Abstract: It is an open question how well tensor network states in the form of an infinite projected entangled-pair states (iPEPS) tensor network can approximate gapless quantum states of matter. In this talk we address this issue for two different physical scenarios: (i) a conformally invariant (2+1)d quantum critical point in the incarnation of the transverse-field Ising model on the square lattice and (ii) spontaneously broken continuous symmetries with gapless Goldstone modes exemplified by the S=1/2 antiferromagnetic Heisenberg and XY models on the square lattice. We find that the energetically best wave functions display finite correlation lengths and we introduce a powerful finite correlation length scaling framework for the analysis of such finite bond dimension (finite-D) iPEPS states. The framework is important (i) to understand the mild limitations of the finite-D iPEPS manifold in representing Lorentz-invariant, gapless many-body quantum states and (ii) to put forward a practical scheme in which the finite correlation length $\xi(D)$ combined with field theory inspired formulas can be used to extrapolate the data to infinite correlation length, i.e., to the thermodynamic limit. The finite correlation length scaling framework opens the way for further exploration of quantum matter with an (expected) Lorentz-invariant, massless low-energy description, with many applications ranging from condensed matter to high-energy physics.
Quantum Criticality with iPEPS (&iMPS) Tensor Networks

Andreas Läuchli  
Institute for Theoretical Physics  
University of Innsbruck, Austria

andreas.laeuchli@uibk.ac.at  
http://www.uibk.ac.at/th-physik/laeuchli-lab

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Quantum Matter

- We would like to understand phase diagrams of complex systems, but whose Hamiltonians are often reasonably well known.

- Quantum phase transitions occur. What is their universality class & field theoretical description?

- New tools welcome to diagnose/characterize QFTs at phase transitions
Example of Microscopic Condensed Matter Models

From microscopic models:

\[ \mathcal{H} = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_3 \sum_{i,j,k \in \triangle} \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k) \]


\[ \mathcal{H} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.) + V_1 \sum_{\langle ij \rangle} (n_i - 1/2)(n_j - 1/2) + V_2 \sum_{\langle\langle ij \rangle\rangle} (n_i - 1/2)(n_j - 1/2) \]


To quantum phase transitions: Wilson Fisher CFTs, QED\(_3\), Gross Neveu, ...
Quantum Criticality of iPEPS Tensor Networks


new tool: iPEPS

- infinite (system size) projected entangled pair states (iPEPS) tensor network

\[ |\psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots} |\sigma_1,\sigma_2,\ldots\rangle \]

- Twofold new approach to quantum many body systems:
  - particular tensor network structure
  - directly in the thermodynamic limit, i.e. infinite system.
    How does that work well for quantum criticality?
    (rather well understood for iMPS, c.f. Tagliacozzo et al. 2008, Pollmann et al. 2009)
Brief iPEPS technicalities

- Optimization by new gradient descent methods

- Contractions using boundary MPS and CTMRG

\[ \rho_1 = \]

\[ \approx \]

bMPS

CTMs

\[ \rho_1 \approx \]
Brief iPEPS technicalities

- Correlation functions:

\[
c(r) = u^{(r-1)} v = u^T A^{r-1} v
\]

\[
j = \lambda_j = j
\]

\[
|\lambda_0| \geq |\lambda_1| \geq \ldots
\]

\[
\xi = -\frac{1}{\log |\lambda_1|} \quad \frac{1}{\xi(\chi)} = \frac{1}{\xi(\infty)} + k \log \left| \frac{\lambda_1(\chi)}{\lambda_2(\chi)} \right|
\]

M. Rams et al, PRX 2018
iPEPS for (2+1)d Ising criticality

- Transverse field Ising model (Hamiltonian formulation)

\[ H_{\text{TFI}} = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x - h_z \sum_i \sigma_i^z \]
Variationally optimised iPEPS tensors

- Ising criticality perturbed in two relevant directions (h-h_c / h_z):

\[ m \]

\[ h \]

\[ h_c \]

\[ D \]
Approach to criticality:
local observables as a function of perturbing coupling
Now: correlation lengths

- tuning $h - h_c$: correlation lengths grow, but do not diverge!

![Graph showing correlation length behavior with respect to $h$ for different dimensions $D$.]
Now: correlation lengths

- tuning $h_z$ at $h_c$:
Correlation lengths: “Casimir effect”
Correlation lengths: "Casimir effect"

- Finite volume (L):

\[ e(L) = e(\infty) - \frac{\alpha^{QCP}_\tau}{L^3} \times \nu \]

\[ \alpha^{(3d \text{ Ising CFT})}_{\tau=i} = +0.35(2) \]

- Our conjecture: Finite correlation length scaling of variational energy:

\[ e(\xi) = e(\infty) - \frac{\alpha^{(3d \text{ Ising CFT})}_{\text{PEPS}}}{\xi^3} \times \nu \]

\[ \alpha^{(3d \text{ Ising CFT})}_{\text{PEPS}} \approx -0.00061, \quad e(\infty) \approx -3.2342623. \]
And now for something completely different:
Continuous symmetry breaking
Different scenario: Continuous symmetry breaking (i.e. magnetic order, superfluids, …)

- Hydrodynamic description based on O(N) non-linear sigma model (collinear order): parameters: velocity, spin stiffness, ordered moment

- Finite volume effects:

\[
\begin{align*}
e(L) &= e(\infty) - \left[ \alpha_{\text{shape/bc}}^{\text{NLSM}} \left( \frac{N - 1}{2} \right) v \right] \frac{1}{L^3} \\
&\quad + \frac{(N - 1)(N - 2)}{8} \frac{v^2}{\rho s L^4} + \mathcal{O}\left( \frac{1}{L^5} \right)
\end{align*}
\]

\[
\frac{m^2(L)}{m^2(\infty)} = 1 + \left[ \mu_{\text{shape/bc}}^{\text{NLSM}} \left( \frac{N - 1}{2} \right) \frac{v}{\rho s} \right] \frac{1}{L} + \mathcal{O}\left( \frac{1}{L^2} \right)
\]
Continuous symmetry breaking
(i.e. magnetic order, superfluids, ...)

- hydrodynamic description based on $O(N)$ non-linear sigma model
  (collinear order): parameters: velocity, spin stiffness, ordered moment

- Conjectured finite correlation length effects:

\[
e(\xi) = e(\infty) - \left[ \alpha_{\text{NLSM}}^{\text{iPEPS}} \left( \frac{N - 1}{2} \right) v \right] \left[ \frac{1}{\xi^3} \right] + \mathcal{O} \left( \frac{1}{\xi^4} \right)
\]

\[
\frac{m^2(\xi)}{m^2(\infty)} = 1 + \left[ \mu_{\text{NLSM}}^{\text{iPEPS}} \left( \frac{N - 1}{2} \right) \frac{v}{\rho_s} \right] \left[ \frac{1}{\xi} \right] + \mathcal{O} \left( \frac{1}{\xi^2} \right)
\]
$S=1/2$ HB magnet / $O(3)$

\[ H_{\text{HB}} = J \sum_{\langle i,j \rangle} \left( S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right) \]

\[ \alpha_{\text{iPEPS}}^{\text{NLSM}} \approx -0.0029 \]

\[ \mu_{\text{iPEPS}}^{\text{NLSM}} \approx +0.045 \]
S=1/2 XY model / O(2)

\[ H_{XY} = -J \sum_{\langle i, j \rangle} (S_i^x S_j^x + S_i^y S_j^y) \]
Overview: D-dependence of correlation lengths
Handwaving understanding:

- Space-time volume required to correctly describe correlation functions becomes D-limited in Lorentz invariant (2+1)d massless behaviour.

\[ |\psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots} \langle \sigma_1,\sigma_2,\ldots | \]

\[ (2+1)d \text{ CFT/QFT} \]

\[ \tau \]

\[ \xi_\tau \sim \xi(D) \]

\[ x \quad \xi_{x,y} \sim \xi_\tau \]

\[ y \]

\[ (2+0)d \text{ Rokhsar – Kivelson} \]

\[ \tau \]

\[ \xi_\tau \approx 0 \]

\[ x \quad \xi_{x,y} = \infty \]

\[ y \]

- Entropic Area-law is not sufficient to decide representability by iPEPS.
Conclusions

- rather accurate energies and critical exponents for d=3 Ising already with bond dimension D=3!

- correlation lengths stay finite for all couplings.

- Finite correlation length is a “blessing”, we can use it to extrapolate energies and order parameters to the “$D \to \infty$” limit.

- Broader qualitative picture: it seems as though the variational iPEPS state is “self-detuned” by a relevant perturbation of the (2+1)d gapless QFT fixed point, rendering the state gapped.

- Space-time volume matters!

- Applications: Superfluids, Superconductors, Gapless Quantum Spin Liquids,…
Finite Entanglement Scaling in iMPS revisited

A. Eberharder. M. Rader and AML, in preparation
Thank you for your attention!