News on tensor network simulations for quantum matter and beyond

Román Orús

Donostia International Physics Center (DIPC)

Multiverse Computing

April 23rd 2021

Outline

1) Some basics

2) Breathing Kagome AF

3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Outline

1) Some basics

2) Breathing Kagome AF

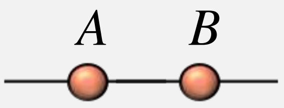
3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Tensor Networks

*e.g. RO, Annals of Physics **349** (2014) 117–158*

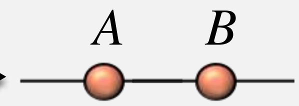
$A \cdot B \rightarrow$ 

$$|\Psi\rangle = \sum_{i's} \Psi_{i_1 i_2 \ldots i_N} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$$

p-level systems

Tensor Networks

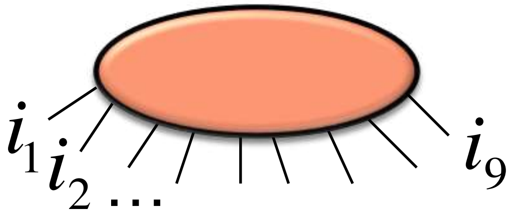
e.g. RO, *Annals of Physics* ***349*** *(2014) 117–158*

$A \cdot B \rightarrow$ 

$$|\Psi\rangle = \sum_{i's} \boxed{\Psi_{i_1 i_2 \ldots i_N}} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$$

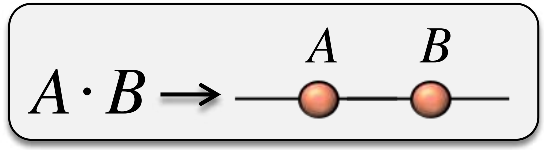
p-level systems

$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6 i_7 i_8 i_9}$$



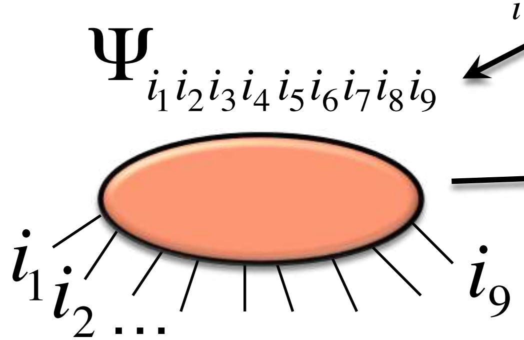
Tensor Networks

*e.g. RO, Annals of Physics **349** (2014) 117–158*



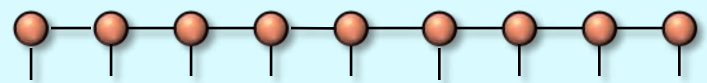
$$|\Psi\rangle = \sum_{i's} \boxed{\Psi_{i_1 i_2 \ldots i_N}} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$$

p-level systems



1d

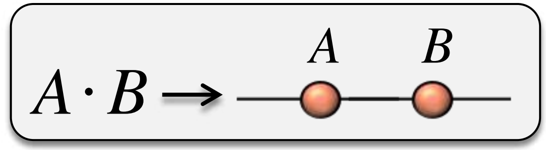
Matrix Product States (MPS)



DMRG, PWFRG, TEBD…

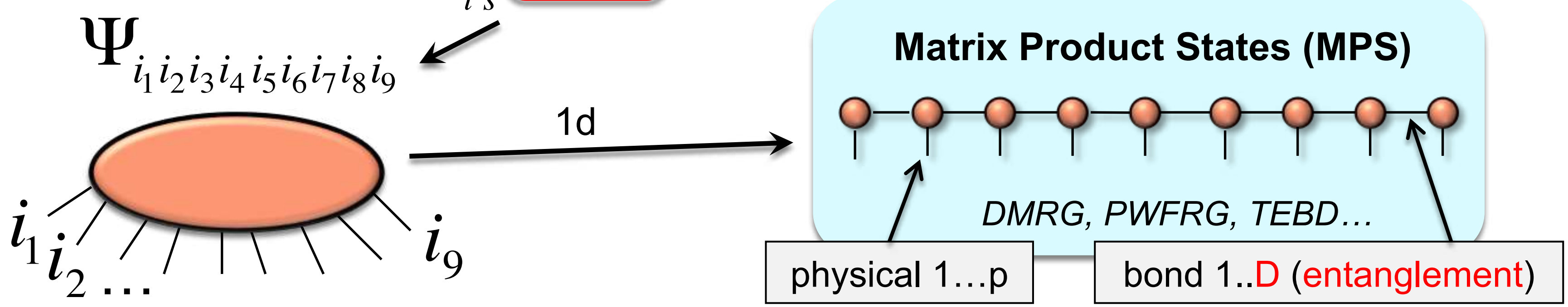
Tensor Networks

*e.g. RO, Annals of Physics **349** (2014) 117–158*



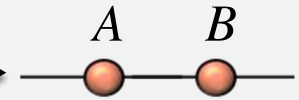
$$|\Psi\rangle = \sum_{i's} \boxed{\Psi_{i_1 i_2 \ldots i_N}} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$$

p-level systems



Tensor Networks

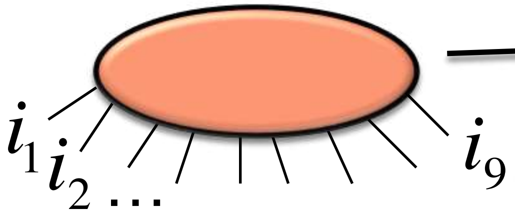
*e.g. RO, Annals of Physics **349** (2014) 117–158*

$A \cdot B \rightarrow$ 

$$|\Psi\rangle = \sum_{i's} \boxed{\Psi_{i_1 i_2 \ldots i_N}} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$$

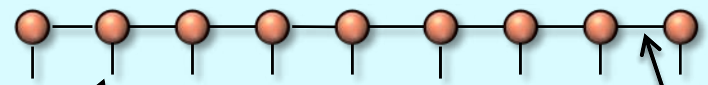
p-level systems

$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6 i_7 i_8 i_9}$



1d

Matrix Product States (MPS)



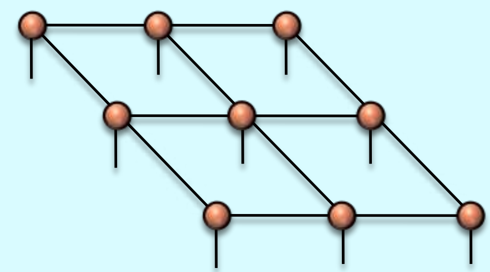
DMRG, PWFRG, TEBD…

physical 1…p

bond 1..D (entanglement)

2d, 3d...

Projected Entangled Pair States (PEPS), Tensor Product States (TPS)

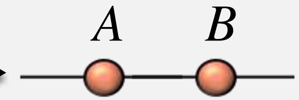


Tensor Product Variational Approach, PEPS & iPEPS algorithms, Tensor-Entanglement Renormalization, TRG/SRG/HOTRG/HOSRG…

Tensor Networks

*e.g. RO, Annals of Physics **349** (2014) 117–158*

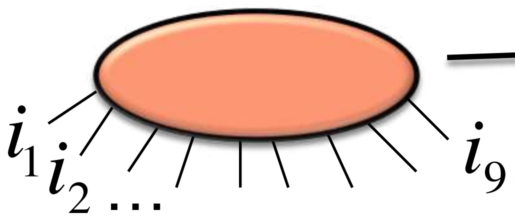
$A \cdot B \rightarrow$



p-level systems

$$|\Psi\rangle = \sum_{i's} \boxed{\Psi_{i_1 i_2 \ldots i_N}} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$$

$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6 i_7 i_8 i_9}$

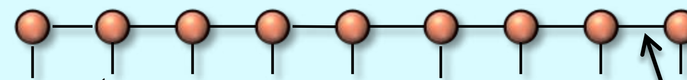


1d

2d, 3d…

Scale-invariant

Matrix Product States (MPS)

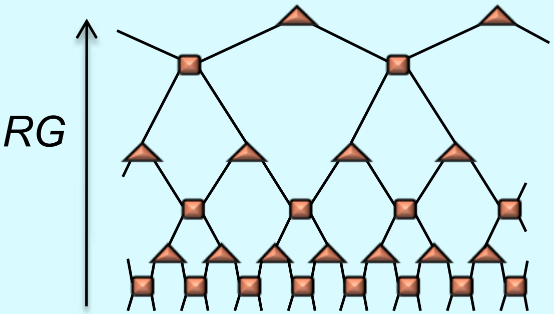


DMRG, PWFRG, TEBD…

physical 1…p

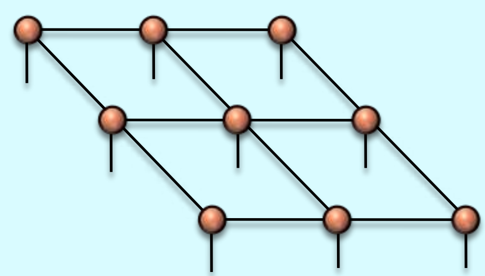
bond 1..D (entanglement)

Multiscale Entanglement Renormalization Ansatz (MERA)



AdS/CFT, Entanglement Renormalization

Projected Entangled Pair States (PEPS), Tensor Product States (TPS)



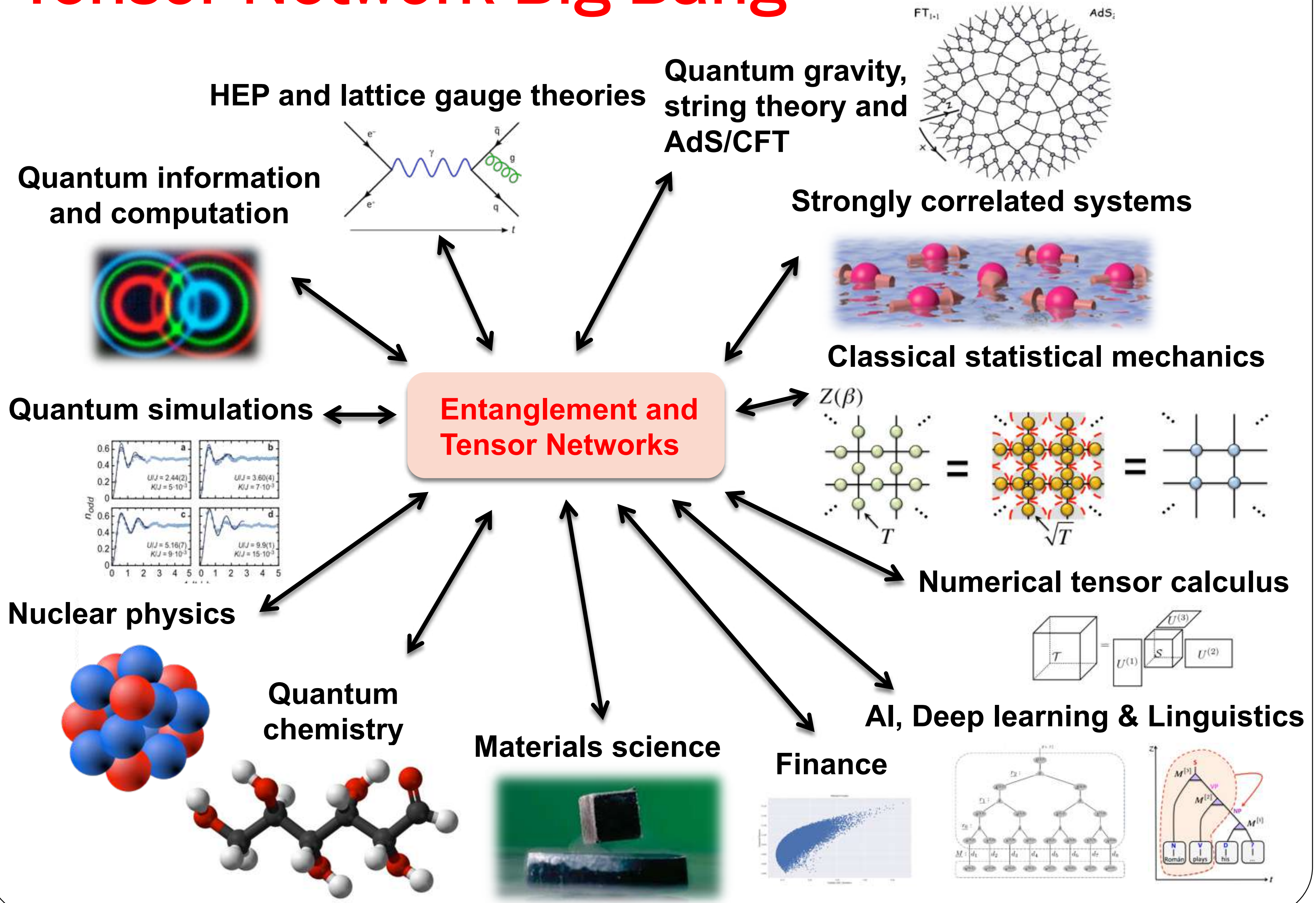
Tensor Product Variational Approach, PEPS & iPEPS algorithms, Tensor-Entanglement Renormalization, TRG/SRG/HOTRG/HOSRG…

Efficient O(poly(N)), satisfy area-law, low-energy eigenstates of local Hamiltonians

Tensor Network Big Bang

Entanglement and Tensor Networks

Tensor Network Big Bang



Outline

1) Some basics

2) Breathing Kagome AF

3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Outline

1) Some basics

2) Breathing Kagome AF

3) 3d thermal bosons and Kitaev models

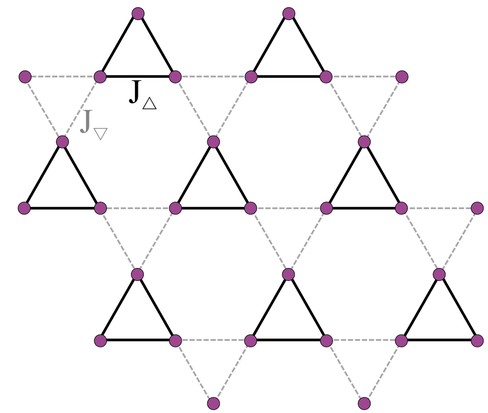
4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Breathing Kagome Heisenberg Antiferromagnet

$$H = J_{\triangle} \sum_{\langle ij \rangle \in \triangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_{\nabla} \sum_{\langle ij \rangle \in \nabla} \mathbf{S}_i \cdot \mathbf{S}_j$$

spin-1/2



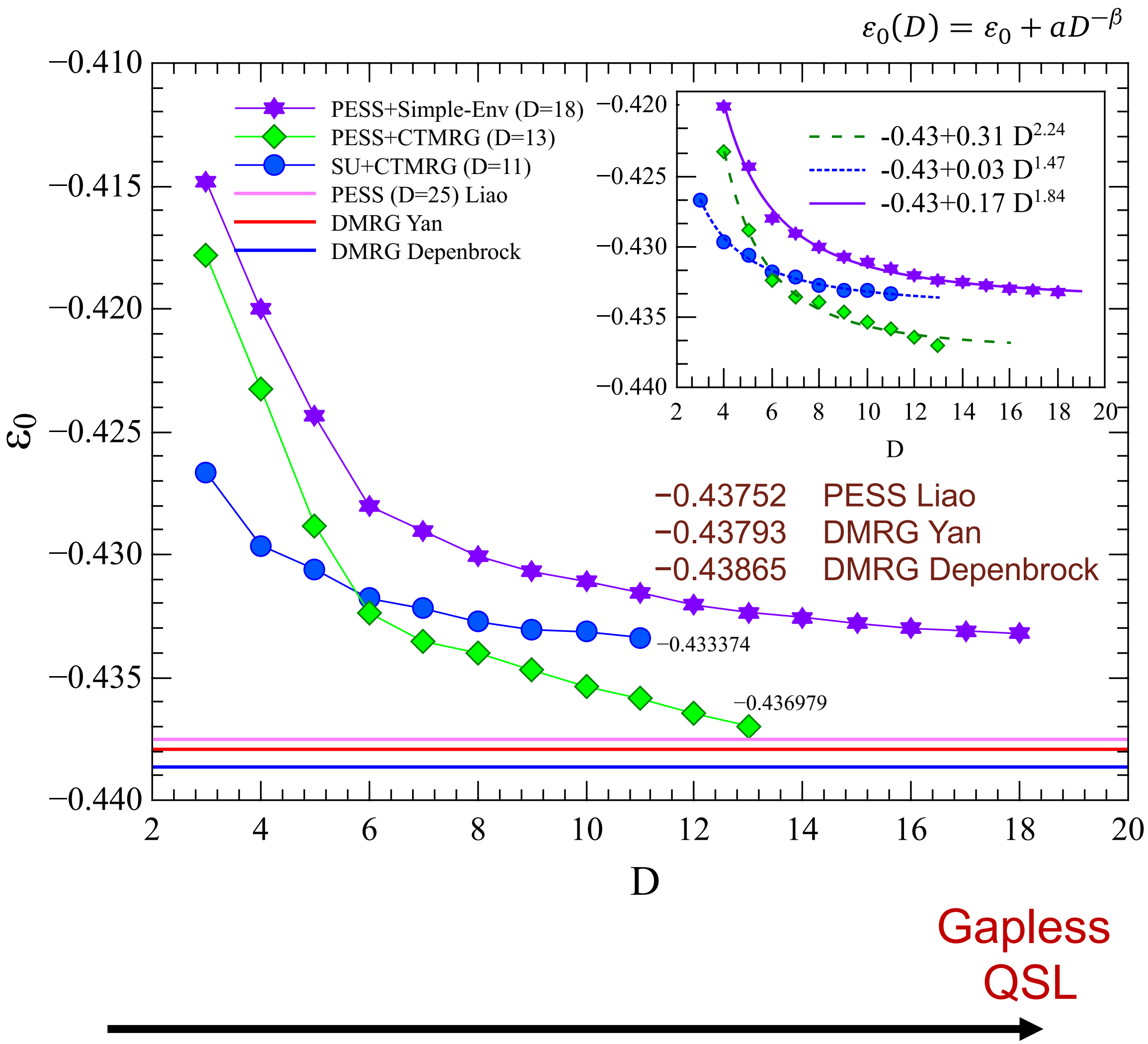
- Kagome compounds tend to be anisotropic in nature
- Candidate Material: Vanadium Oxyfluoride compound $[NH_4]_2[C7H_{14}N][V_7O_6F_{18}]$ *Clark et al, PRL, (2013)* *Aidoudi et al, Nat. Chem. (2011)* *Orian et al, PRL, (2017)*
- Can Heisenberg antiferromagnets with Breathing anisotropy host QSL?
- Experimental Signatures of a QSL at $J_{\nabla}/J_{\triangle} \approx 0.55$ *Orian et al, PRL, (2017)*

Phase transition?

iPEPS, small breathing limit

$J_\triangledown / J_\triangle = 1$

S. S. Jahrmi, RO, D. Poilblanc, F. Mila, SciPst Phys. 9 092 (2020)



$J_\triangledown / J_\triangle \ll 1$ $J_\triangledown / J_\triangle = 1$

Gapless U(1) QSL (DMRG)

Y.C.He et al, PRX (2017)
Repellin et al, PRB (2017)

Gapless U(1) QSL (PEPS)

Xie et al, PRX (2014)
Picot et al, PRB (2016)
Liao et al, PRL (2017)

Gapless U(1) QSL (VMC)

Ran et al, PRL (2007)
Y. Iqbal et al, PRB (2013)
Y. Iqbal et al, PRB (2014)
Y. Iqbal et al, PRB (2015)

Gapped Z_2 QSL (PEPS)

Poilblanc et al, PRB (2012)
Schuch et al, PRB (2012)
Poilblanc et al, PRB (2013)

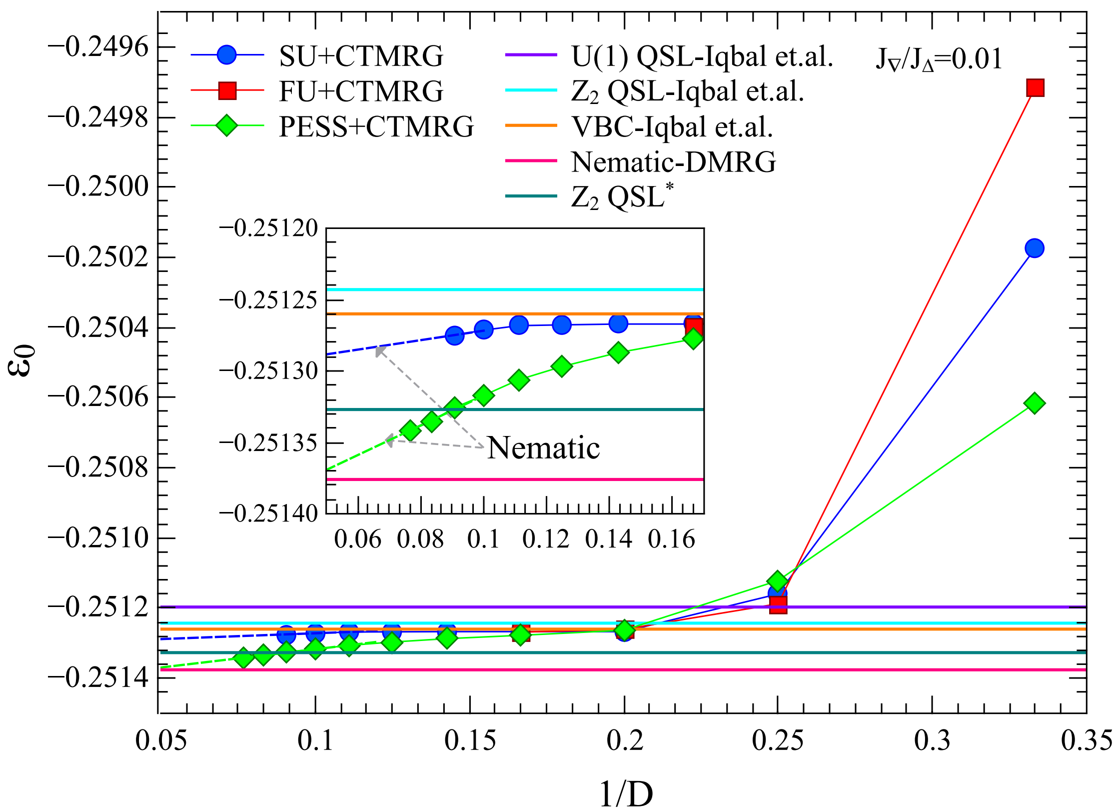
Gapped Z_2 QSL (DMRG)

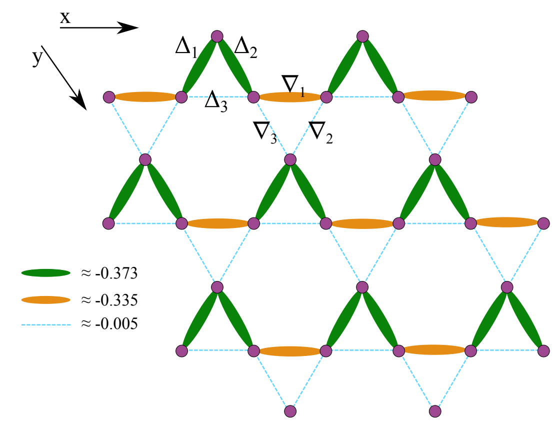
Jiang et al, Science (2008)
Yan et al, Science (2011)
Depenbrock et al, PRL (2012)

iPEPS, large breathing limit

$J_\nabla / J_\Delta = 0.01$

S. S. Jahrmi, RO, D. Poilblanc, F. Mila, SciPst Phys. 9 092 (2020)





Lattice Nematic state:
Preserves Translational Symmetry
Breaks Rotational Symmetry

Gapless Nematic

$J_\nabla / J_\Delta \ll 1$ → $J_\nabla / J_\Delta = 1$

VBC (VMC+PEPS)

Y. Iqbal et al, PRB (2018)

Gapped Z_2 QSL (PEPS)

M. Iqbal et al, arXiv:1912.08284 (2019)

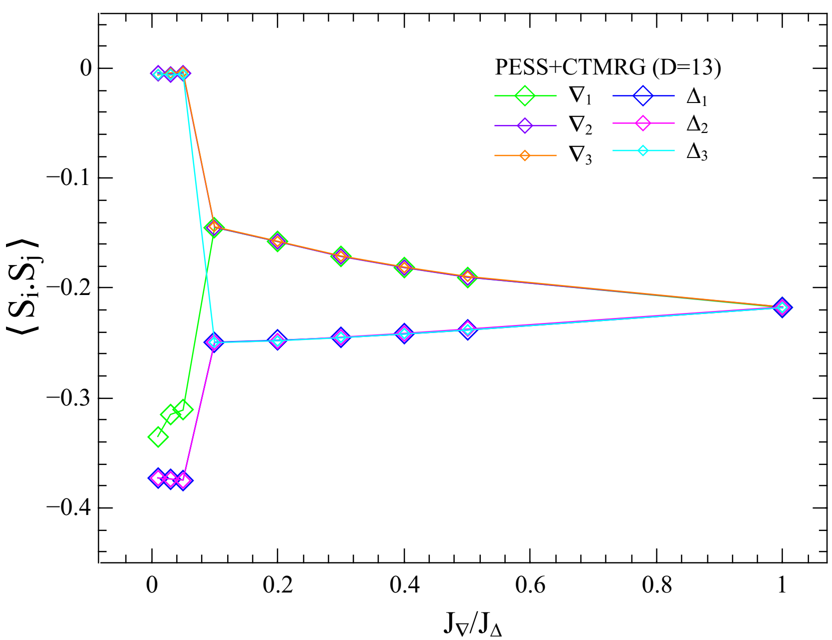
Nematic (DMRG)

Repellin et al, PRB (2017)

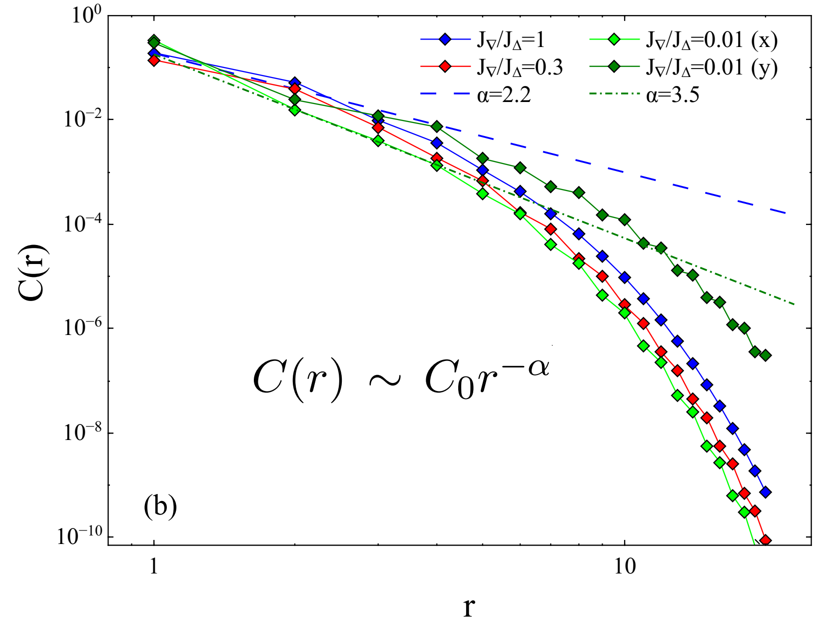
iPEPS, transition and criticality

S. S. Jahrmi, RO, D. Poilblanc, F. Mila, SciPst Phys. 9 092 (2020)

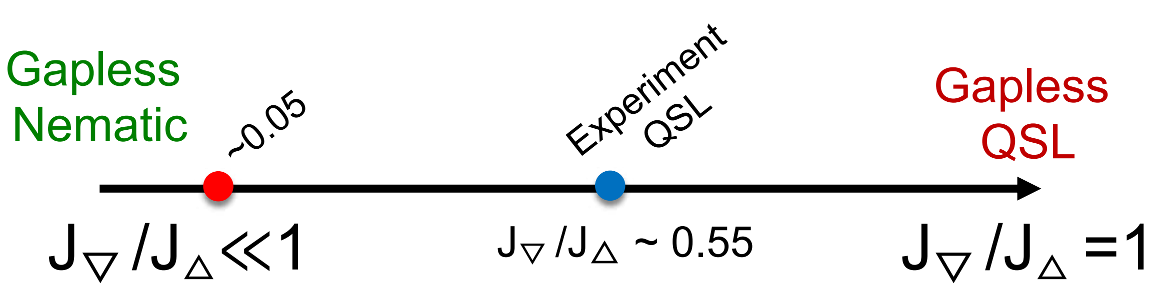
$J_\nabla / J_\Delta \sim 0.05$

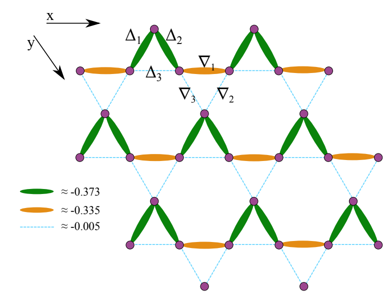


Nematic is critical



$$C(r) = \langle \mathbf{S}_{(x,y)} . \mathbf{S}_{(x+r,y)} \rangle - \langle \mathbf{S}_{(x,y)} \rangle . \langle \mathbf{S}_{(x+r,y)} \rangle$$





Outline

1) Some basics

2) Breathing Kagome AF

3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Outline

1) Some basics

2) Breathing Kagome AF

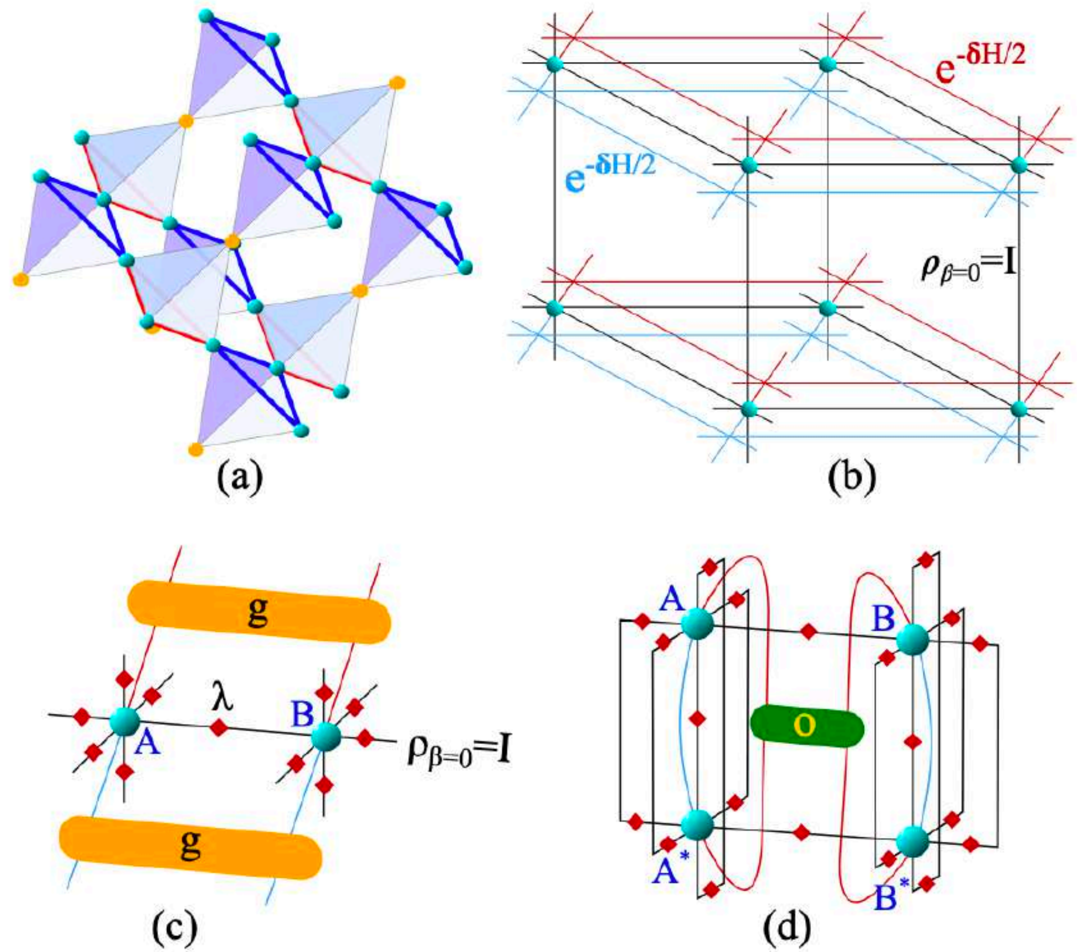
3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

3d Thermal iPEPS

S. S. Jahrmi, RO, SciRep 20 29052 (2020)



(a) (b) (c) (d)

Thermal states in cubic and pyrochlore lattices

Simple update

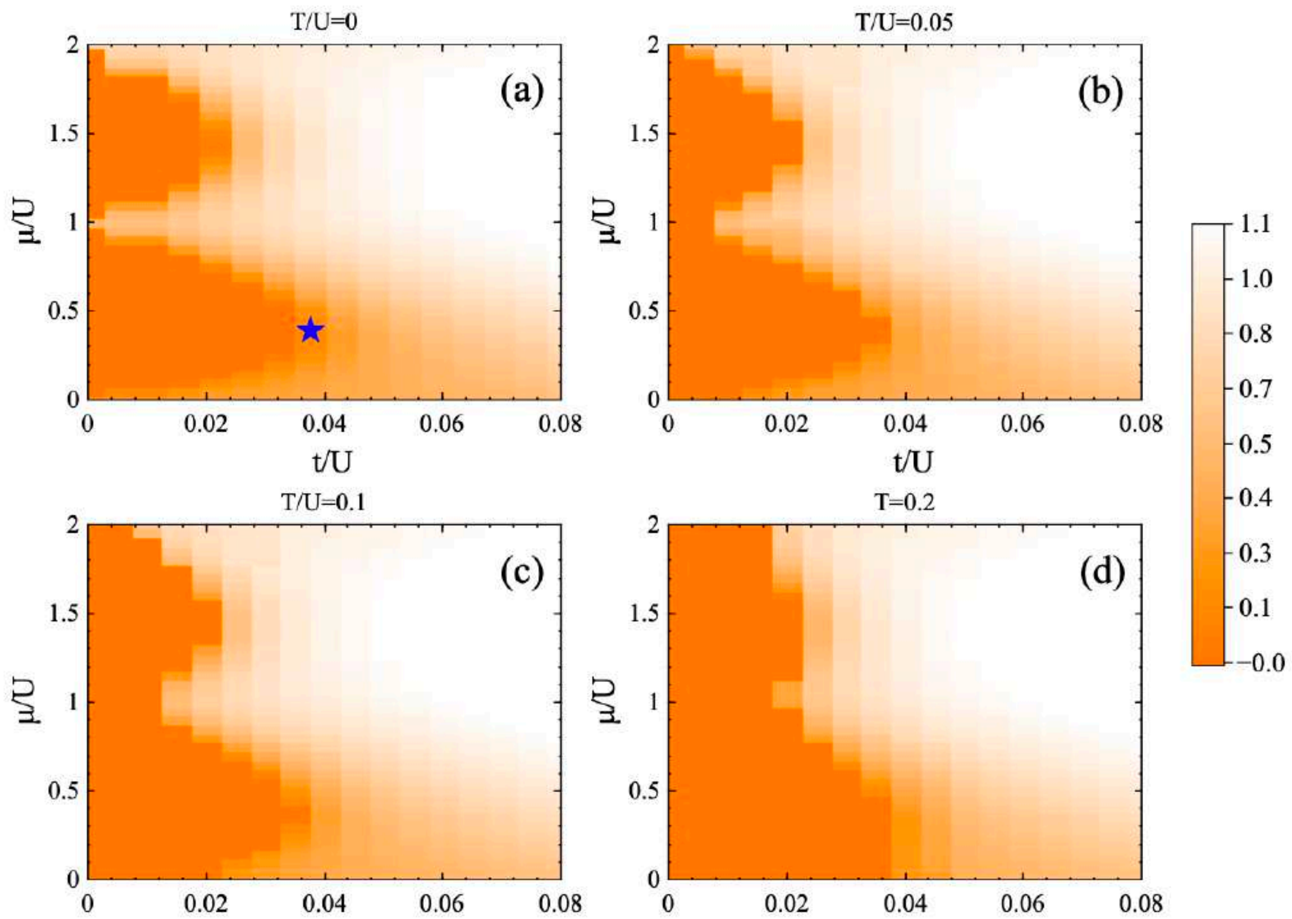
Mean-Field environment

3d Thermal Bosons

Hard- and soft-core

S. S. Jahrmi, RO, SciRep 20 29052 (2020)

$$H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i$$



Soft-core

Cubic lattice

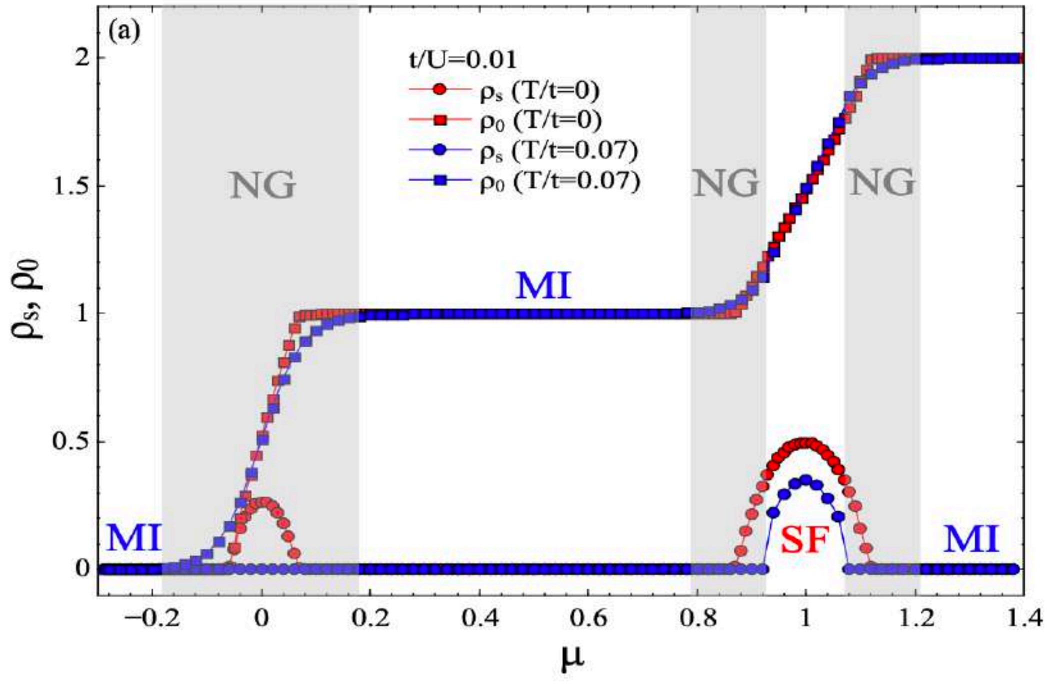
3d Thermal Bosons

Hard- and soft-core

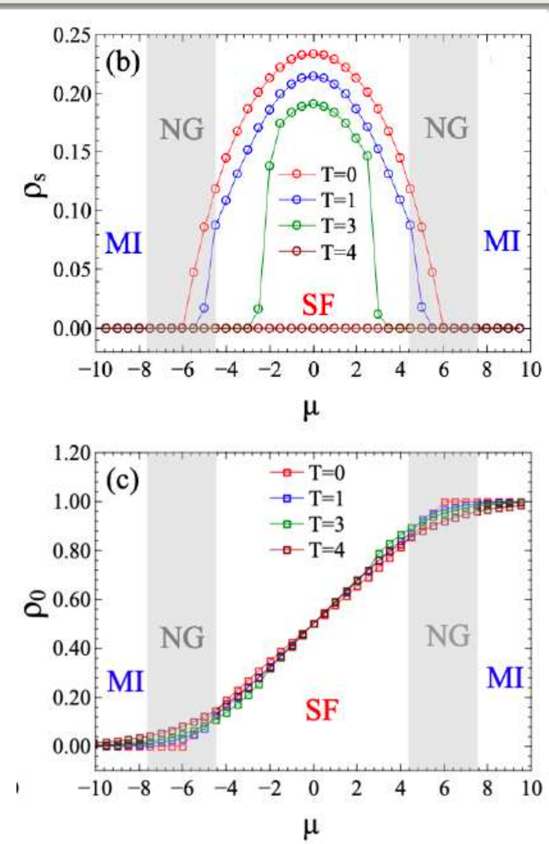
S. S. Jahrmi, RO, SciRep 20 29052 (2020)

$$H = -t\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U}{2}\sum_i n_i(n_i-1) - \mu\sum_i n_i$$

Soft-core, cubic lattice



Hard-core, pyrchlore lattice



3d Thermal Kitaev

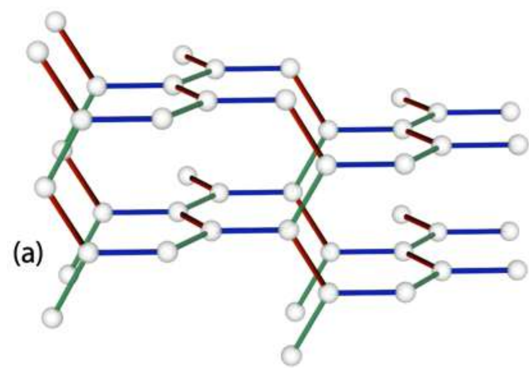
S. S. Jahrmi, H. Yarloo, RO, arXiv:2011.11577

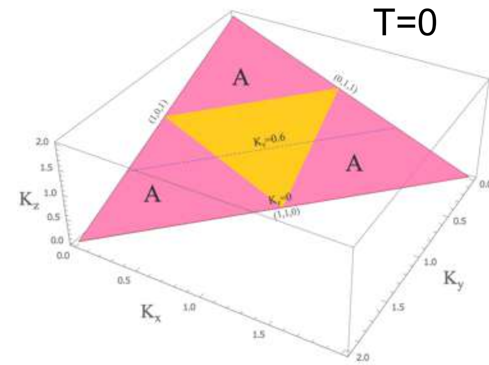
Hyperhoneycomb lattice

$$\mathcal{H}_{\mathrm{Kitaev}} = \sum_{\langle i,j\rangle,\gamma} K_\gamma\, S_i^\gamma S_j^\gamma$$

$\gamma = x, y, z$

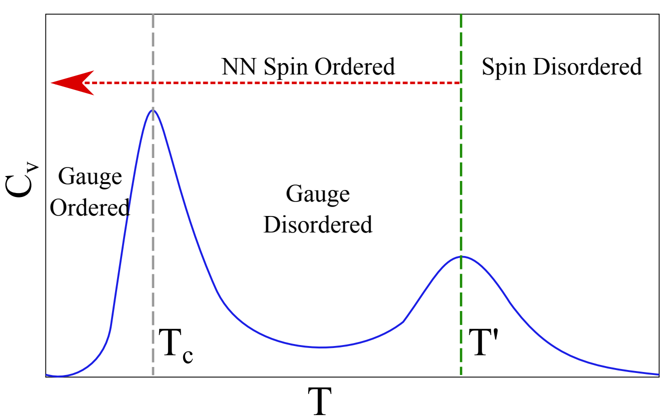
β-Li_2IrO_3 gs vortex-free

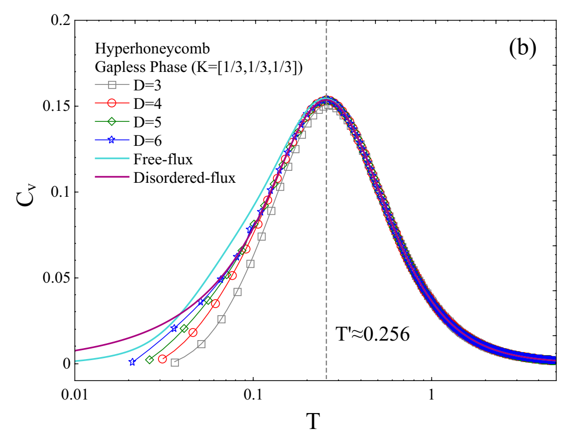


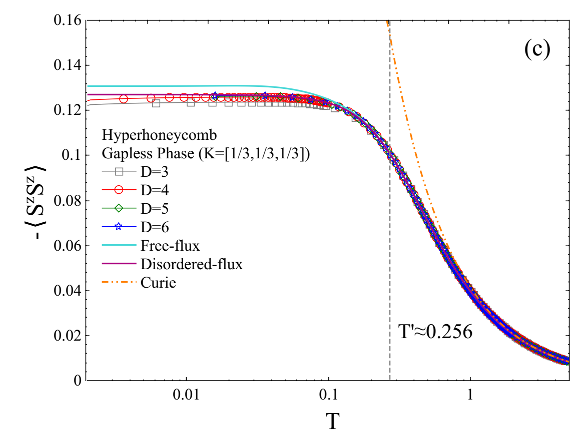


K. O'Brien, M. Hermanns, S. Trebst, PRL 93 085101 (2016)
T. Takayama et al, PRL 114 077202 (2015)

- Specific heat C_v exhibits a double-peak behavior
- High-T crossover: ordering of spins (Majoranas) at T ′~K
- Low-T transition: ordering of gauge fields at Tc ~ K/100







3d Thermal Kitaev

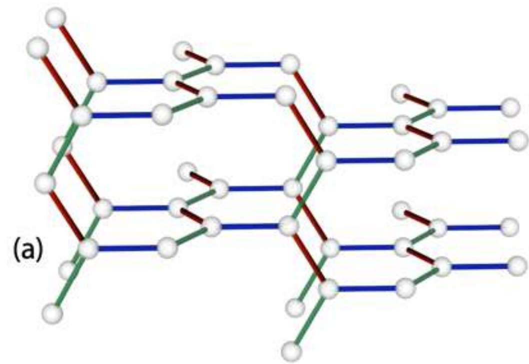
S. S. Jahrmi, H. Yarloo, RO, arXiv:2011.11577

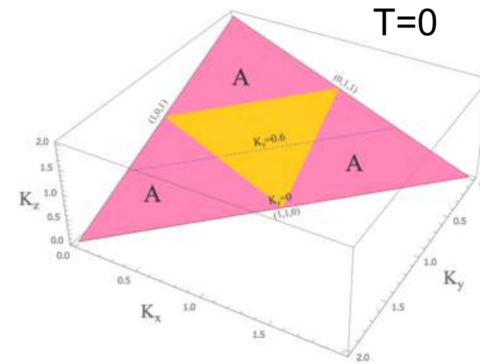
Hyperhoneycomb lattice

$$\mathcal{H}_{\mathrm{Kitaev}} = \sum_{\langle i,j\rangle,\gamma} K_\gamma \, S_i^\gamma S_j^\gamma$$

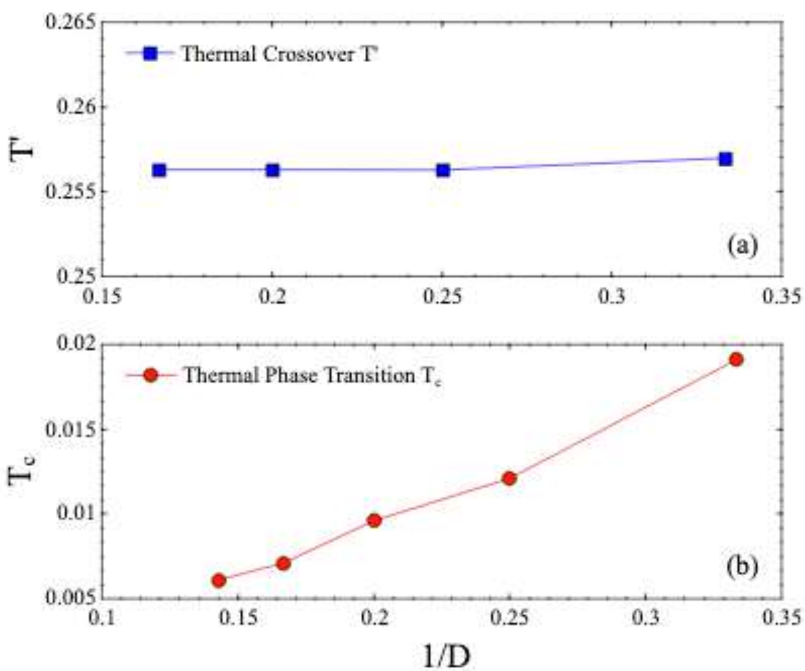
$\gamma = x, y, z$

β-Li_2IrO_3 gs vortex-free





K. O'Brien, M. Hermanns, S. Trebst, PRL 93 085101 (2016)
T. Takayama et al, PRL 114 077202 (2015)



Entanglement scaling of high-T thermal crossover and low-T thermal phase transition

(also studied Kitaev-Heisenberg on hyperoctagon lattice)

Outline

1) Some basics

2) Breathing Kagome AF

3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Outline

1) Some basics

2) Breathing Kagome AF

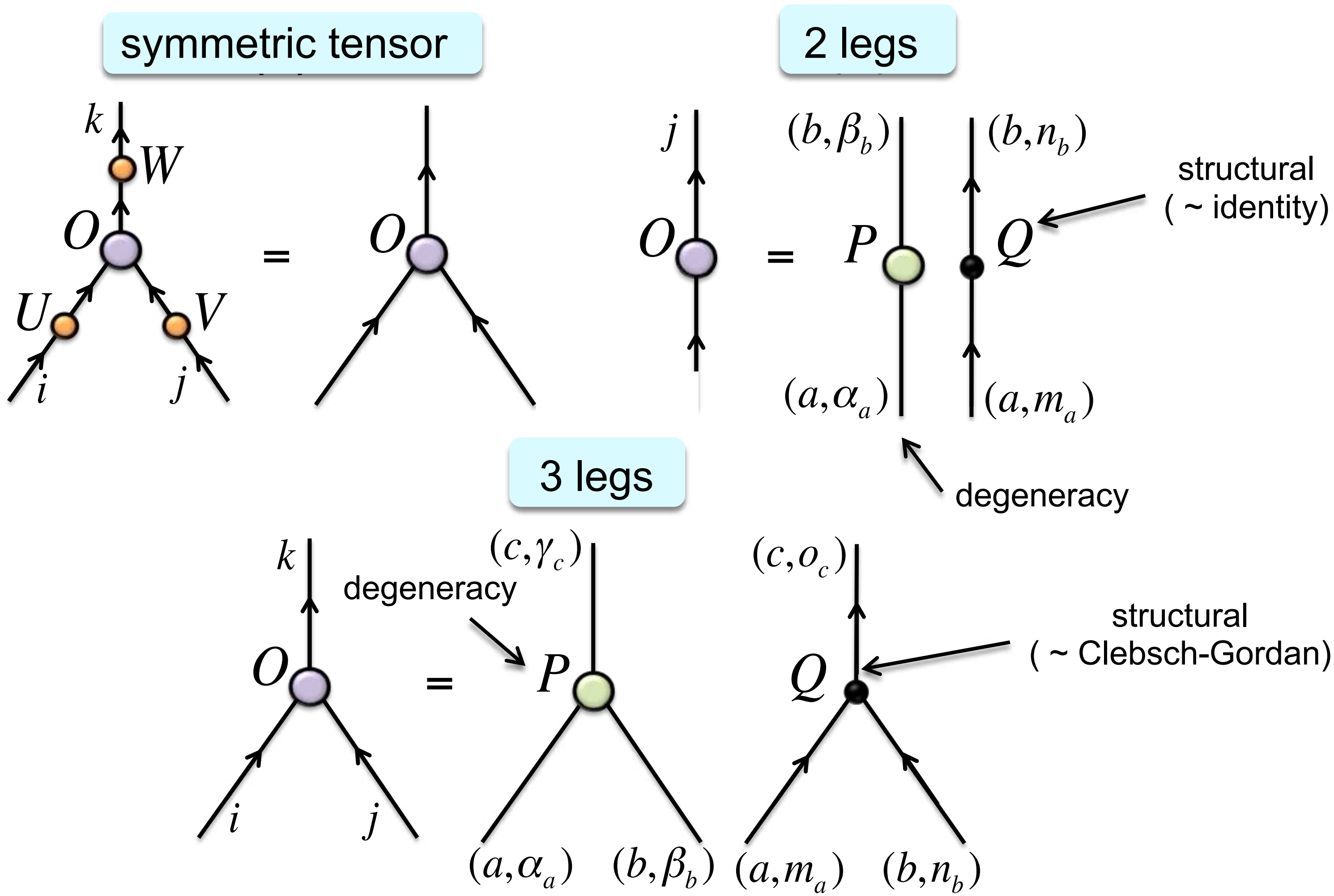
3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Symmetric tensors and Schur’s lemma

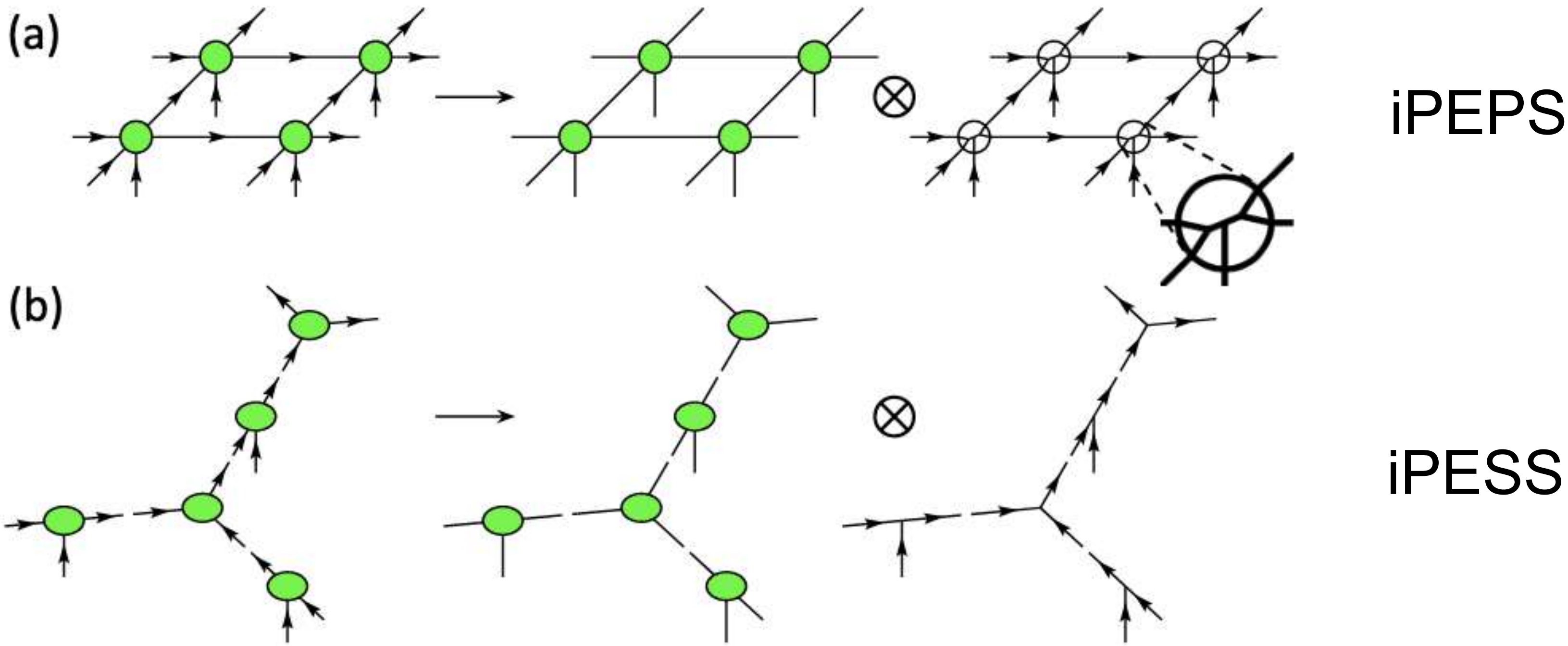
e.g., S. Singh, R. N. C. Pfeifer, G. Vidal, PRA 82, 050301 (2010)



Structural part depends only on the group properties (intertwiners)

SU(2) iPEPS and iPESS

P. Schmoll, RO, PRB 102 241101 (2020)

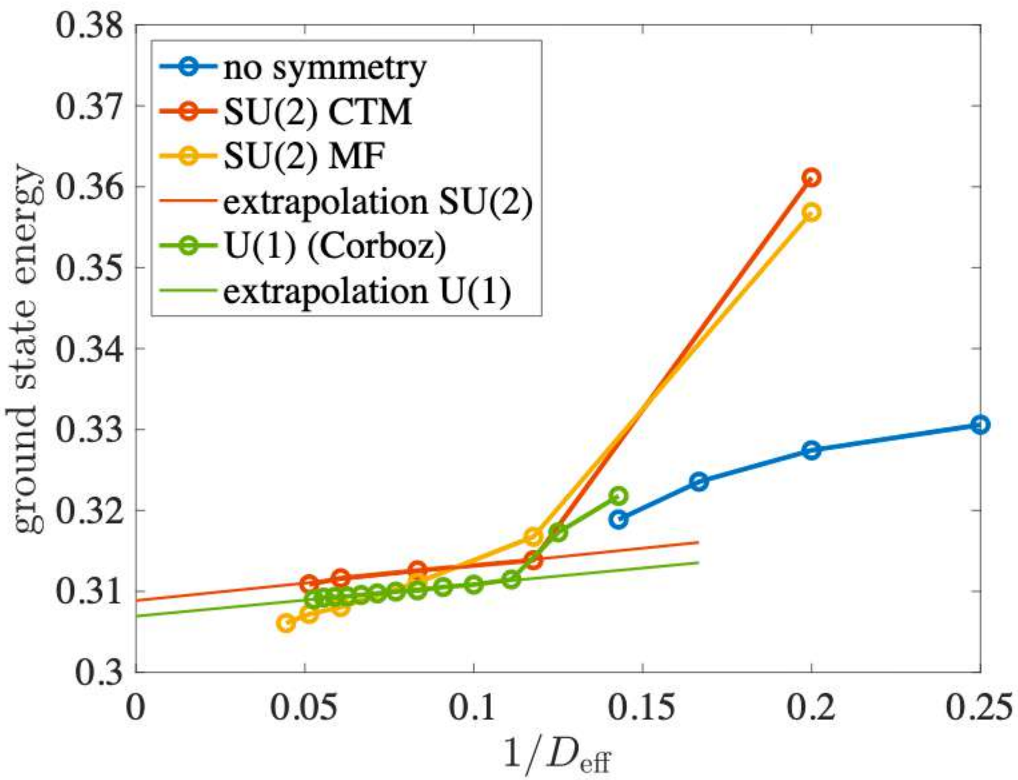


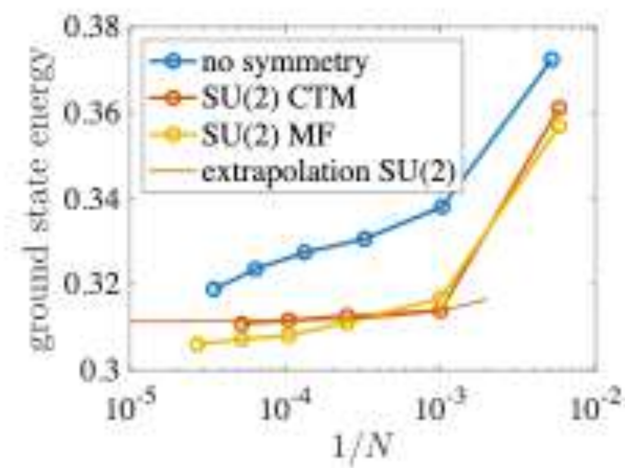
Benchmarking SU(2) iPEPS and iPESS

P. Schmoll, RO, PRB 102 241101 (2020)

$$H = \sum_{\langle i,j \rangle} \left(\cos(\theta)\, (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + \sin(\theta)\, (\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2 \right)$$

Spin-1 BLBQ
square lattice





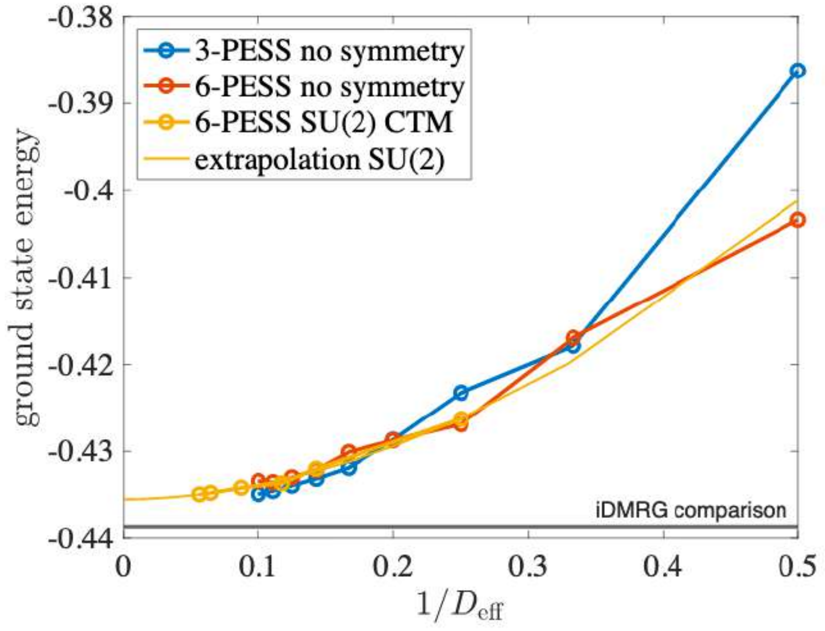
SU(2) may be too restrictive

I. Niesen, P. Corboz, SciPost 3 030 (2017)

Benchmarking SU(2) iPEPS and iPESS

P. Schmoll, RO, PRB 102 241101 (2020)

Spin-1/2 KHAF



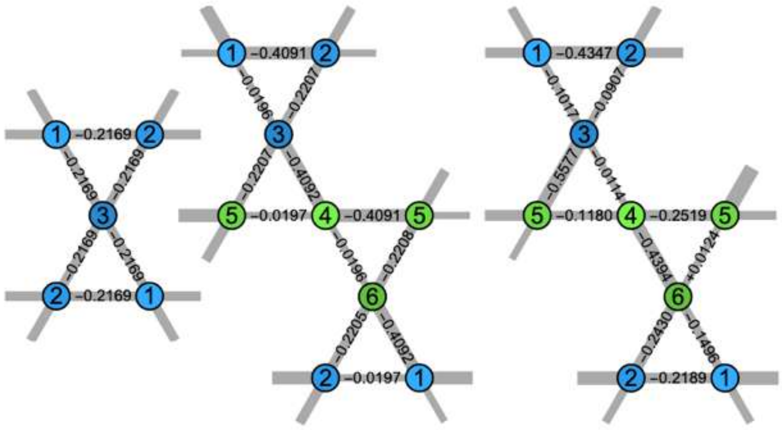


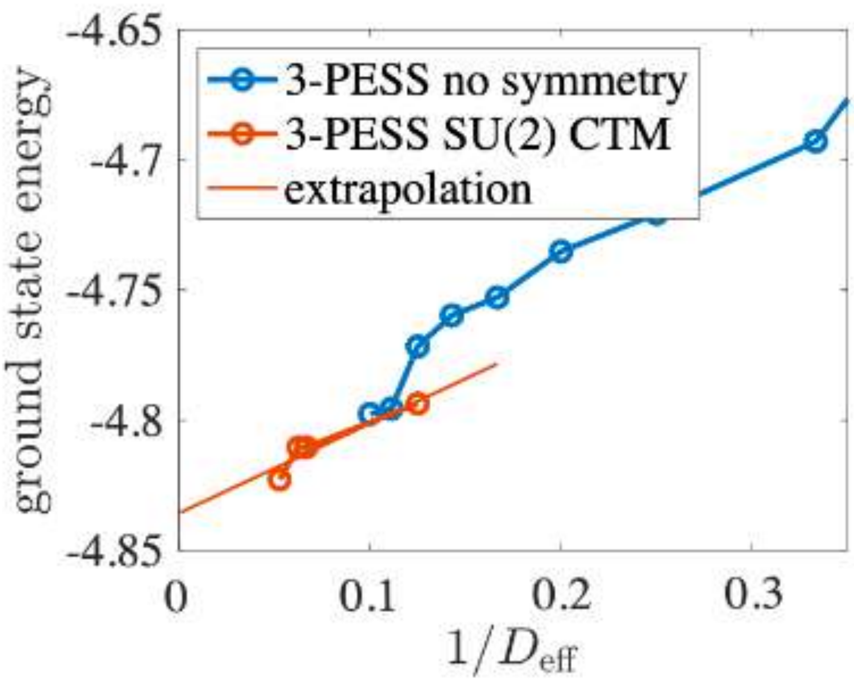
FIG. 7: (Color online) Spin-spin correlation $\langle \boldsymbol{S}_i \boldsymbol{S}_j \rangle$ on each link of the unit cell for the non-symmetric 3-PESS, the non-symmetric 6-PESS and the $SU(2)$-invariant 6-PESS (from left to right).

Clean extrapolation

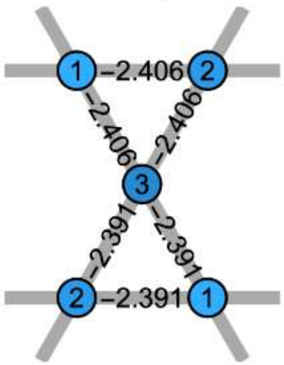
Benchmarking SU(2) iPEPS and iPESS

P. Schmoll, RO, PRB 102 241101 (2020)

Spin-2 KHAF

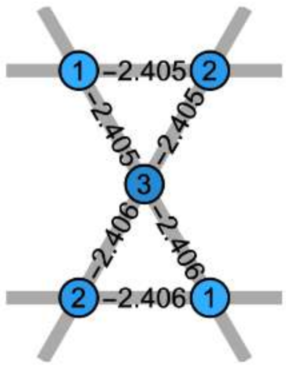


No symmetry



&

SU(2) symmetry



Quantum spin liquid?

Benchmarking SU(2) iPEPS and iPESS

P. Schmoll, RO, PRB 102 241101 (2020)

SU(2) lowest-energy summary

Model	No symmetry	$SU(2)$
$s=1$ BLBQ	$(7, 0.3188)$	$(6, 19.5, 0.3108)$
$s=1/2$ KHAF	$(10, -0.4348)$	$(7, 17.75, -0.4349)$
$s=2$ KHAF	$(10, -4.7975)$	$(5, 19, -4.8227)$

SU(2) improves energies, but sometimes may be too restrictive

Outline

1) Some basics

2) Breathing Kagome AF

3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Outline

1) Some basics

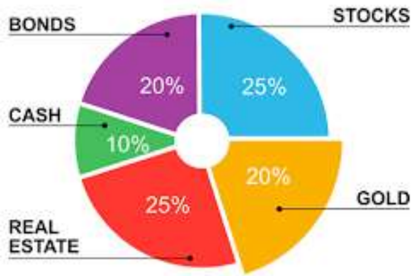
2) Breathing Kagome AF

3) 3d thermal bosons and Kitaev models

4) 2d iPEPS with SU(2)

5) Optimizing investment portfolios

Dynamic Portfolio Optimization



Find optimal trajectory in the portfolio space, taking into account transaction costs and other constraints

Forecasted profits (vector)

Asset weights (vector)

$$\text{Return} \equiv \sum_{t=t_i}^{t_f} \mu_t^T \overline{\omega}_t$$

Asset's covariance (matrix)

$$\text{Risk} \equiv \frac{1}{2} \sum_{t=t_i}^{t_f} \overline{\omega}_t^T \Sigma_t \overline{\omega}_t$$

Constraints

$\sum_{n=1}^{N} \overline{\omega}_{n,t} = K \quad \forall t$	Fixed amount of total investing at each time
$\omega_{n,t} \leq K'/K$	Maximum amount of investment per asset

$$\omega_{n,t} \equiv \frac{\overline{\omega}_{n,t}}{K}$$

G. Rosenberg et al, IEEE Journal of Selected Topics in Signal Processing 10, 1053 (2016)

See also P. Rebentrost, S. Lloyd, arXiv:1811.03975

Hamiltonian Cost Function

$$\mathcal{H} = \sum_{t=t_i}^{t_f} -\mu_t^T \omega_t + \underbrace{\frac{\gamma}{2}}_{\text{Risk aversión (controls volatility)}} \omega_t^T \Sigma_t \omega_t + \underbrace{\lambda}_{\text{Transaction costs}} (\Delta\omega_t)^2 + \underbrace{\rho}_{\text{Lagrange multiplier}} \left(\underbrace{u}_{\text{Vector of ones}}^T \omega_t - 1 \right)^2$$

TO MINIMIZE

Discrete formulation

$$\omega_{n,t} = \frac{1}{K} \sum_{q=0}^{N_q - 1} 2^q x_{n,t,q} \qquad N_{tot} = N \times N_t \times N_q$$

Quadratic Unconstrained Binary Optimization (QUBO)

$$\mathcal{H} = x^T Q x \qquad x \in \{0,1\}^{N_{tot}} \qquad Q \in \mathbb{R}^{N_{tot} \times N_{tot}}$$

Ising magnet

$$\mathcal{H} = \sum_{i,j=0}^{N_{tot}-1} J_{ij} s_i s_j \qquad x_i = (1 + s_i)/2 \qquad s_i = \pm 1$$

NP-Hard Optimization Problem

MULTIVERSE
COMPUTING

BBVA

Dynamic Portfolio Optimization with Real Datasets Using Quantum Processors and Quantum-Inspired Tensor Networks

Samuel Mugel,[1] Carlos Kuchkovsky,[2] Escolástico Sánchez,[2] Samuel Fernández-Lorenzo,[2] Jorge Luis-Hita,[2] Enrique Lizaso,[3] and Román Orús[3,4,5]

[1]*Multiverse Computing, Banting Institute, 100 College Street, ONRamp Suite 150, Toronto, ON M5G 1L5 Canada*
[2]*BBVA Research & Patents, Calle Sauceda 28, 28050 Madrid, Spain*
[3]*Multiverse Computing, Paseo de Miramón 170, E-20014 San Sebastián, Spain*
[4]*Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain*
[5]*Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain*

In this paper we tackle the problem of dynamic portfolio optimization, i.e., determining the optimal trading trajectory for an investment portfolio of assets over a period of time, taking into account transaction costs and other possible constraints. This problem, well-known to be NP-Hard, is central to quantitative finance. After a detailed introduction to the problem, we implement a number of quantum and quantum-inspired algorithms on different hardware platforms to solve its discrete formulation using real data from daily prices over 8 years of 52 assets, and do a detailed comparison of the obtained Sharpe ratios, profits and computing times. In particular, we implement classical solvers (Gekko, exhaustive), D-Wave Hybrid quantum annealing, two different approaches based on Variational Quantum Eigensolvers on IBM-Q (one of them brand-new and tailored to the problem), and for the first time in this context also a quantum-inspired optimizer based on Tensor Networks. In order to fit the data into each specific hardware platform, we also consider doing a preprocessing based on clustering of assets. From our comparison, we conclude that D-Wave Hybrid and Tensor Networks are able to handle the largest systems, where we do calculations up to 1272 fully-connected qubits for demonstrative purposes. Finally, we also discuss how to mathematically implement other possible real-life constraints, as well as several ideas to further improve the performance of the studied methods.

arXiv:2007.00017, first implementation with real data up to 52 assets and 8 years on D-Wave, VQE, and Tensor Networks (quantum-inspired)

Sharpe ratios

Method	XS	S	M	L	XL	XXL
VQE	3.59	-	-	-	-	-
Exhaustive	6.31	8.90	-	-	-	-
VQE Constrained	6.31	6.04	4.81	-	-	-
Gekko	5.98	8.90	8.39	15.83	20.76	-
D-Wave Hybrid	5.98	8.90	8.39	7.47	9.70	12.16
Tensor Networks	5.98	8.90	9.54	16.36	15.77	15.83

Profits

Method	XS	S	M	L	XL	XXL
VQE	2.4 %	-	-	-	-	-
Exhaustive	5.1 %	13.9 %	-	-	-	-
VQE Constrained	5.1 %	9.1 %	7.1 %	-	-	-
Gekko	5.8 %	13.9 %	13.6 %	54.1 %	71.6 %	-
D-Wave Hybrid	5.8 %	13.9 %	13.6 %	18.9 %	29.3 %	67.6 %
Tensor Networks	5.8 %	13.9 %	15.4 %	38.2 %	39.6 %	39.7 %

Run times (in sec.)

Method	XS	S	M	L	XL	XXL
VQE	278	-	-	-	-	-
Exhaustive	0.005	34	-	-	-	-
VQE Constrained	123	412	490	-	-	-
Gekko	24	27	21	221	261	-
D-Wave Hybrid	8	39	19	52	74	171
Tensor Networks	0.838	51	120	26649	82698	116833

- Not all figures of merit are equivalent
- D-Wave Hybrid and TNs: best
- D-Wave Hybrid extremely fast
- TNs highly improbable (GPUs, etc)
- VQE (in NISQ) highly limited

Largest portfolio optimization so far with quantum and TN methods and with real data

Improvable, promising

Conclusions

- Breathing Kagome compatible with gapless nematic phase and transition at $J_{\triangledown} / J_{\triangle} \approx 0.05$
- 3d thermal iPEPS allows accurate simulation of the thermodynamics of complex bosonic systems and Kitaev materials
- SU(2) symmetry improves energies, but may sometimes be too stringent for 2d simulations
- Spin-2 KHAF compatible with a QSL
- Quantum and Tensor Network optimization works for portolio optimization with real data

Thanks!