Re-entrance and entanglement in the one-dimensional Bose-Hubbard model

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Re-entrance is a novel feature where the phase boundaries of a system exhibit a succession of transitions between two phases A and B, like A-B-A-B, when just one parameter is varied monotonically. This type of re-entrance is displayed by the 1D Bose Hubbard model between its Mott insulator (MI) and superfluid phase as the hopping amplitude is increased from zero. Here we analyse this counter-intuitive phenomenon directly in the thermodynamic limit by utilizing the infinite time-evolving block decimation algorithm to variationally minimize an infinite matrix product state (MPS) parameterized by a matrix size χ. Exploiting the direct restriction on the half-chain entanglement imposed by fixing χ, we determined that re-entrance in the MI lobes only emerges in this approximate when $\chi \geq 8$. This entanglement threshold is found to be coincident with the ability an infinite MPS to be simultaneously particle-number symmetric and capture the kinetic energy carried by particle-hole excitations above the MI. Focussing on the tip of the MI lobe we then applied, for the first time, a general finite-entanglement scaling analysis of the infinite order Kosterlitz-Thouless critical point located there. By analysing χ's up to a very moderate $\chi = 70$ we obtained an estimate of the KT transition as $t_{\mathrm{KT}} = 0.30 \pm 0.01$, demonstrating the how a finite-entanglement approach can provide not only qualitative insight but also quantitatively accurate predictions.

Overview

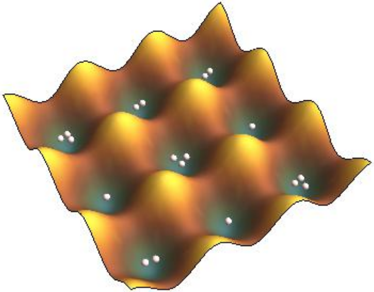
Bose-Hubbard model for a 1D chain

$$\hat{H} = \frac{U}{2}\sum_j \hat{n}_j(\hat{n}_j - 1) - t\sum_j \left(\hat{b}_j^\dagger \hat{b}_{j+1} + h.c.\right) - \mu \sum_j \hat{n}_j$$

- The BHM favors delocalized particles for large t. How to explain re-entrance?
- Use infinite time-evolving block decimation (iTEBD) algorithm to variationally minimize the infinite matrix product state (MPS) ansatz.

Mott Insulator - Superfluid Quantum Phase Transition

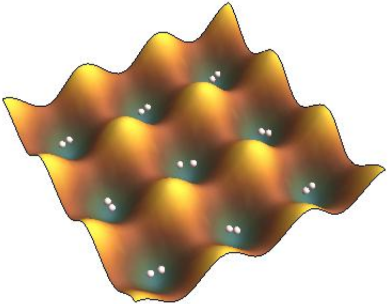
Superfluid



Atom number uncertain and well defined macroscopic phase

Gapless excitation spectrum and finite compressibility

Mott Insulator



Atom number exactly known but no phase coherence

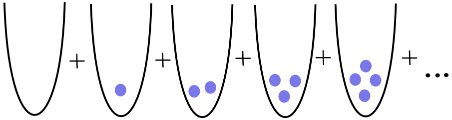
Gapped excitation spectrum and vanishing compressibility

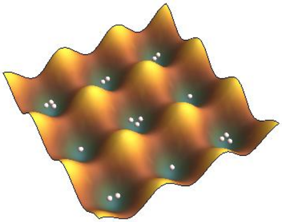
Superfluid Limit

$$H = -J \sum_{(i,j)} \hat{a}_i^\dagger \hat{a}_j$$

$$\Psi_{SF} = \frac{\left(\hat{c}_0^\dagger\right)^N}{\sqrt{N!}} |0\rangle \propto \left(\sum_{j=1}^{L} \hat{b}_j^\dagger\right)^N |0\rangle,$$

Atom number uncertain and well defined macroscopic phase



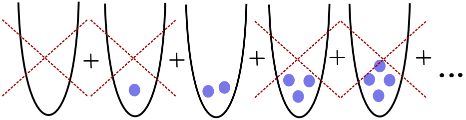


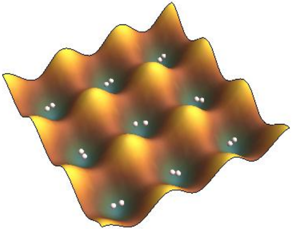
Strong Interactions Limit

$$H = \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)$$

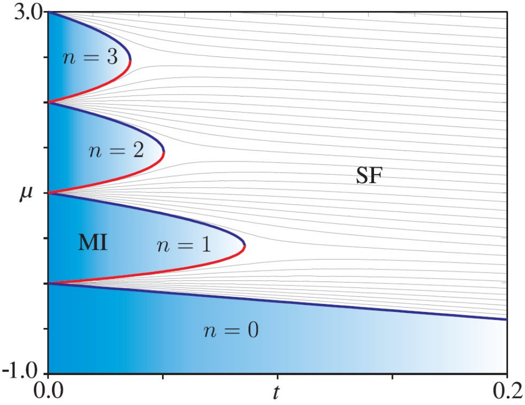
$$\Psi_{Mott} \propto \prod_{j=1}^{L} \left(\hat{b}_j^\dagger \right)^{N/L} |0\rangle$$

Atom number exactly known but no phase coherence



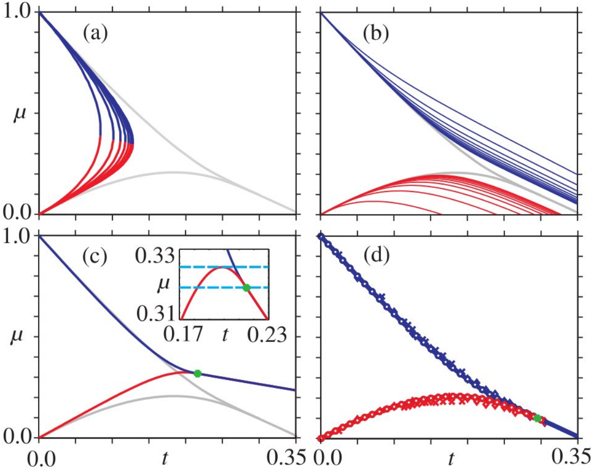


Mean-Field Phase Diagram of the BHM



- Areas with vanishing compressibility are MI
- Density Contours have negative slope for large t
- Integer density contours meet the tips of the Mott lobes

Phase Diagram of the 1D BHM



(a) small-cluster MF (b) periodic bc's with 2 to 11 sites
(c) real-space RG (d) DMRG and QMC

Matrix Product States

Interpolate between

$$|\Psi\rangle = \sum_{s_1 \ldots s_N} C(s_1 \ldots s_N)|s_1 \ldots s_N\rangle$$

and

$$|\Psi\rangle_{MF} = \left(\sum c_{s_1}|s_1\rangle\right)\left(\sum c_{s_2}|s_2\rangle\right)\ldots\left(\sum c_{s_N}|s_N\rangle\right)$$

via Matrix product states:

$$|\Psi\rangle = \sum_{s_1 \ldots s_N} \mathrm{tr}\left[A_1(s_1)\Sigma_1 A_2(s_2)\ldots A_N(s_N)\right]|s_1 \ldots s_N\rangle$$

It's possible because the entanglement is bound by area laws.

Vidal, Phys.Rev.Lett. **93**, 040502 (2004) & Phys.Rev.Lett. **98**, 070201 (2007)

Finite-Entanglement infinite MPS

Recall Schmidt decomposition via a SVD,

$$
\begin{aligned}
|\Psi\rangle &= \sum_{ij} c_{ij} |i^{\triangleleft}\rangle \otimes |j^{\triangleright}\rangle = \sum_{ij} \sum_{\alpha} U_{i\alpha} \Lambda_{\alpha\alpha} V^{*}_{j\alpha} |i^{\triangleleft}\rangle \otimes |j^{\triangleright}\rangle \\
&= \sum_{\alpha=1}^{\chi} \lambda_{\alpha} |\Phi^{\triangleleft}_{\alpha}\rangle \otimes |\Phi^{\triangleright}_{\alpha}\rangle
\end{aligned}
$$

and the von-Neumann entropy

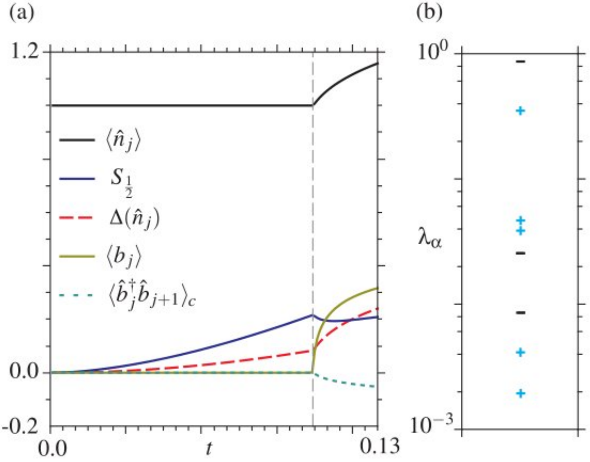
$$
E_{\frac{1}{2}} = -\sum_{\alpha=1}^{\chi} \lambda_{\alpha}^{2} \log_{2}\left(\lambda_{\alpha}^{2}\right)
$$

The elements of Σ are the Schmidt coefficients.

$\Rightarrow$ The size of the A's determines the maximal entanglement!

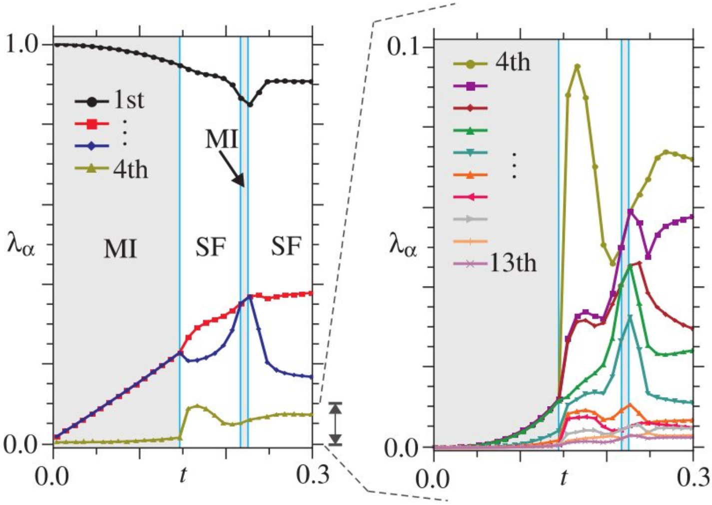
Schollwöck, Annals of Physics **326** (2011) 96-192

Signatures of Criticality at Finite Entanglement



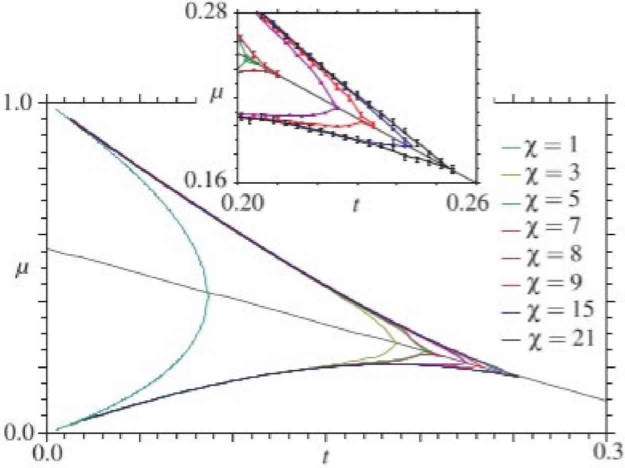
(a) $\chi = 3$ calculation: Pseudo-critical point ($\mu = 0.6$)
(b) $\chi = 13$ Entanglement spectrum ($\mu = 0.6$, $t = 0.22$)

Utility of the Schmidt Spectrum



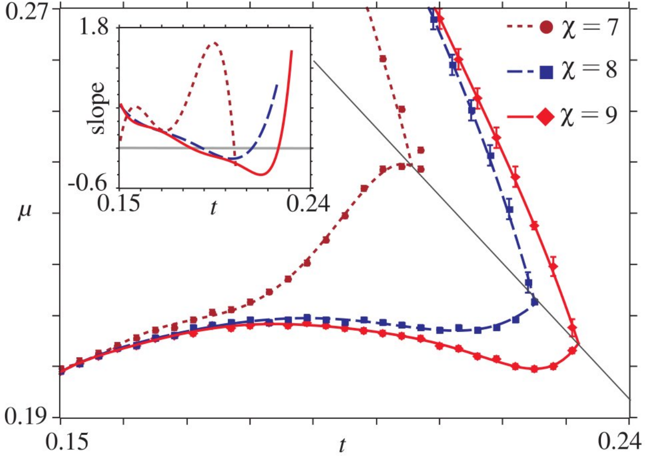
$\chi = 13$ calculation: Re-entrance!

Phase boundaries for different χ



Works much better than small-cluster MF and $\chi = 21$ is tiny for DMRG standards

A Zoom to the Tip



$\chi = 8$ is the minimal entanglement needed to see re-entrance

Kinetic and Interaction energies

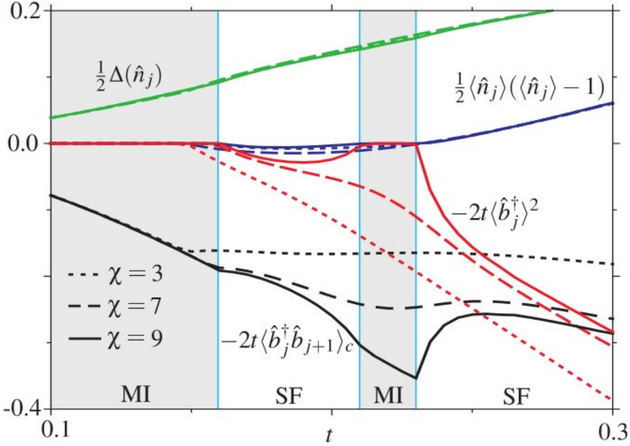
Rewrite the energy density of the BHM

$$\begin{aligned}\epsilon &= -t\left(\langle \hat{b}_j^\dagger \hat{b}_{j+1}\rangle_c + \langle \hat{b}_j^\dagger\rangle^2 + c.c.\right) - \mu\langle \hat{n}_j\rangle \\ &+ \frac{U}{2}\Delta(\hat{n}_j) + \frac{U}{2}\langle \hat{n}_j\rangle(\langle \hat{n}_j\rangle - 1)\end{aligned}$$

where

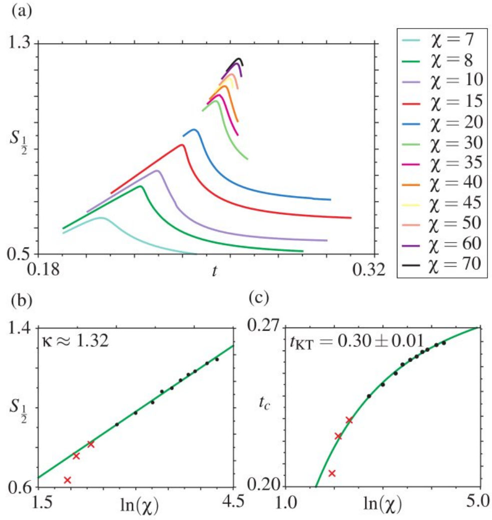
$$\Delta(\hat{n}_j) = \langle \hat{n}_j \hat{n}_j\rangle - \langle \hat{n}_j\rangle^2 \quad \text{and} \quad \langle \hat{b}_j^\dagger \hat{b}_{j+1}\rangle_c = \langle \hat{b}_j^\dagger \hat{b}_{j+1}\rangle - \langle \hat{b}_j^\dagger\rangle\langle \hat{b}_{j+1}\rangle$$

Fluctuations and correlation distributions for $\mu = 0.204$



In the MI phase MF neglects $\langle\hat{b}_j^\dagger\hat{b}_{j+1}\rangle_c$ and $\Delta(\hat{n}_j)$.

Entanglement Scaling of the KT point



(b) $S_{1/2} \sim \kappa \ln(\chi)$ (c) $t_c(\chi) = B_1/(\ln(\chi) + B_2)^2 + t_{KT}$

Conclusions

- "Utilizing the iTEBD algorithm we have performed a finite-entanglement analysis of the MI-SF transition in the BHM in 1D."
- Extrapolation beyond MF by restricting the entanglement
- What is the "entanglement needed for an infinite MPS to be both particle-number symmetric and effectively capture intricate particle-hole excitations above the MI state carrying kinetic energy."
- Low cost iTEBD calculations can provide qualitative and quantitative insight into the lobe structure and accurate estimations of critical points.