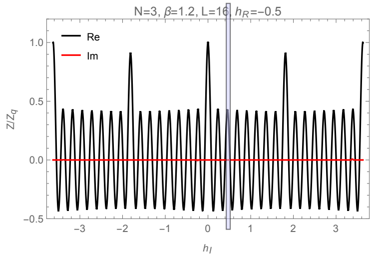

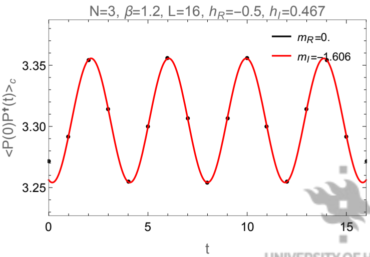

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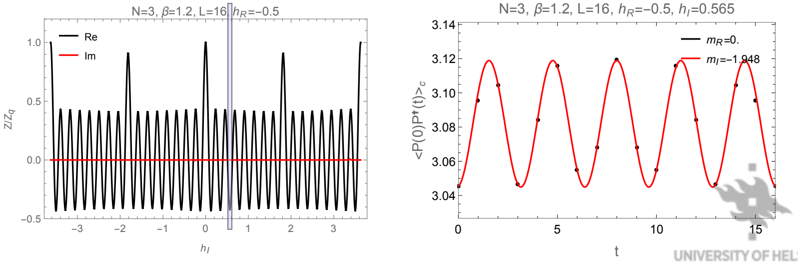

3. Alternative representations

- How well do different representations of the same partition function (spin-, cluster-, or flux-variable rep.) deal with different types of sign-problems?

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- Sign-problem is irreducible at zeroes of partition function (must be present in all representations)!
- Benchmark for severity of sign-problem in different representations:

  $\rightarrow$ how quick does sign-problem develop when approaching first edge-singularity?

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- Will consider case 1 of external field coupling ($h' = 0$ and $h \in \mathbb{C}$):

$$Z_N(\beta,h) = \sum_{\{s\}} \exp\bigg(\sum_x \Big(\beta \sum_{\nu=1}^{d} \big(2\,\delta_{s_x,s_{x+\widehat{\nu}}} - 1\big) + h\,\mathrm{e}^{\frac{2\pi\mathrm{i}s_x}{N}}\Big)\bigg)$$

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$$Z(\beta,h) = \Big(\cosh(h)\cosh(\beta)^d\Big)^V$$
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with:

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- Dual formulation for $N = 3$ $\rightarrow$ [Y. Delgado et al., Comp. Phys. Commun. 183 (2012), 1920-1927]

- Obtaining the cluster representation: [M. Alford et al., Nucl. Phys. B 602 (2001) 61-86]

$$Z_N(\beta, h_0, \ldots, h_{N-1}) = \sum_{\{s\}} \exp\bigg(\sum_x \bigg(\beta \sum_{\nu=1}^{d} \big(2\,\delta_{s_x, s_{x+\hat{\nu}}} - 1\big) + \sum_{n=0}^{N-1} h_n\, \delta_{n, s_x}\bigg)\bigg) \,,$$

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3. Alternative representations: cluster representation

- Example: case 1 from before,

$$h_n = h\,\mathrm{e}^{\frac{2\pi\mathrm{i}n}{N}} = |h|\,\mathrm{e}^{\mathrm{i}\arg(h)+\frac{2\pi\mathrm{i}n}{N}}\;,$$

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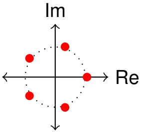
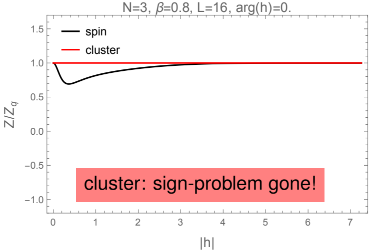
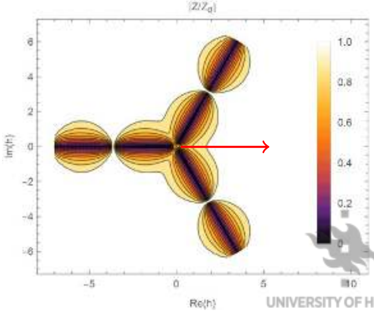
→ if k even : h_n with largest real part is purely real $\Rightarrow W_{N,h}(V_C) \in \mathbb{R}_+$,



1D system, $L = 16$, $\beta = 0.8$, $N = 3$





[M. Alford et al., Nucl. Phys. B 602 (2001) 61-86]

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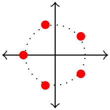
- Example: case 1 from before,

$$h_n = h\,\mathrm{e}^{\frac{2\pi \mathrm{i} n}{N}} = |h|\,\mathrm{e}^{\mathrm{i}\arg(h) + \frac{2\pi \mathrm{i} n}{N}} ,$$

$\rightarrow$ non-real h_n occur in complex conjugate pairs if $\arg(h) = \frac{\pi k}{N}$ with $k \in \mathbb{Z}$,

$\rightarrow$ if k even : h_n with largest real part is purely real $\Rightarrow W_{N,h}(V_C) \in \mathbb{R}_+$,

$\rightarrow$ if k odd : h_n with largest real part is not purely real $\Rightarrow W_{N,h}(V_C) \in \mathbb{R}$.



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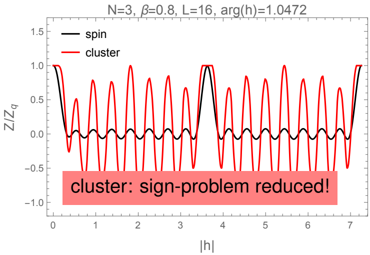

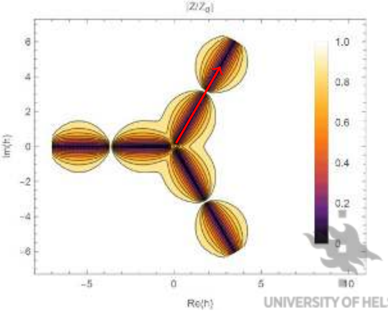

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- Benchmark for sign-problem in different representations:

  $\longrightarrow$ how fast does sign-problem develop when approaching first edge-singularity?

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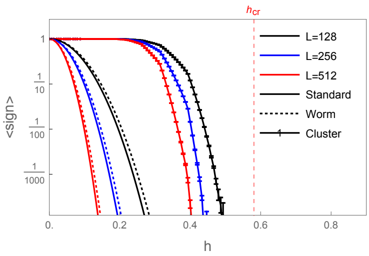
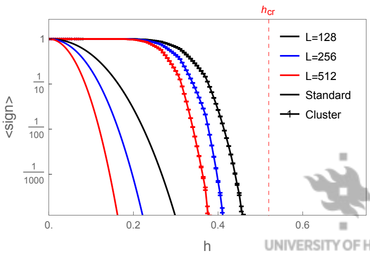
  → how fast does sign-problem develop when approaching first edge-singularity?

- Example, case 1 ($h_n = h\,\mathrm{e}^{\frac{2\pi i n}{N}}$ with $\arg(h) = \frac{\pi}{N}$) in 1D:

$\beta = 0.3$, $N = 2$



$\beta = 0.5$, $N = 3$



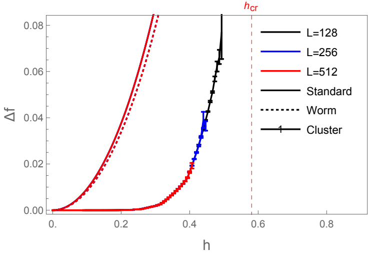
- Benchmark for sign-problem in different representations:
  → how fast does sign-problem develop when approaching first edge-singularity?

- Example, case 1 ($h_n = h\, e^{\frac{2\pi i n}{N}}$ with $\arg(h) = \frac{\pi}{N}$) in 1D:
  - Free energy difference (full vs. phase-quenched systems) for different representations:

$$\Delta f = -\frac{1}{V}\log(Z_N) + \frac{1}{V}\log(Z_{N,q}) = -\frac{1}{V}\log(\langle \text{sign} \rangle) \,.$$

→ Cluster representation allows to go much closer to edge singularity!

$\beta = 0.3$, $N = 2$



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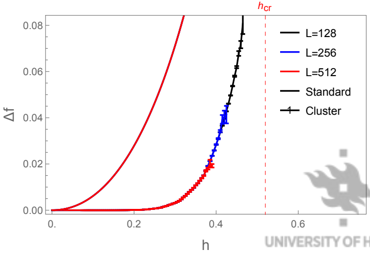
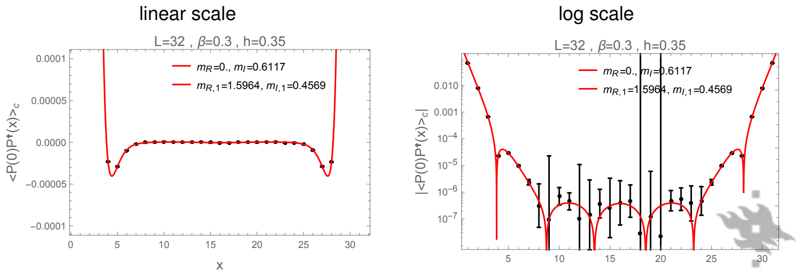


- Connected point-to-point correlation function:

$$\left\langle P_x^\dagger P_y \right\rangle_c = \left\langle P_x^\dagger P_y \right\rangle - \left\langle P_x^\dagger \right\rangle \left\langle P_y \right\rangle .$$

- Direct measurement for case 1 ($h' = 0$, $h \in \mathbb{C}$) using "cluster algorithm" (improved estimators):
    - for $\arg(h) = 0$ (liquid phase) ,



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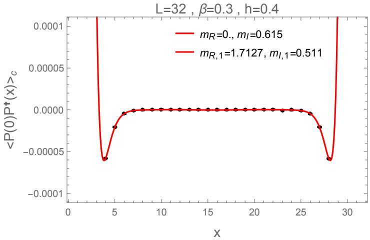
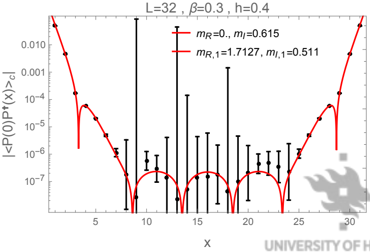
linear scale



log scale

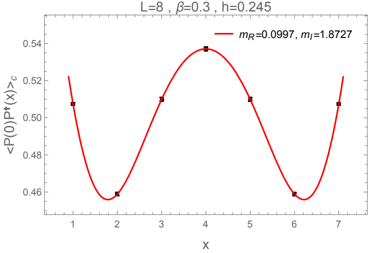


- Connected point-to-point correlation function:

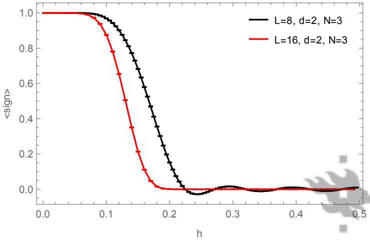
$$\langle P_x^\dagger P_y \rangle_c = \langle P_x^\dagger P_y \rangle - \langle P_x^\dagger \rangle \langle P_y \rangle \ .$$

- Direct measurement for case 1 ($h' = 0$, $h \in \mathbb{C}$) using "cluster algorithm" (improved estimators):
  - for $\arg(h) = 0$ (liquid phase) ,
  - and $\arg(h) = \pi/N$ (gaseous & crystalline phases) .

linear scale



average sign



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5. Conclusion & outlook

- Conclusion:
  - Reviewed different possibilities to couple N-state Potts models to complex external fields.
  - Reviewed relation between zeros of partition function and non-monotonic two-point functions.
  - While sign-problem in general representation-dependent, it is irreduzible at zeroes of partition function.
  - Cluster representation solves many sign-problems and drastically reduces others.

  → Even if new representations are found to not completely solve the sign-problem, they might still drastically reduce it, which should be tested.

- Outlook:
  - "Edge singularity benchmark" in higher dimensions.
  - Determination of properties of cluster algorithm (auto-correlation time, scalability).
  - Better understanding of "crystalline" phase in higher dimensions?

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