Tensor network algorithms for 3D quantum systems

Patrick Vlaar

University of Amsterdam

Benasque 2022

European Research Council

Established by the European Commission

UvA

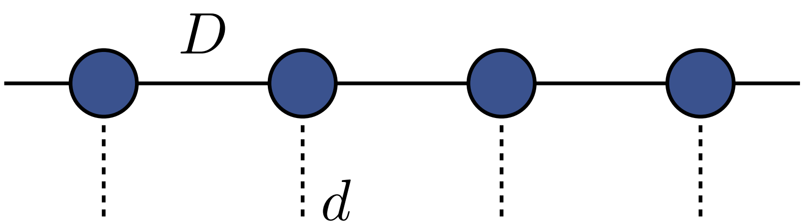
Delta Institute for Theoretical Physics

Overview

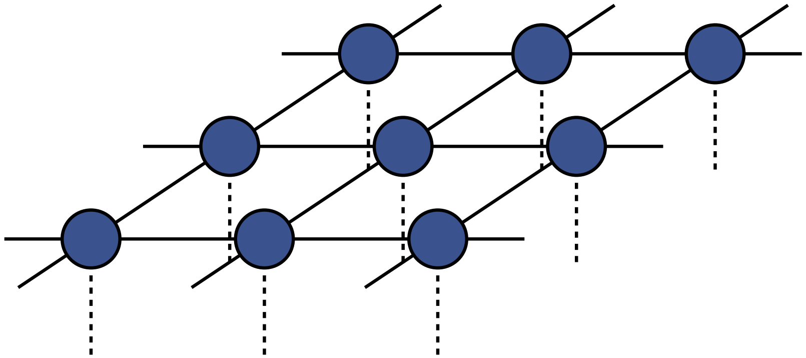
- iPEPS
  - CTMRG
  - Imaginary time evolution
- iPEPS for 3D quantum systems
- iPEPS for layered systems
- Conclusion

iPEPS

- Generalization of iMPS to higher dimensions
- Variational ansatz
- Satisfies area law
- Thermodynamic limit
- No canonical form in higher dimensions
  - Use contraction methods, e.g. CTMRG, TRG, ….

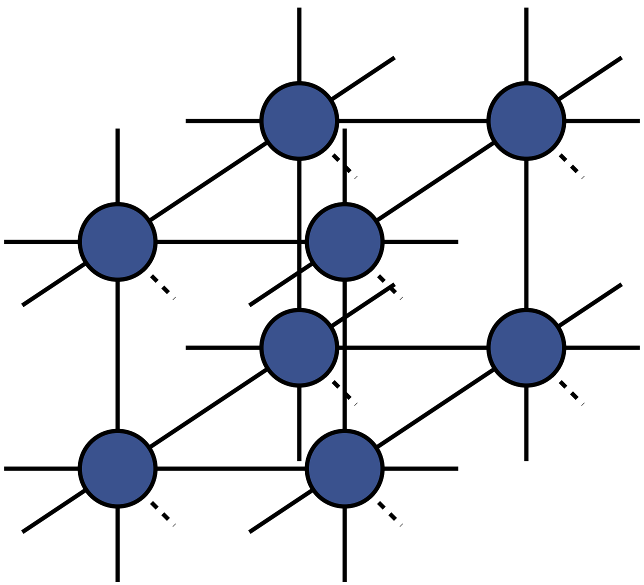


White, PRL 69, 2863 (1992); Fannes, et al., CMP 144, 443 (1992); Östlund & Rommer, PRL 75, 3537 (1995)



Verstraete & Cirac, arXiv:cond-mat/0407066 (2004); Nishio, et al., arXiv:cond-mat/0401115 (2004)

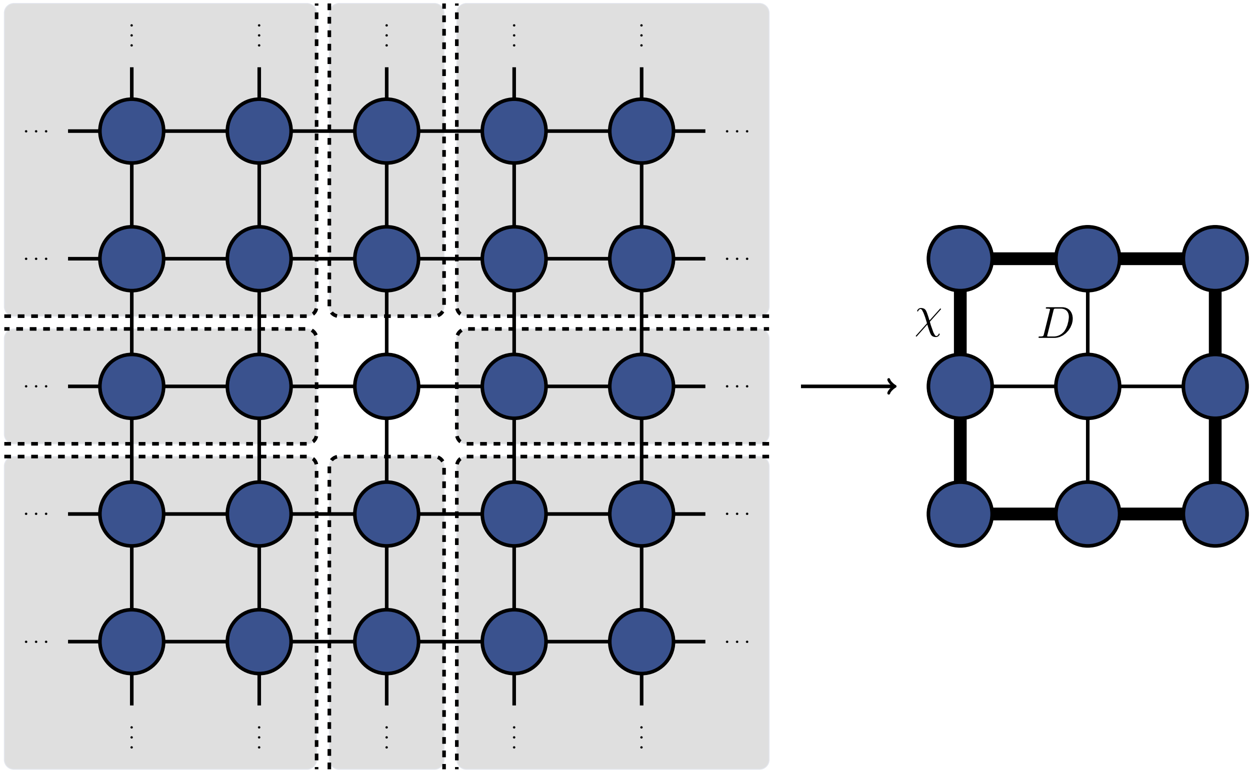
iPEPS in 3D



- Can iPEPS be used to simulate 3D quantum models?
- Applications to classical systems[1]
- Contraction is challenging

[1] Nishino, Okunishi, Hieida, Maeshima, & Akutsu, NPB 575, 504 (2000); Nishino, Hieida, Okunishi, Maeshima, Akutsu, & Gendiar, PTP 105, 409 (2001); Gendiar & Nishino, PRE 65, 046702 (2002); Gendiar, Maeshima, & Nishino, PTP 110, 691 (2003); Gendiar & Nishino, PRB 71, 024404 (2005); Vanderstraeten, Vanhecke, & Verstraete, PRE 98, 042145 (2018)

CTMRG



Nishino & Okunishi, JPSJ 65, 891 (1996); Orús & Vidal, PRB 80, 094403 (2009); Corboz, Rice & Troyer, PRL 113, 046402 (2014)

Imaginary time evolution

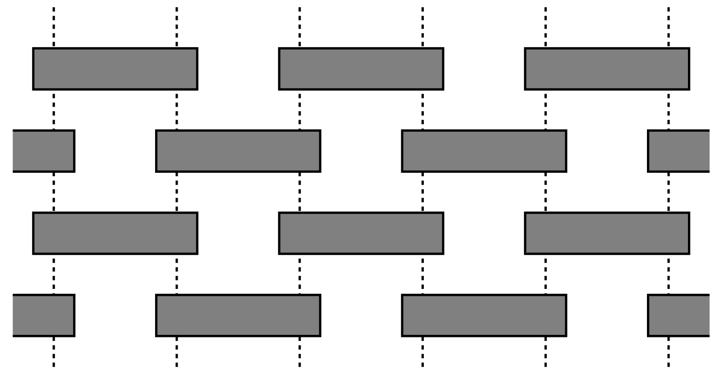
- Project to ground state

$$e^{-\beta \hat{H}} |\phi\rangle \xrightarrow{\beta \to \infty} |\psi_0\rangle$$

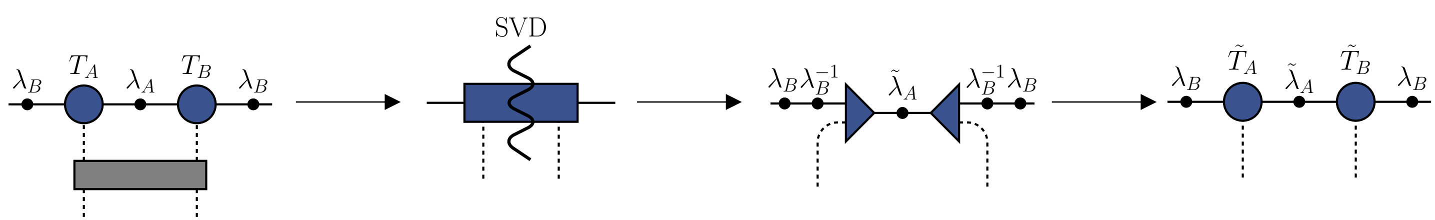
- Trotter-Suzuki decomposition

$$e^{-\beta \sum_i \hat{H}_i} = \left(e^{-\tau \sum_i \hat{H}_i}\right)^M$$

$$= \left(\prod_i e^{-\tau \hat{H}_i}\right)^M + \mathcal{O}(\tau)$$



- In 1D: TEBD[1]



[1] Vidal, PRL 91, 147902 (2003)

Imaginary time evolution

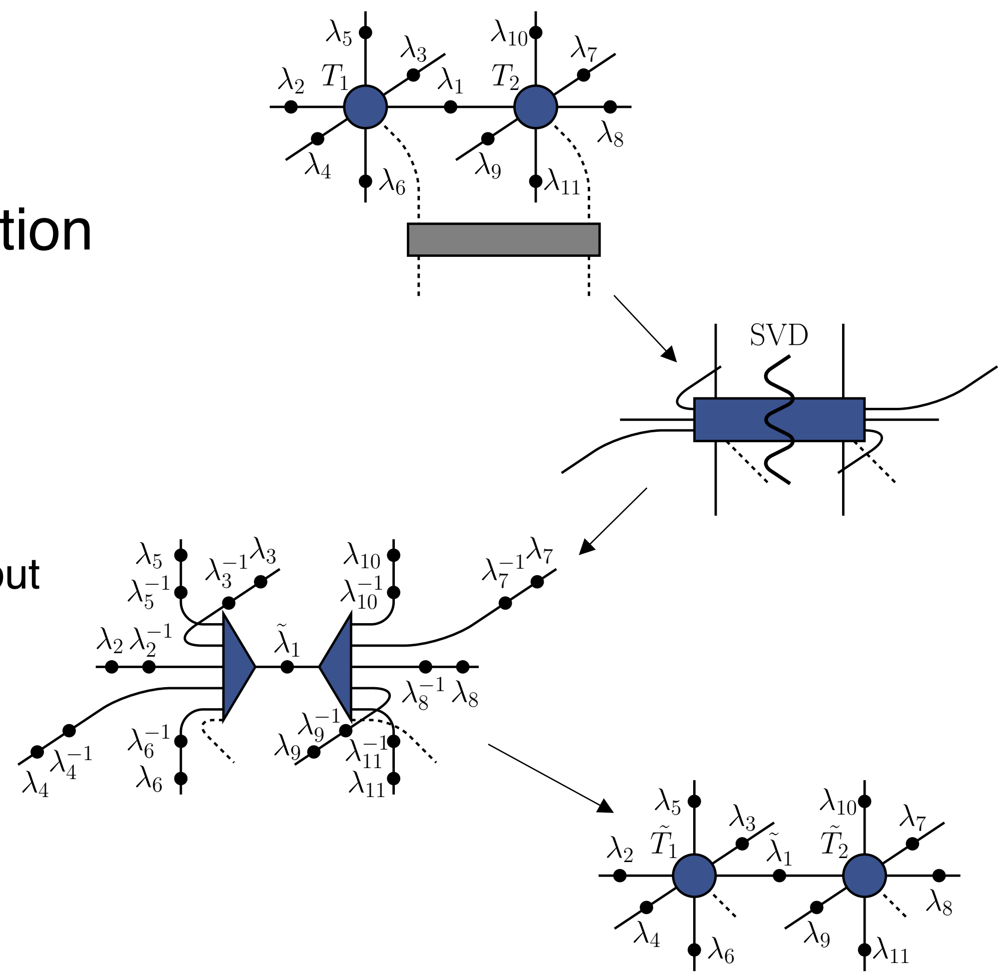
- Project to ground state

$$e^{-\beta \hat{H}}|\phi\rangle \xrightarrow{\beta \to \infty} |\psi_0\rangle$$

- Trotter-Suzuki decomposition

$$e^{-\tau \sum_i \hat{H}_i} \approx \prod_i e^{-\tau \hat{H}_i}$$

- For higher dimensions
  - Simple update (SU)[1]
    - Computationally cheap, but limited accuracy



[1] Jiang, Weng, & Xiang, PRL 101, 090603 (2008)

Imaginary time evolution

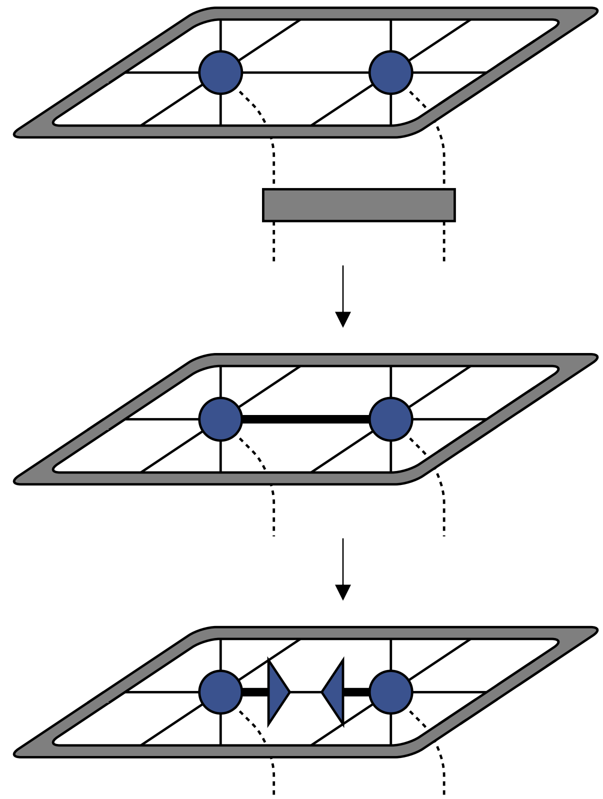
- Project to ground state

$$e^{-\beta \hat{H}} |\phi\rangle \xrightarrow{\beta \to \infty} |\psi_0\rangle$$

- Trotter-Suzuki decomposition

$$e^{-\tau \sum_i \hat{H}_i} \approx \prod_i e^{-\tau \hat{H}_i}$$

- For higher dimensions
  - Simple update (SU)[1]
    - Computationally cheap, but limited accuracy
  - Full update (FU)[2]
    - More accurate, but more expensive



[1] Jiang, Weng, & Xiang, PRL 101, 090603 (2008)
[2] Jordan, Orús, Vidal, Verstraete, & Cirac, PRL 101, 250602 (2008)

Imaginary time evolution

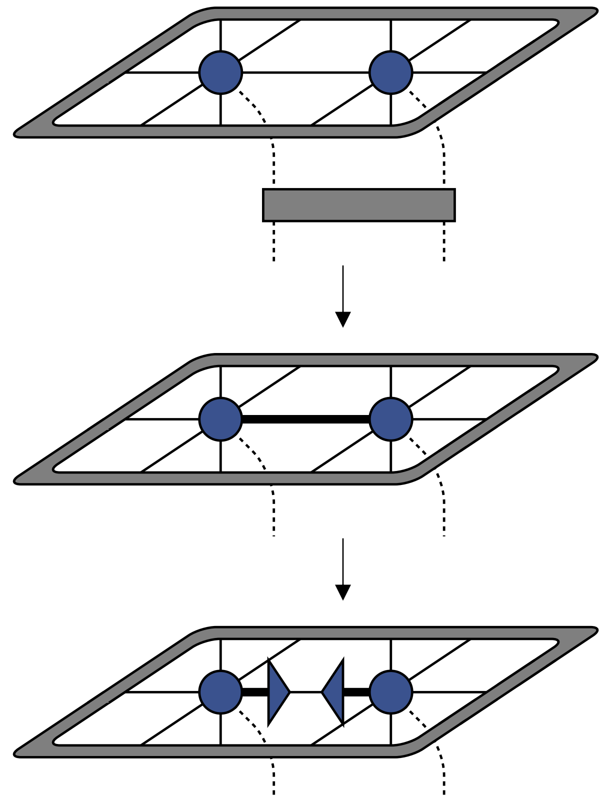
- Project to ground state

$$e^{-\beta \hat{H}}|\phi\rangle \xrightarrow{\beta\to\infty} |\psi_0\rangle$$

- Trotter-Suzuki decomposition

$$e^{-\tau \sum_i \hat{H}_i} \approx \prod_i e^{-\tau \hat{H}_i}$$

- For higher dimensions
  - Simple update (SU)[1]
    - Computationally cheap, but limited accuracy
  - Full update (FU)[2]
    - More accurate, but more expensive
  - Fast FU[3]



[1] Jiang, Weng, & Xiang, PRL 101, 090603 (2008)
[2] Jordan, Orús, Vidal, Verstraete, & Cirac, PRL 101, 250602 (2008)
[3] Phien, Bengua, Tuan, Corboz, & Orús, PRB 92, 035142 (2015)

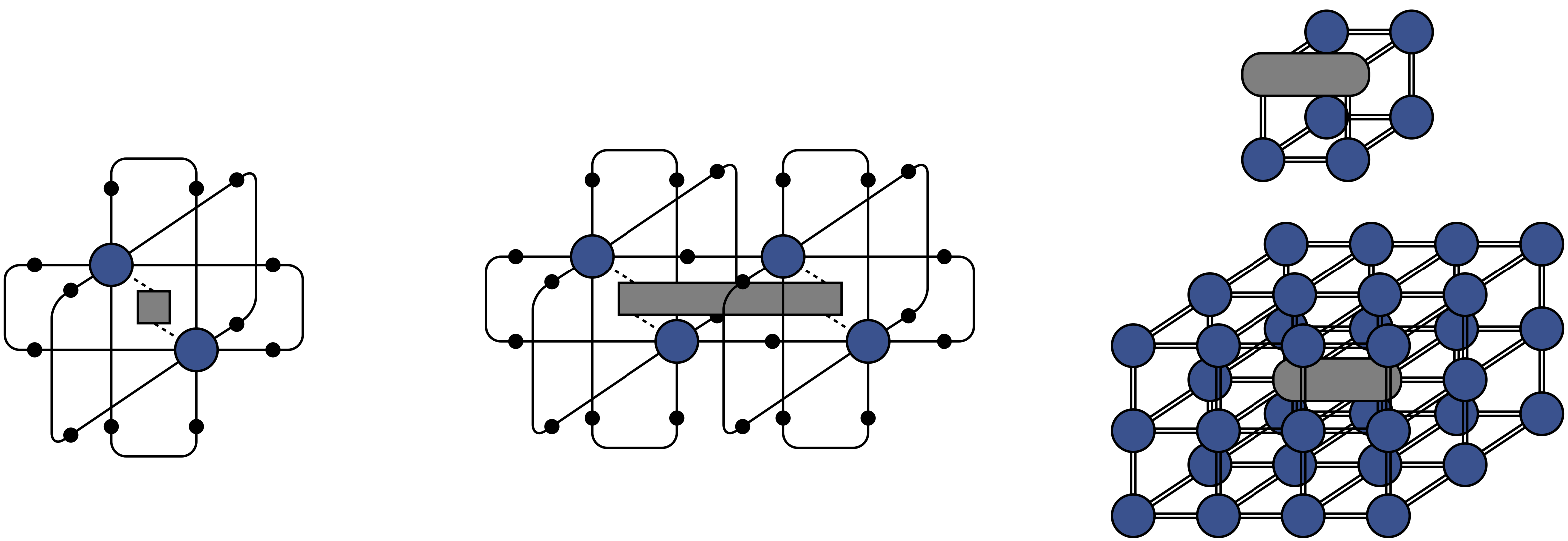
Simulation of 3D quantum systems with PEPS

PV and P. Corboz, PRB 103, 205137 (2021)

- Optimize iPEPS with SU
- Contraction
  - Cluster contraction
  - SU+CTMRG

Cluster contraction

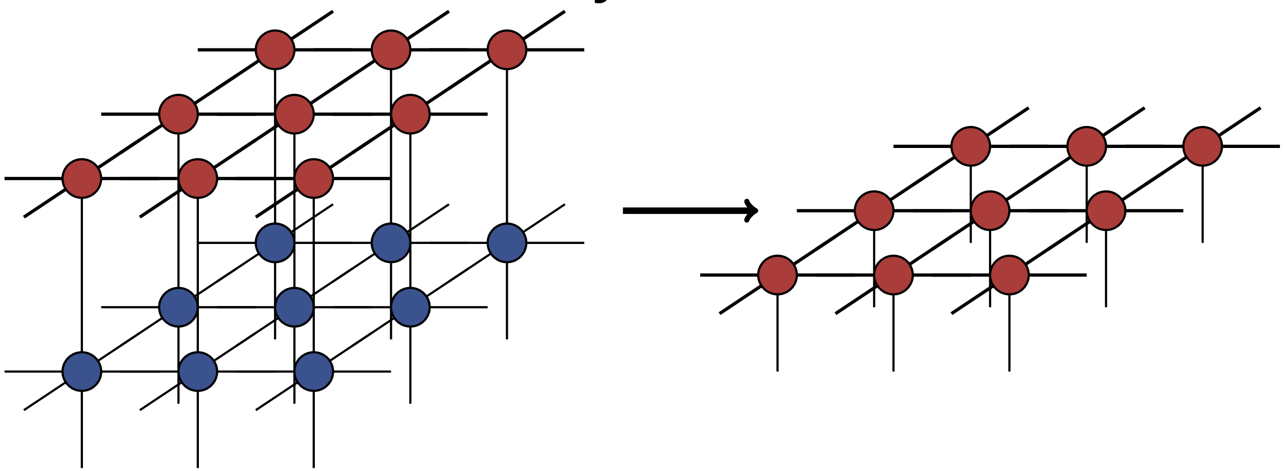
- Approximate through local contraction
- Smallest cluster used before[1]



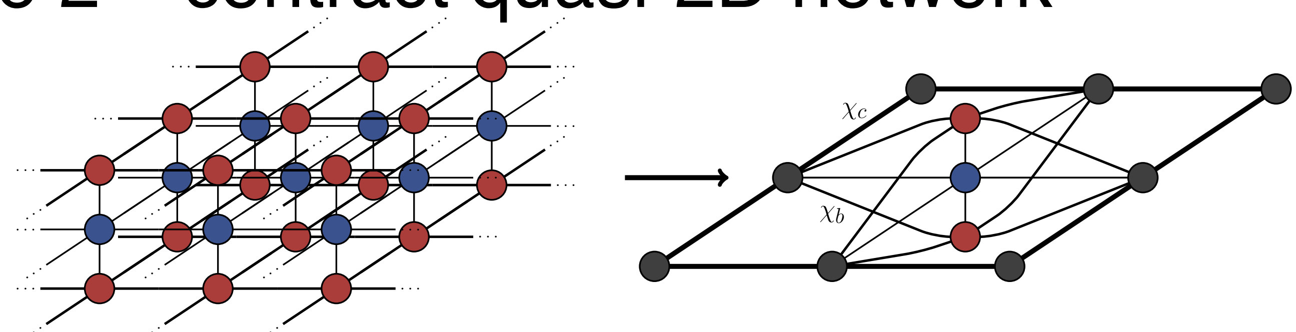
[1] S. S. Jahromi and R. Orús, Phys. Rev. B 99, 195105 (2019); T. Picot and D. Poilblanc, Phys. Rev. B 91, 064415 (2015)

SU+CTMRG

Stage 1 – use boundary iPEPS

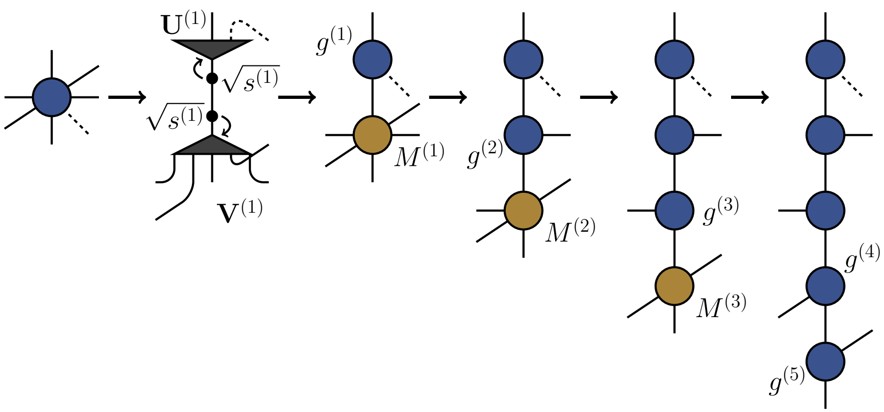


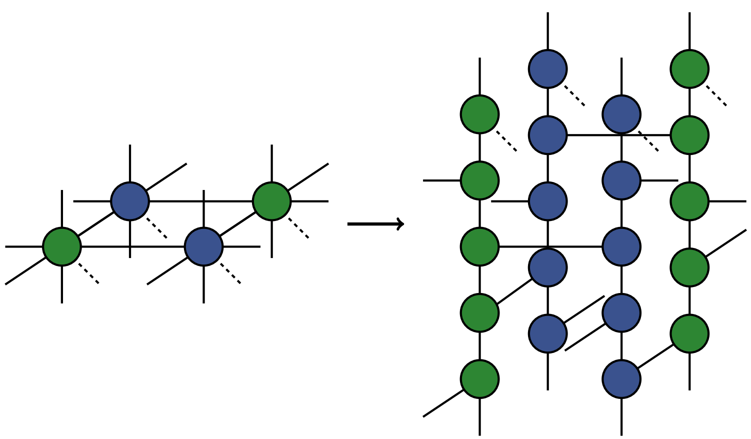
Stage 2 – contract quasi-2D network



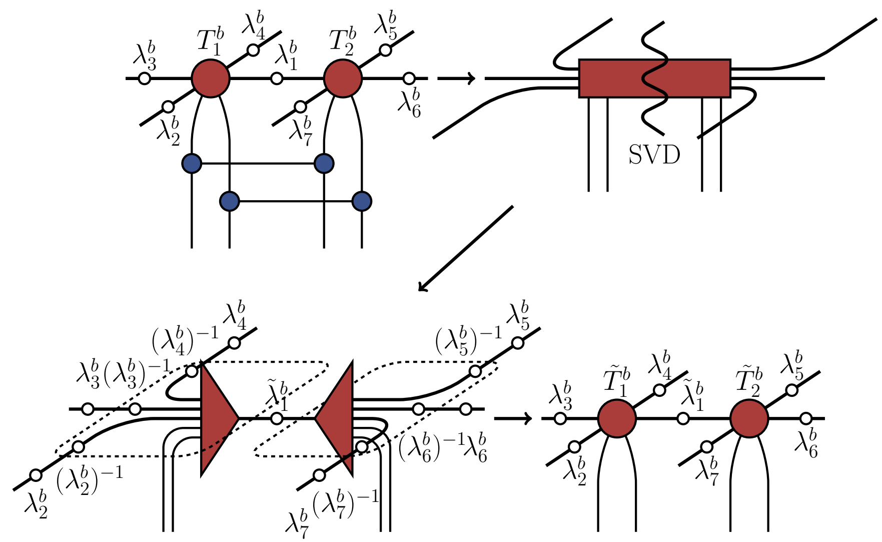
SU+CTMRG – boundary contraction

Decompose tensor

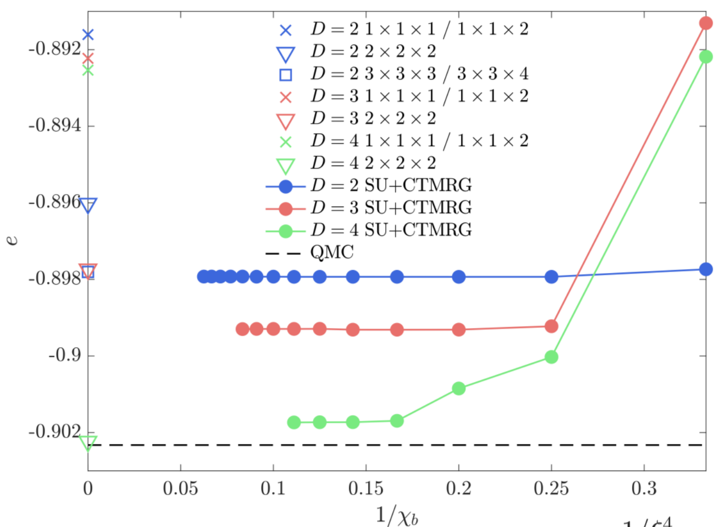


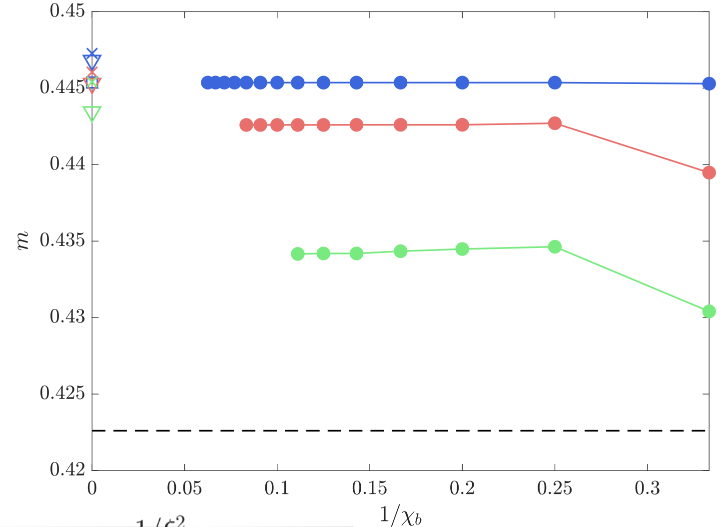


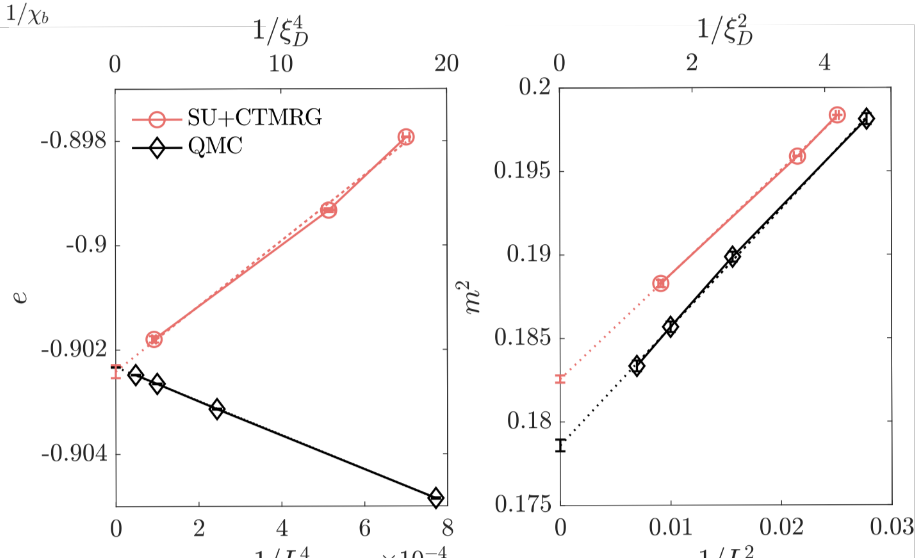
Apply to boundary



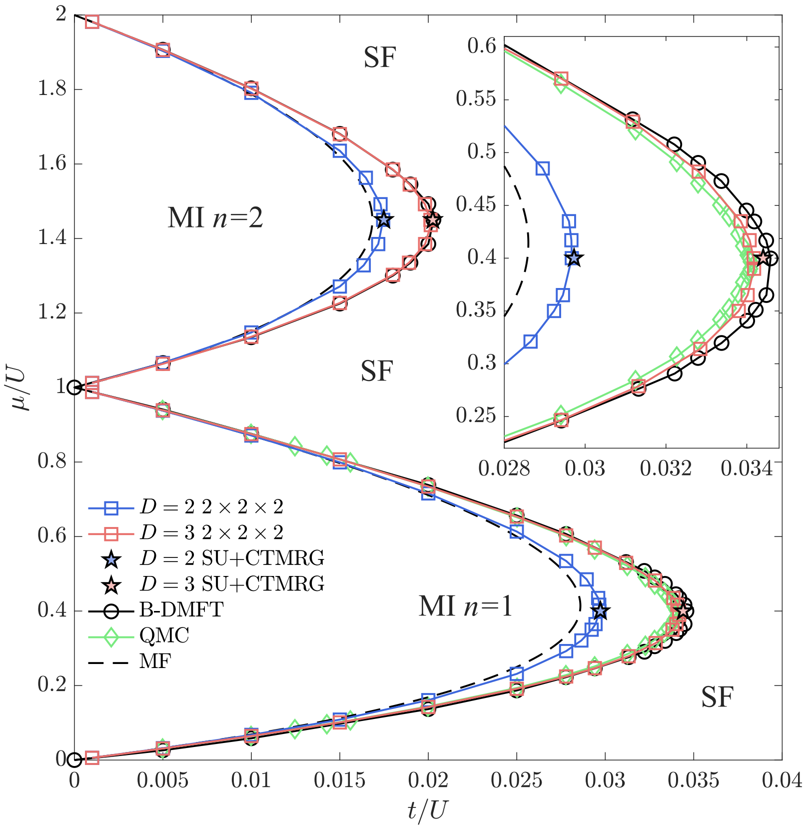
Results Heisenberg model







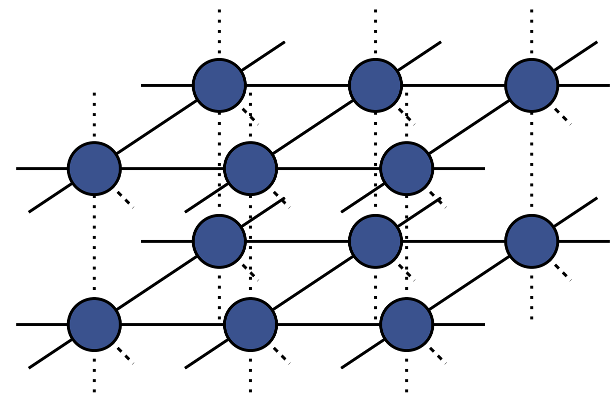
Results Bose-Hubbard model



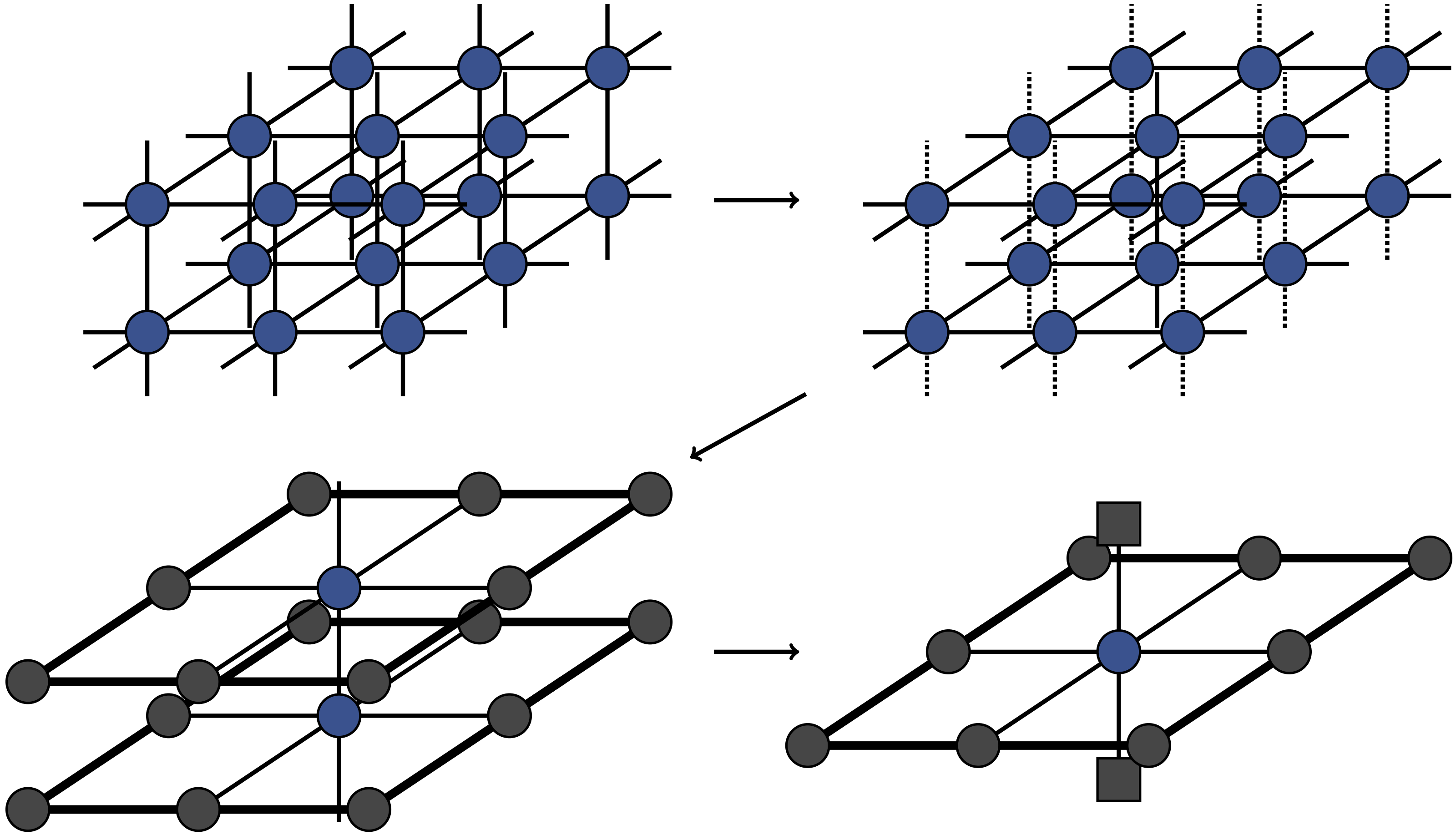
B-DMFT - Anders, Gull, Pollet, Troyer, & Werner, PRL 105, 096402 (2010); QMC - Capogrosso-Sansone, Prokof'ev, & Svistunov, PRB 75, 134302 (2007)

2D systems with interlayer coupling

- Strong anisotropy between xy- and z-correlations
- Examples
  - Triangular lattice compounds, e.g. $\mathrm{Ba_3CoSb_2O_9}$, $\mathrm{Ba_3CoNb_2O_9}$
  - Herbertsmithite
  - Cuprates
  - $\mathrm{SrCu_2(BO_3)_2}$
  - ….
- In contraction treat xy-plane and z-direction differently

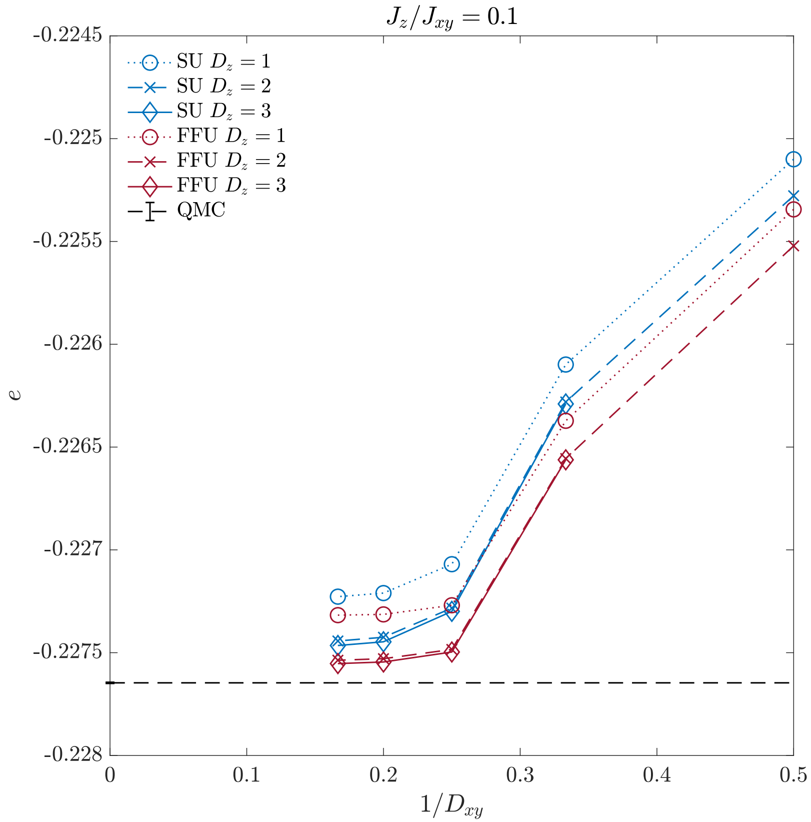


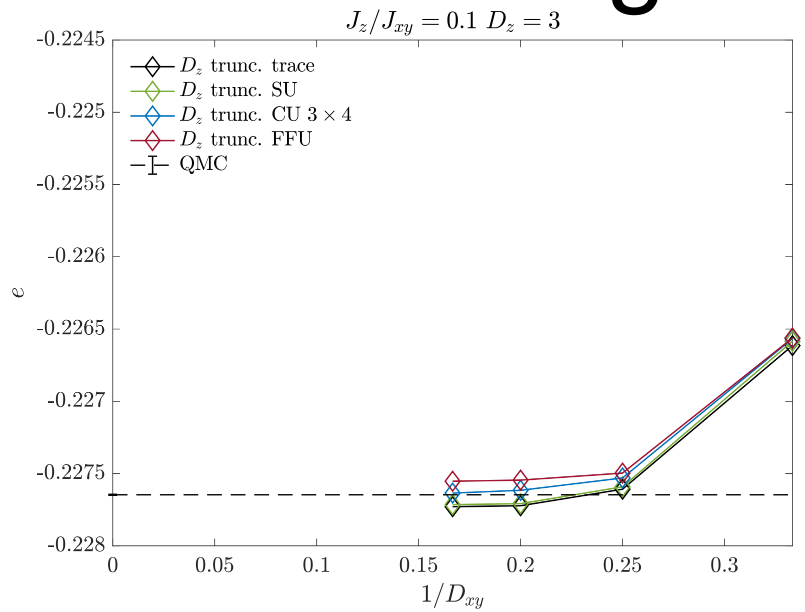
Layered CTM

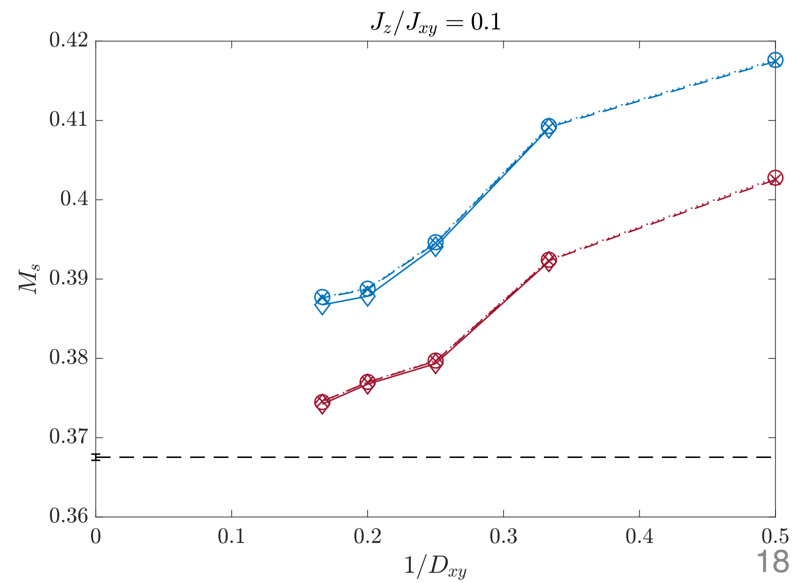


Results anisotropic Heisenberg model

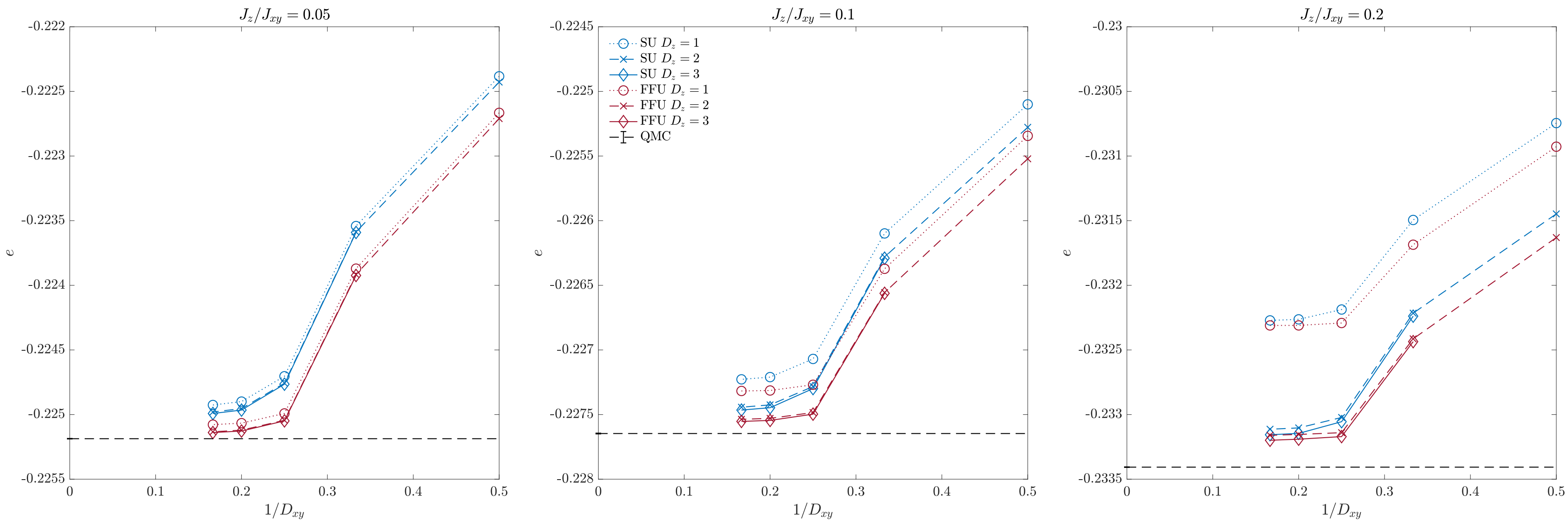
$$\hat{H} = J_{xy} \sum_{\langle i,j \rangle_{xy}} S_i S_j + J_z \sum_{\langle i,j \rangle_z} S_i S_j$$





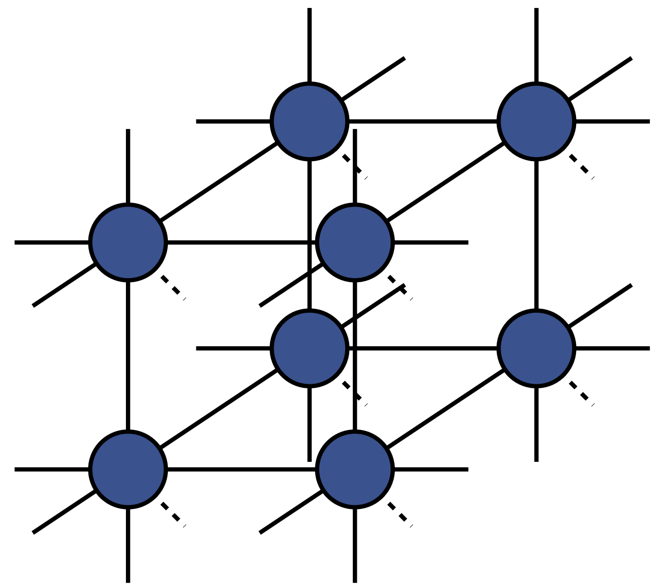


Results anisotropic Heisenberg model



Conclusion

- Tensor network methods promising tool to study challenging 3D quantum systems
- We developed methods for
  - 3D systems
    - Cluster contraction
    - SU+CTMRG
  - Layered systems
    - Layered CTM



Thank you for your attention!