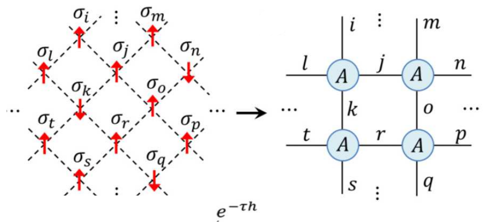
Tensor Renormalization Group (TRG)

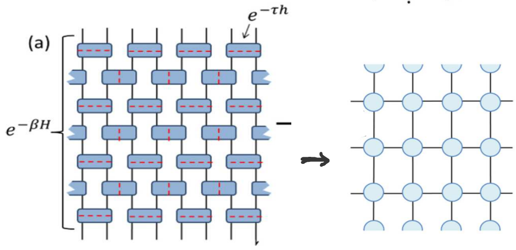
Goal: Compute 2D contractions by coarse-graining RG schemes (instead of transfer matrix schemes)

Applications:

Partition functions of
2D classical models:



Imaginary time evolution of
1D quantum models:



[Levin2007] Levin, Nave: proposed original idea for TRG for classical lattice models.
Local approach: truncation error is minimized only locally.

[Jiang2008] Jiang, Weng, Xiang: adapted Levin-Nave idea to 2D quantum ground state projection via imaginary time evolution. Local approach: truncation is done via 'simple update'. TRG is used to compute expectation values.

[Xie2009] Jiang, Chen, Weng, Xiang; and [Zhao2010] Zhao, Xie, Chen, Wei, Cai, Xiang:
Propose 'second renormalization' (SRG), a global approach taking account renormalization of environmental tensor ('full update'). Reduced truncation error significantly.

[Xie2012] Xie, Qin, Zhu, Yang, Xiang: different coarse-graning scheme, using higher-order SVD, employing both local and global optimization schemes.

[Zhao216] Zhao, Xie, Xiang, Imada: coarse-graining on finite lattices.

[Evenbly2019] Lan, Evenbly: propose core tensor renormalization group (CTRG), which rescales lattice size linearly (not exponentially), but at much lower cost, $\mathcal{O}(\chi^4)$ (rather than $\mathcal{O}(\chi^6)$).

1.TRG for 2D classical lattice models

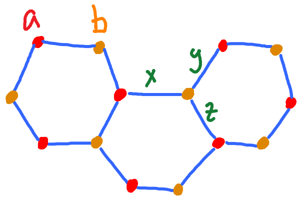
[Levin2007] Levin, Nave

Goal: compute partition function of 2D classical model.

Strategy: Express partition function as 2D tensor network, contract it by coarse-graining procedure.

<u>Example</u> 2D classical Ising model on honeycomb lattice [Zhao2010, Sec. II.B]

Honeycomb lattice is bipartite:



unit cell contains two sites, labeled a, b

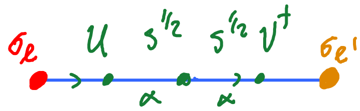
three bond directions: x, y, z

Hamiltonian: $$H = -\sum_{\langle \ell,\ell'\rangle} \sigma_\ell \sigma_{\ell'} \,, \qquad \sigma_\ell = \pm 1 \quad \text{Ising variable} \tag{1}$$

nearest neighbors, with $\ell \in a$, $\ell' \in b$

Partition function: $$Z = \sum_{\{\vec\sigma\}} e^{-\beta H} = \sum_{\{\vec\sigma\}} \prod_{\langle \ell,\ell'\rangle} \underbrace{e^{\beta \sigma_\ell \sigma_{\ell'}}}_{\substack{\equiv\, \Theta_{\ell\ell'} \\ 2\times 2}} = \sum_{\{\vec\sigma\}} \prod_{\langle \ell,\ell'\rangle} \Theta_{\ell\ell'} \tag{2}$$

'Factorize' the dependence on σ_ℓ and $\sigma_{\ell'}$ by performing an SVD:



$$\Theta_{\underset{a}{\ell}\,\underset{b}{\ell'}} = \sum_{\alpha=1,2} \underbrace{U_{\sigma_\ell \alpha} (S_\alpha)^{1/2}}_{\substack{\equiv\, Q^a_{\sigma_\ell \alpha} \\ 2\times 2}} \underbrace{(S_\alpha)^{1/2} V^\dagger_{\alpha \sigma_{\ell'}}}_{\substack{Q^b_{\sigma_{\ell'} \alpha} \\ 2\times 2 \text{ matrices}}} \tag{3}$$

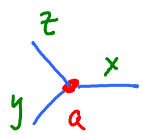
classical model: no need to distinguish upper/lower indices

Advantage of this representation: spin dependence has been factorized.

Price to pay: additional 2-dimensional bond index, $\alpha \in \{1,2\}$ has been introduced.

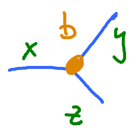
Group all Q's connected to site ℓ on a -lattice, and sum over σ_ℓ , for given $x, y, z \in \{1,2\}$

$$T^a_{[\ell]xyz} = \sum_{\sigma_\ell} Q^a_{\sigma_\ell x} Q^a_{\sigma_\ell y} Q^a_{\sigma_\ell z} \tag{4}$$

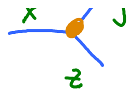


Ditto for site ℓ' on b -lattice, sum over $\sigma_{\ell'}$:

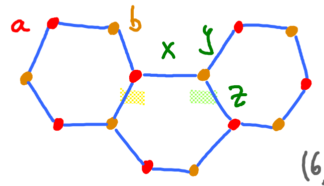
$$T^b_{[\ell']xyz} = \sum_{\sigma_{\ell'}} Q^b_{\sigma_{\ell'} x} Q^b_{\sigma_{\ell'} y} Q^b_{\sigma_{\ell'} z} \tag{5}$$



$$T_{[\ell']xyz} = \sum_{\sigma_{\ell'}} Q_{\sigma_{\ell'}x}\, Q_{\sigma_{\ell'}y}\, Q_{\sigma_{\ell'}z} \qquad (5)$$



Then partition function takes the form



$$Z \overset{(2)}{=} \sum_{\{\vec\sigma\}} \prod_{\langle \ell,\ell'\rangle} \Theta_{\ell\ell'} = \mathrm{Tr} \prod_{\ell\in a,\, \ell'\in b} T^{a}_{[\ell]\, x_\ell y_\ell z_\ell}\, T^{b}_{[\ell']\, x_{\ell'} y_{\ell'} z_{\ell'}} \qquad (6)$$

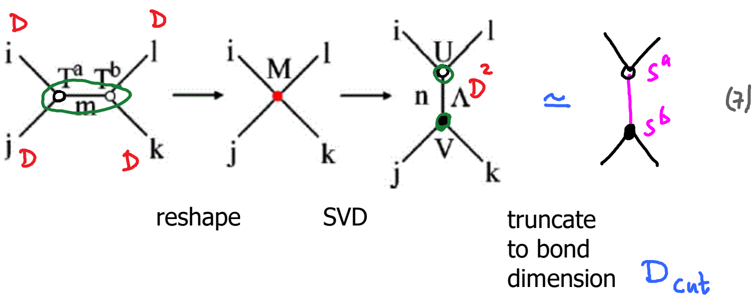
sum over virtual indices on all (suitably contracted) nearest-neighbor bonds

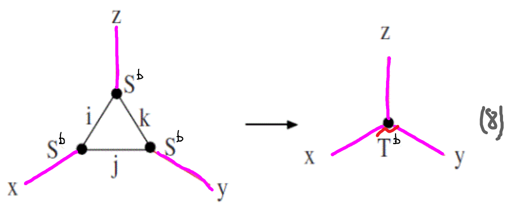
All statistical physics models with short-range interactions can be expressed as tensor network models, i.e.

$Z = \mathrm{Tr} \prod T$ (for more examples, see [Zhao2010, section II]).

<u>Contract out the tensor network by course-graining</u> [Levin2007]

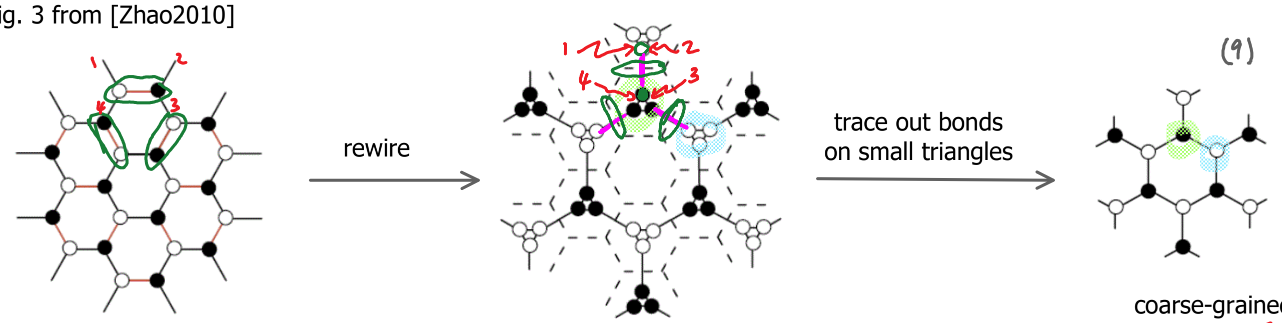
'rewire': switch from T-vertices with external leg pairings (i,j), (l,k) to S-vertices with pairings (i,l), (j,k):





coarse-grain:
trace out bonds on small triangle
to define updated T^b-tensor

Fig. 3 from [Zhao2010]

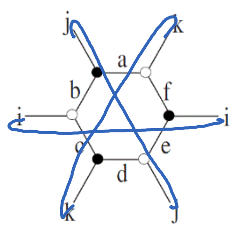


dashed lines depict original bonds,
solid lines depict rewired bonds

coarse-grained
lattice, $\tilde{T}$

Iterate this procedure, thereby coarse-graining lattice step by step, until T^a, T^b reach fixed point values,

T^{a*}, T^{b*} . Use these to compute partition function via $Z =$



and from there the free energy per spin, $F = -\frac{1}{N\beta} \ln Z$

and the magnetization, etc.

Goal: compute ground state of 2D quantum lattice model

Strategy: iterative projection via $e^{-H\tau}$, compress by 'simple update';

compute $\langle\psi|\psi\rangle$ and $\langle\psi|\hat{O}|\psi\rangle$ using TRG of Levin & Nave.

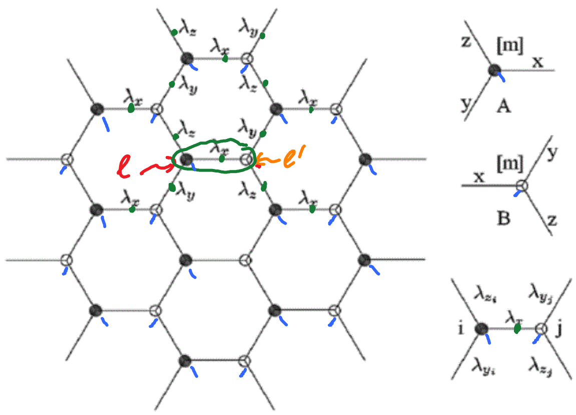
Model: $S = 1/2$ Heisenberg on honeycomb lattice.

vertices: A or B tensors
bonds: diagonal λ-tensors (weights)

iPEPS-type tensor network Ansatz for ground state:

$$|\psi\rangle = \mathrm{Tr} \prod_{l \in b} \prod_{l' \in w} \overbrace{\lambda_{x_l} \lambda_{y_l} \lambda_{z_l}}^{\text{weight factors associated with bonds}} \underbrace{A^{\sigma_l}_{x_l y_l z_l} B^{\sigma_{l'}}_{x_{l'} y_{l'} z_{l'}}}_{\text{tensors associated with vertices}} |\sigma_l \sigma_{l'}\rangle \qquad (1)$$

black white

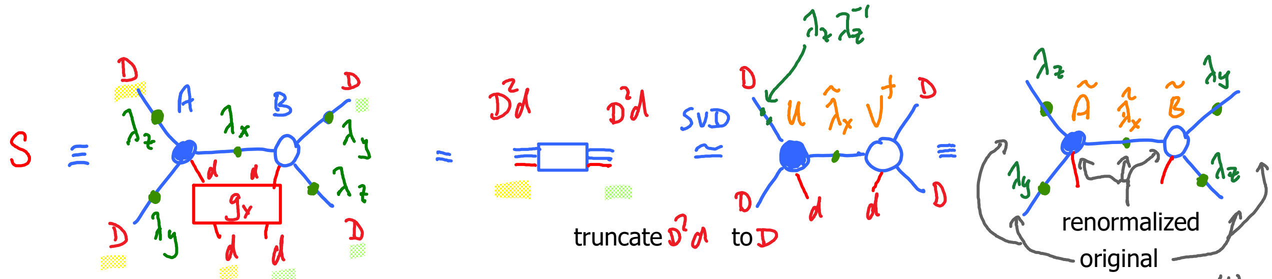


Ground state projection via simple update

$$H = H_x + H_y + H_z \qquad \text{(living on x, y, or z bonds)} \qquad (2)$$

Suzuki-Trotter: $$e^{-H\tau} \simeq \underbrace{e^{-H_x\tau}}_{g_x} \underbrace{e^{-H_y\tau}}_{g_y} \underbrace{e^{-H_z\tau}}_{g_z} + O(\tau^2) \qquad (3)$$

Sequentially update x, y, z bonds using these three gates.



(4)

$$S \simeq U \hat{\lambda}_x V^\dagger, \quad \tilde{A} = \lambda_z^{-1} \lambda_y^{-1} U, \quad \tilde{B} = \lambda_z^{-1} \lambda_y^{-1} V^\dagger \qquad (5)$$

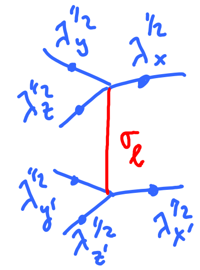
SVD, truncate

'simple update': outer legs of [A–B] contain λ, which account for the 'environment' of [A–B]

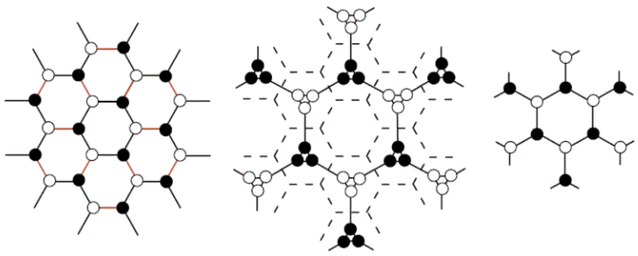
in mean-field fashion. Without including these λ factors in definition of S, procedure does not converge.

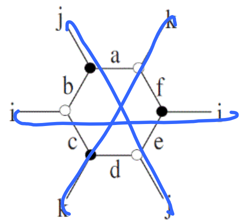
- Similarly update y and z bonds. This concludes one iteration.
- Iterate simple update many times.
- Start with $\tau \sim 10^{-3}$, gradually reduce it to $\tau \sim 10^{-5}$.
- Number of iterations needed until convergence: $10^5 - 10^6$

$\langle \psi | \psi \rangle$ is a double-layer tensor network.

$T_{[\ell]} =$ 

Use TRG (á la Levin & Nave) to contract bond indices of double-layer network:



$Z =$ 

Start with a finite system, and iterate until only ~~size~~ six sites are left; then trace out final bond indices.

<u>Results</u> [Jiang2008]

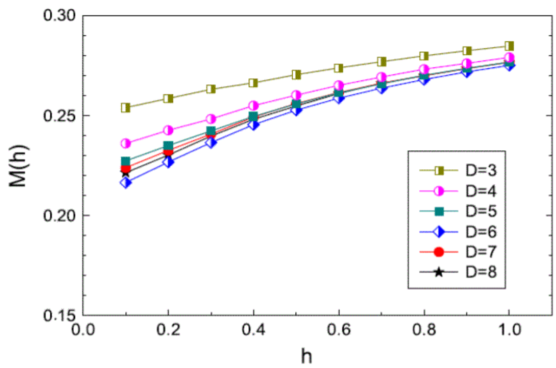


FIG. 5 (color online). The staggered magnetization $M(h)$ as a function of the staggered magnetic field, at different D.

TABLE II. Comparison of our results with those obtained by other approaches for the ground state energy per site E and the staggered magnetization M of the Heisenberg model with $h = 0$.

Method	E	M
Spin wave [12]	−0.5489	0.24
Series expansion [13]	−0.5443	0.27
Monte Carlo [14]	−0.5450	0.22
Ours $D = 8$	−0.5506	0.21 ± 0.01

3. Second renormalization (SRG) of tensor network states

[Xie2009],
more details: [Zhao2010]

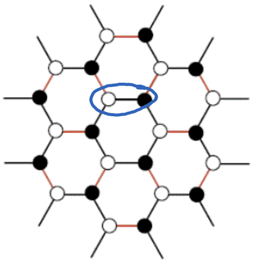
Goal: include influence of environment when doing update   'global optimization', 'full update'.

Two applications:	(i) partition function of classical 2D models
	(ii) 2D quantum ground states

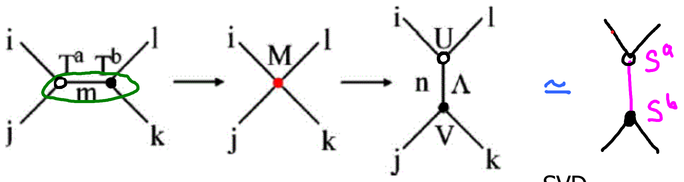
(i) Classical tensor network model

(TRG.1.6)

$$Z = \mathrm{Tr} \prod_{l \in a,\, l' \in b} T^{a}_{[l]\, x_l y_l z_l} \; T^{b}_{[l']\, x_{l'} y_{l'} z_{l'}}$$



rewire: $M_{ij,kl}$



(1)

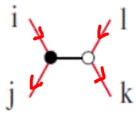
SVD minimizes truncation error for rewiring M . However, we should minimize truncation error of Z.

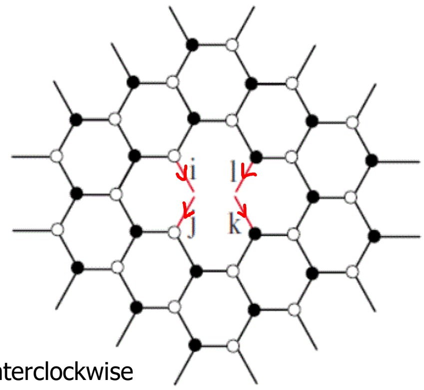
Renormalize environment

Partition function:

$$Z = \mathrm{Tr}\, M E$$

$$= \sum_{ijkl} M^{li}{}_{jk}\, E^{jk}{}_{li} \qquad (2)$$





convention: counterclockwise
assignment of indices

Goal: minimize truncation error of Z.

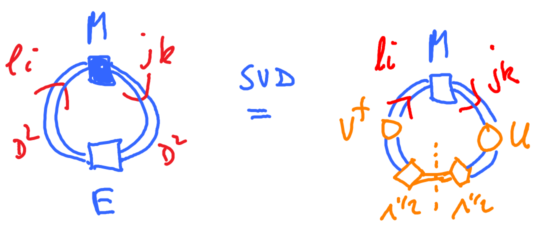
Strategy:

(i) Compute E
- (a) cheap mean-field approach ('single update')
- (b) on finite lattices
- (c) more expensive forward/backward TRG ('full update')

(ii) Do SVD on ME,   Let's discuss (ii) first.

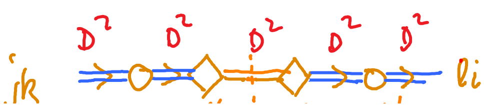
Minimize truncation error of ME   [Zhao2010, Sec. III.B]

$$Z = M^{li}{}_{jk}\, E^{jk}{}_{li} =$$



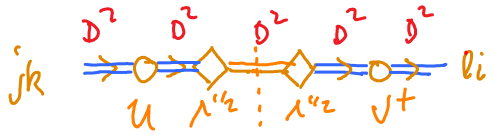
$$= \mathrm{Tr}\, \tilde{M} \qquad (3)$$

with $E \overset{SVD}{=} U \Lambda V^\dagger$



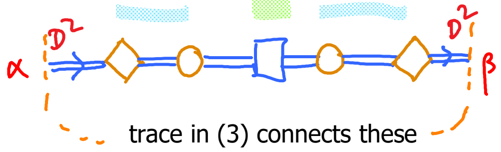
(4)

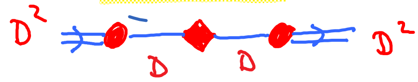
with $E \overset{SVD}{=} U \underbrace{\Lambda}_{\Lambda^{1/2}\cdot\Lambda^{1/2}} V^\dagger$



(4)

and $\tilde{M} \equiv \Lambda^{1/2} V^\dagger \; M \; U \; \Lambda^{1/2} \overset{SVD}{\simeq} \tilde{U} \; \tilde{\Lambda} \; \tilde{V}^\dagger = \tilde{\tilde{M}}$ (5)





truncate from D^2 back to D (6)

Since $Z = \mathrm{Tr}\,\tilde{M}$, this truncation directly controls error in partition function!

It knows not only about M, but also about its environment, via $U, \Lambda, V^\dagger$

Now express M in terms of truncated objects, $\tilde{U}, \tilde{\Lambda}, \tilde{V}^\dagger$

To this end, first invert relation between M and $\tilde{M}$, using $U^\dagger U = V^\dagger V = \mathbb{1}$

$$M \overset{(5)}{=} V \Lambda^{-1/2} \; \tilde{\tilde{M}} \; \Lambda^{-1/2} U^\dagger$$

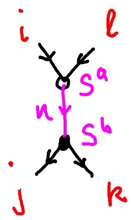
then insert truncated version of $\tilde{M}$:

$$\overbrace{\tilde{U}\tilde{\Lambda}^{1/2} \; \tilde{\Lambda}^{1/2}\tilde{V}^\dagger}$$

and write as product of two vertices:

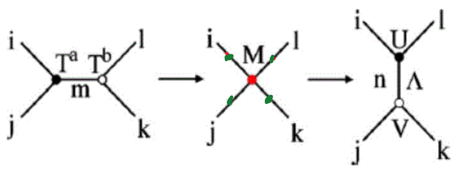
$$= \underbrace{V \Lambda^{-1/2}\tilde{U}\tilde{\Lambda}^{1/2}}_{S^a} \; \underbrace{\tilde{\Lambda}^{1/2}\tilde{V}^\dagger \Lambda^{-1/2} U^\dagger}_{S^b}$$

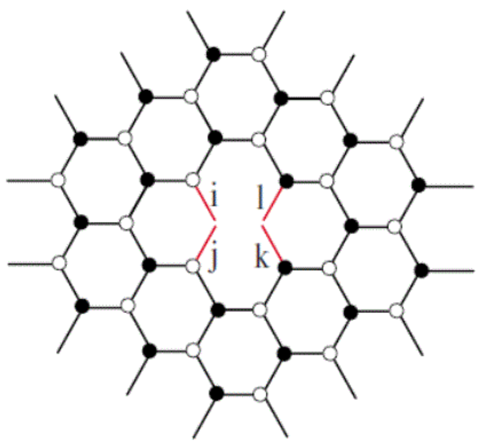
with indices: $M^{li}{}_{jk} = S^{a\,li}{}_{n} \; S^{b\,n}{}_{jk}$



Now we return to (i): actually computing the environment

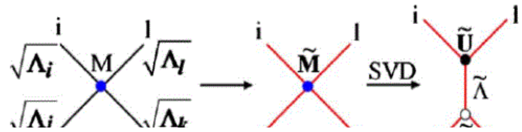
<u>(a) Computing environment tensor E using simple update (mean-field approach)</u> [Xie2009]





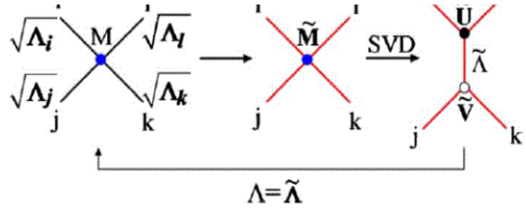
$M = U \Lambda V^\dagger$ defines the 'singular bond vector' Λ, which measures entanglement between two sites. It can be used directly to obtain a cheap, mean-field approximation of environment ('simple update'):

- Take $E^{li}{}_{jk} \simeq \sqrt{\Lambda_i \Lambda_j \Lambda_k \Lambda_l}$



- Compute $\tilde{M}$ $= M \cdot E$, then do SVD: $\tilde{M} = \tilde{U}\tilde{\Lambda}\tilde{V}^\dagger$

new bond vector

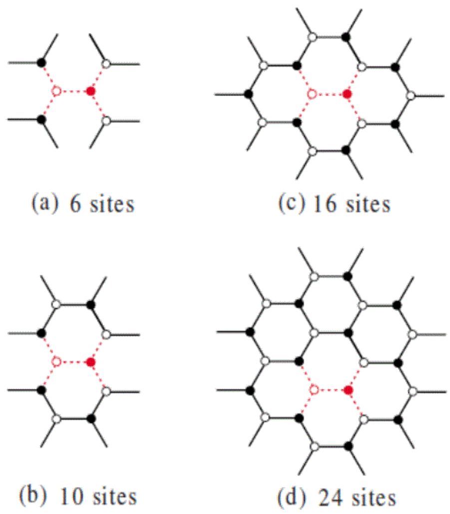


- Use new $\Lambda = \tilde{\Lambda}$ to recalculate E, $\tilde{M}$, $\tilde{\Lambda}$, etc.

- Iterate until convergence (typically 2 to 3 iterations suffice; near critical point, more are needed).

(b) Computing environment tensor E using finite lattices

$$\delta f(T) = 1 - \frac{f(T)}{f_{exact}(T)}$$



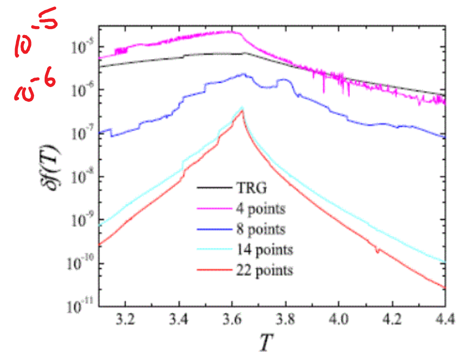


FIG. 10. (Color online) Relative errors of the free energy for the Ising model on a triangular lattice obtained by considering the second renormalization effect from four finite environment lattices which contains 4, 8, 14, and 22 sites, respectively. The configurations of these environments are shown in Fig. 9. The TRG result is also shown for comparison.

Including even just a few environmental sites already leads to big improvements!

(c) Computing environment tensor E using TRG

[Zhao2010]

'Forward iteration':

(a) → (b): Rewire environment $E^{jk}{}_{li}$ using data at iteration n:

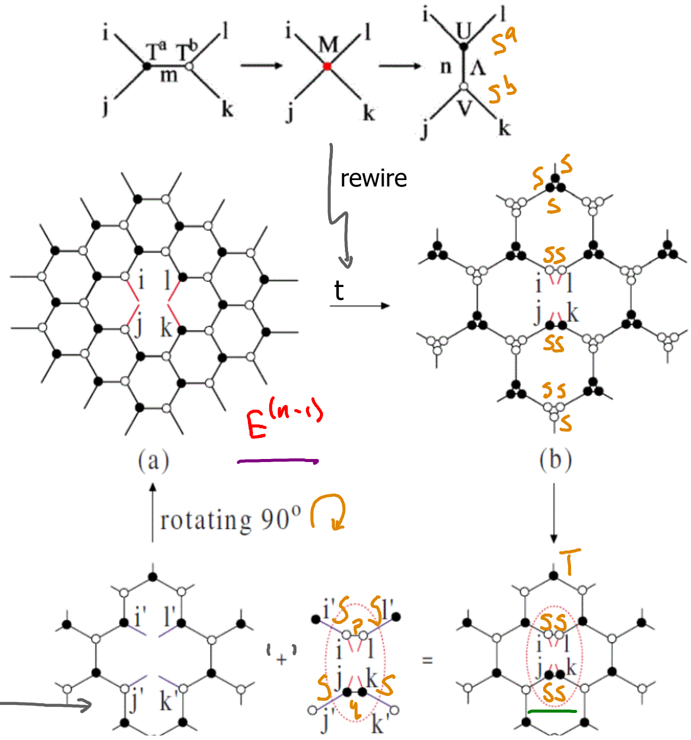
$$T^{[n]}T^{[n]} = M^{[n]} = U^{[n]}\Lambda^{[n]}V^{\dagger[n]}$$

(b) → (c): Trace out small triangles, $T = SSS$ four S are left over

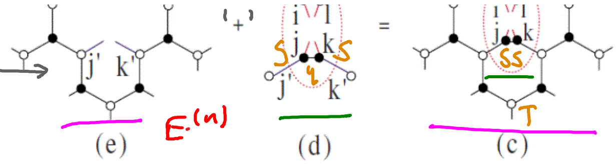
(c) → (d) + (e): Identify new environment

(e) looks same as (a), only rotated by 90 degrees, and rescaled.

Iteration relation, expressing old through new environment:



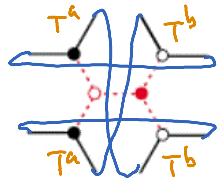
Iteration relation, expressing
old through new environment:



$$E^{[n-1]}_{\ell i, jk} = E^{[n]}_{\ell' i', j' k'} \, S^{a}_{\ell p \ell'} \, S^{a}_{i i' p} \, S^{b}_{q j j'} \, S^{b}_{k' q k}$$

- Start with a very large but finite number of sites.
- Iterate until only 4 environmental sits are left:
- Compute final environment, $E^{(N)}$, by tracing out open indices:

$$E^{(N)} = \mathrm{Tr}\; T^a T^b T^a T^b$$



'Backward iteration':

- Start from current values of tensors T^a, T^b and bond vectors Λ .
- Use them to compute $E^{(N)}$, $E^{(N-1)}$, etc., all the way back to $E^{(0)} = E$ = desired result.

This completes step (i). Now go to step (ii), compute $\tilde{M}$, $\tilde{\Lambda}$, M , and iterate, until $\tilde{\Lambda}$ have converged.

Results for SRG (2nd renormalization) for classical 2D system

Ising model on triangular lattice:

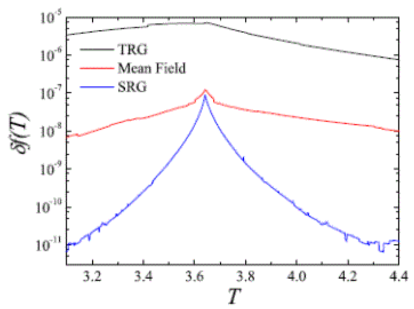
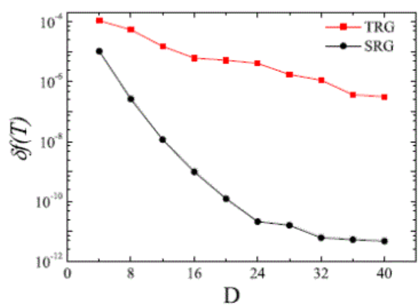


FIG. 12. (Color online) Comparison of the relative error of the free energy for the Ising model on triangular lattices obtained using TRG (red), the mean-field approximated SRG (blue), and the SRG (black) methods with D_{cut}=24, respectively. The critical temperature is T_c=4/ln 3.

critical state is hardest to simulate



mean field
SRG

FIG. 13. (Color online) The relative error of the free energy as a function of the truncation dimension D_{cut} for the Ising model on triangular lattices obtained using the TRG (black) and SRG (blue), respectively. T=3.2.

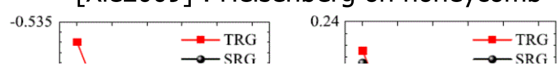
error drops with increasing D
much more quickly for SRG than TRG

Results for SRG (2nd renormalization) for quantum ground state search

Optimize by imaginary time evolution; contractions performed using SRG.

Compute expectation values such as $\langle \psi | \psi \rangle$, $\langle \psi | \hat{O} | \psi \rangle$ using SRG, too.

[Xie2009] : Heisenberg on honeycomb



SRG yields more stable results than TRG!

[Xie2009] : Heisenberg on honeycomb

SRG yields more stable results than TRG!

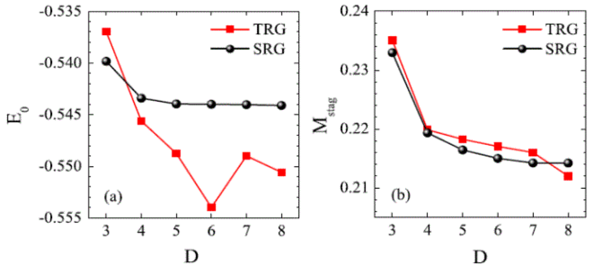


FIG. 5 (color online). (a) The ground state energy per site E_0 and (b) the staggered magnetization M_{stag} as functions of the bond degrees of freedom D on honeycomb lattices.

[Zhao2010]

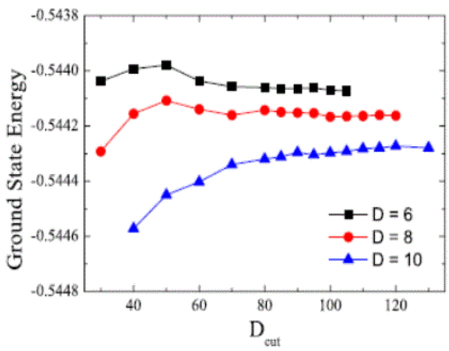


FIG. 19. (Color online) The SRG result of the ground-state energy as a function of the truncation dimension D_{cut} for the Heisenberg model on a honeycomb lattice. D is the bond dimension of the wave function.

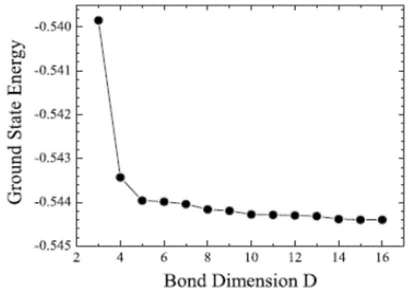


FIG. 20. The ground-state energy of the Heisenberg model on a honeycomb lattice as a function of the bond dimension D obtained by the SRG with $D_{cut}=130$.

$E^{SRG} = -0.54440 \qquad E^{QMC} = -0.54455(20)$

Energy does not decrease with D_cut, because imaginary time-evolution / SRG is not variational!

Goal: reduce computational cost of TRG from $\mathcal{O}(\chi^6)$ to $\mathcal{O}(\chi^4)$

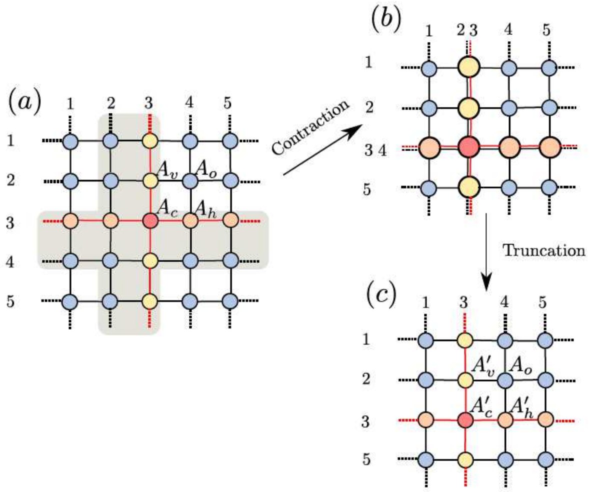


FIG. 1. A depiction of the CTRG iteration, which maps an $L \times L$ lattice of tensors to an $(L-1) \times (L-1)$ lattice. (a) The initial network is everywhere composed of copies of the bulk tensor A_0, except for a single 'core' row and column containing tensors $\{A_c, A_h, A_v\}$ as indicated. (b) An adjacent row and column of the network has been contracted into the core row/column, thus growing the index dimension of the core tensors. (c) The indices of the core tensors are truncated to dimension χ, as to obtain new core tensors $\{A'_c, A'_h, A'_v\}$.

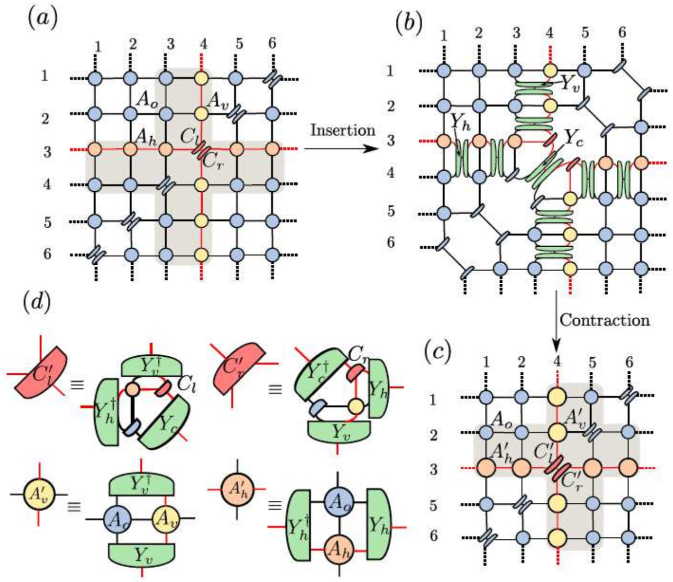


FIG. 2. At iteration of the CTRG algorithm. (a) The initial square lattice network is homogeneous except for a core row/column which contains core tensors $\{A_v, A_h, C_l, C_r\}$ and a diagonal line through the core along in which the bulk tensors have been decomposed into products of 3-index tensors. (b) Pairs of isometries $\{Y_v, Y_h, Y_c\}$ and their conjugates have been inserted into the core row/column of the network. (c) Isometries are contracted with their neighboring tensors, effectively absorbing a bulk row/column into the core row/column, as to produce new core tensors $\{A'_v, A'_h, C'_l, C'_r\}$. (d) Definitions of the new core tensors.

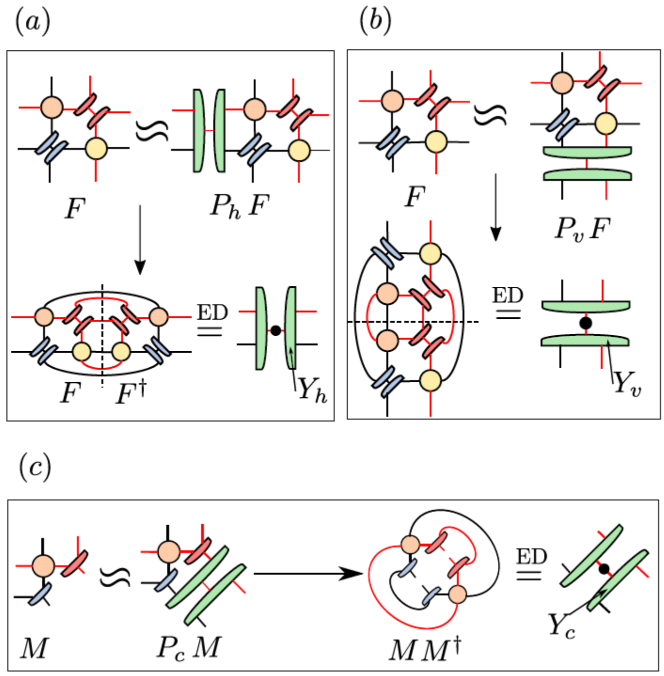


FIG. 3. (a) The projector $P_h \equiv Y_h Y_h^\dagger$ should be chosen to (approximately) leave invariant the network F, which is the network formed from the central tensors of the initial lattice in Fig. 2(a). The optimal isometry Y_h is formed by taking the eigenvalue decomposition (ED) of $FF^\dagger$, when F is viewed as a matrix between its left two and remaining indices, and truncating to retain only the χ dominant eigenvectors. (b) The optimal isometry Y_v is obtained from the ED of $FF^\dagger$, when F is viewed as a matrix between its bottom two and remaining indices. (c) The optimal isometry Y_c is obtained from the ED of $MM^\dagger$, when M is half of the F network.

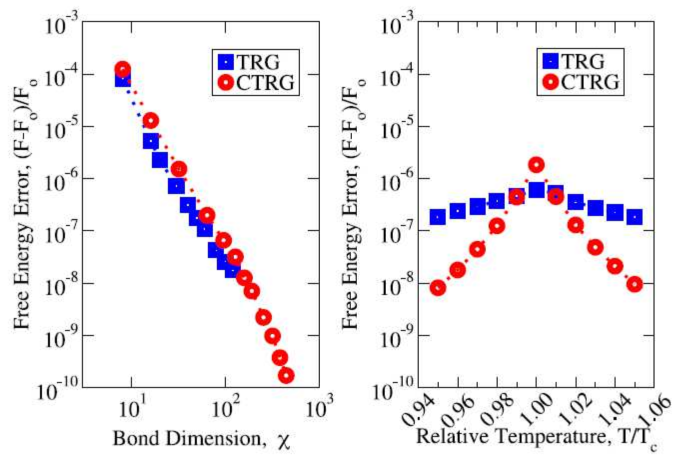


FIG. 5. (a) A comparison of the accuracy of the free energy density produced by TRG and CTRG for the Ising model on an infinite strip of width $L = 128$ sites at critical temperature. Both methods produce comparable accuracy for the same bond dimension χ, with TRG giving only slightly more accurate energies. (b) Comparison between TRG and CTRG for accuracy of the free energy density as a function of temperature with fixed bond dimension $\chi = 30$.