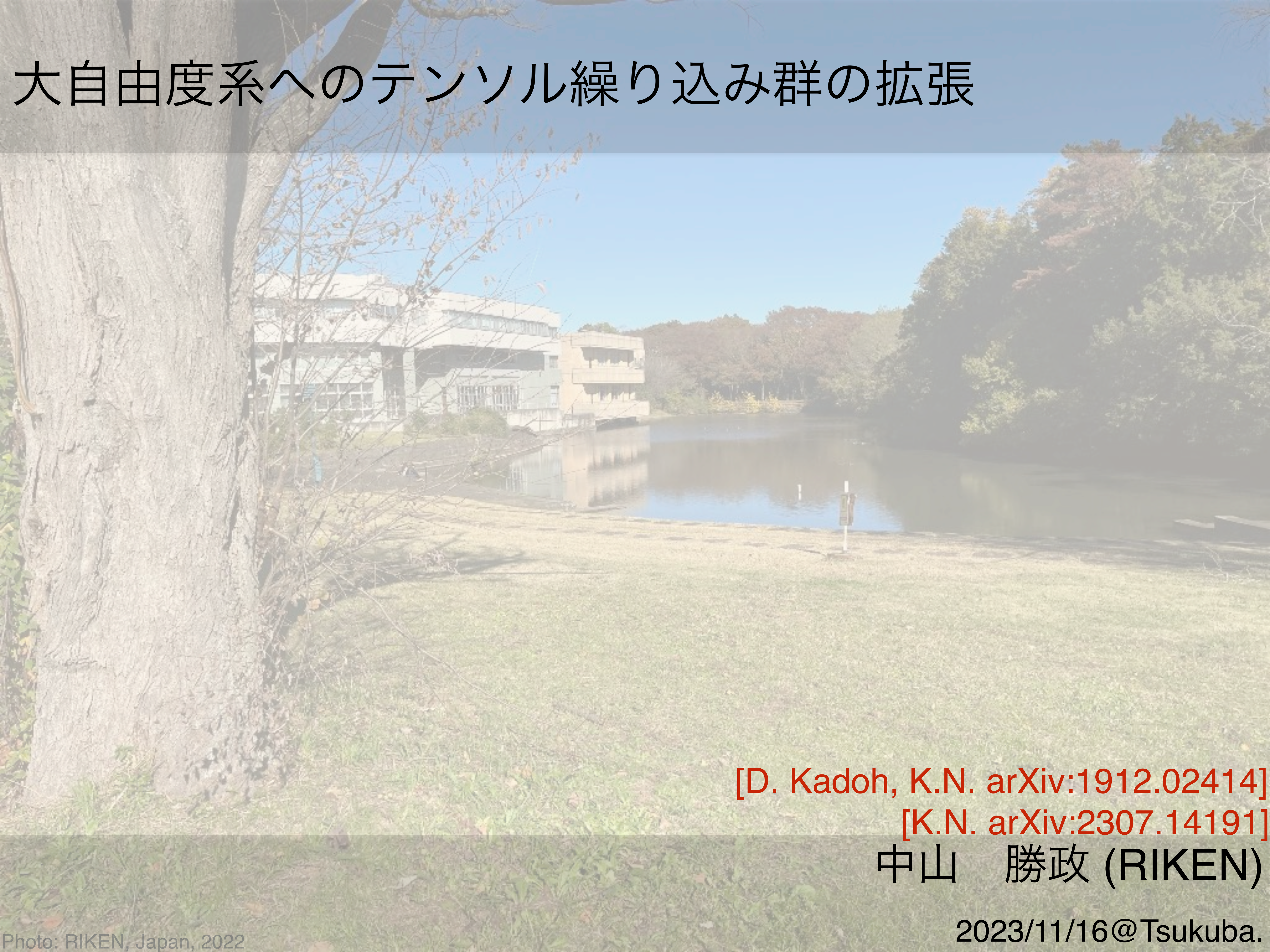
大自由度系へのテンソル繰り込み群の拡張



[D. Kadoh, K.N. arXiv:1912.02414]
[K.N. arXiv:2307.14191]

中山　勝政 (RIKEN)

2023/11/16＠Tsukuba.

Photo: RIKEN, Japan, 2022

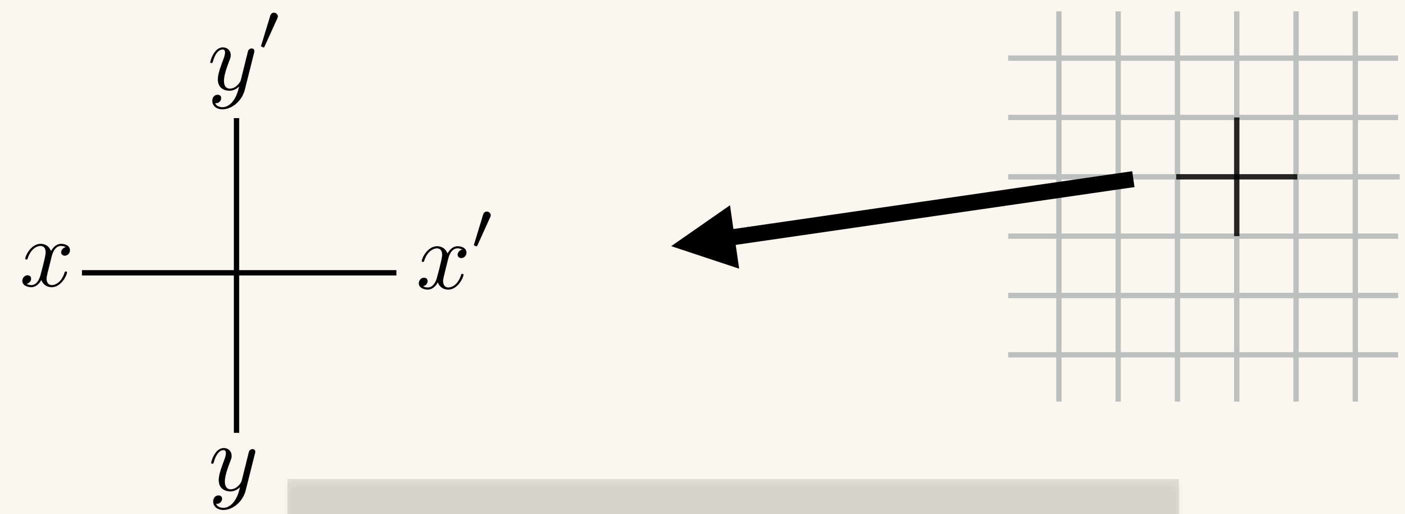
◉ テンソル繰り込み群 (TRG)

[M. Levin, C. P. Nave. arXiv:cond-mat/0611687]

◇ TRGはテンソルのトレースとして物理量を計算する

$$Z = \mathrm{Tr} \sum_{i \in \mathrm{lattice}} A_{x_i y_i x_i' y_i'}$$

$$A_{xyx'y'} =$$



○原理的には符号問題なし

○テンソル表現

×高コスト $(\mathrm{dim} \geq 3)$

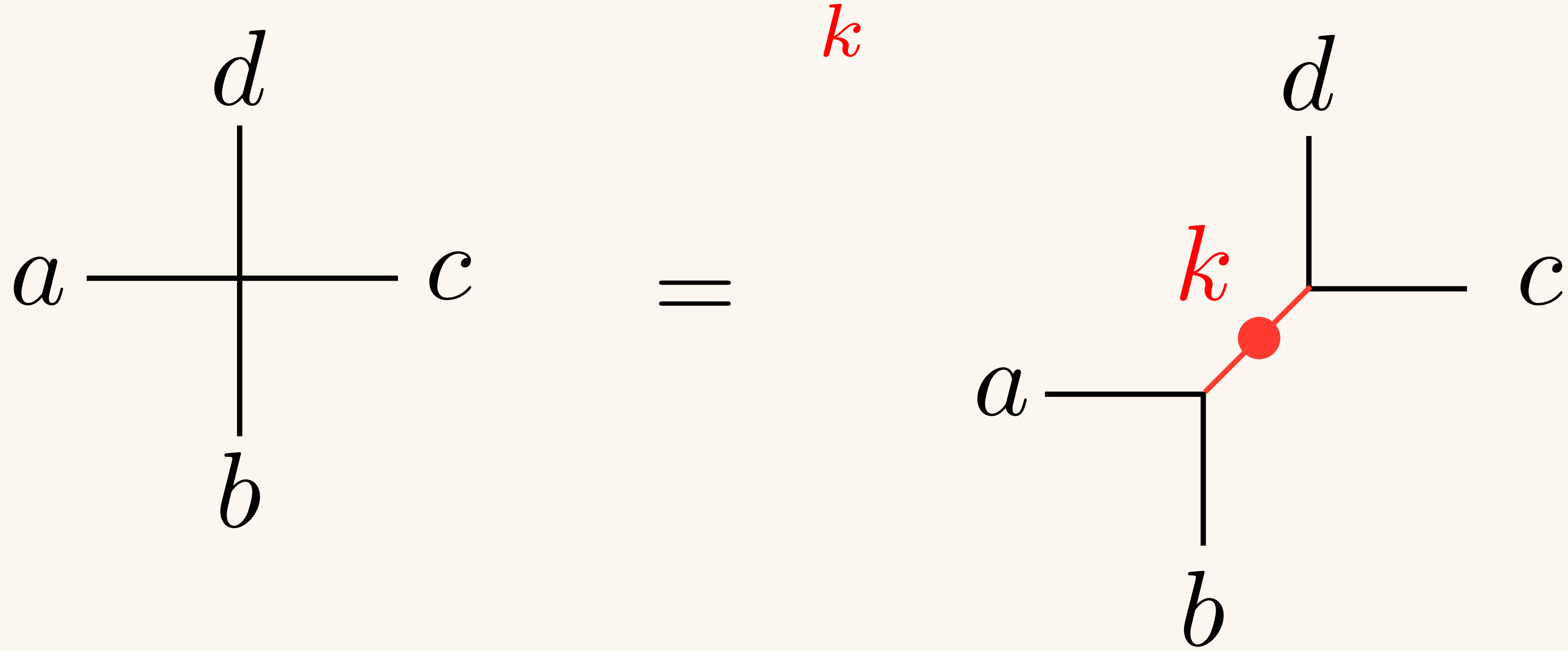
△複雑な系統誤差

厳密な縮約は現実的ではないので近似が必要。

→ 特異値分解 (SVD) (Frobenius norm)

◉ 特異値分解 (SVD)

$$T_{abcd} = \sum_{k}^{D} A_{ab}{}^{k} \lambda^{k} B_{cd}{}^{k}$$

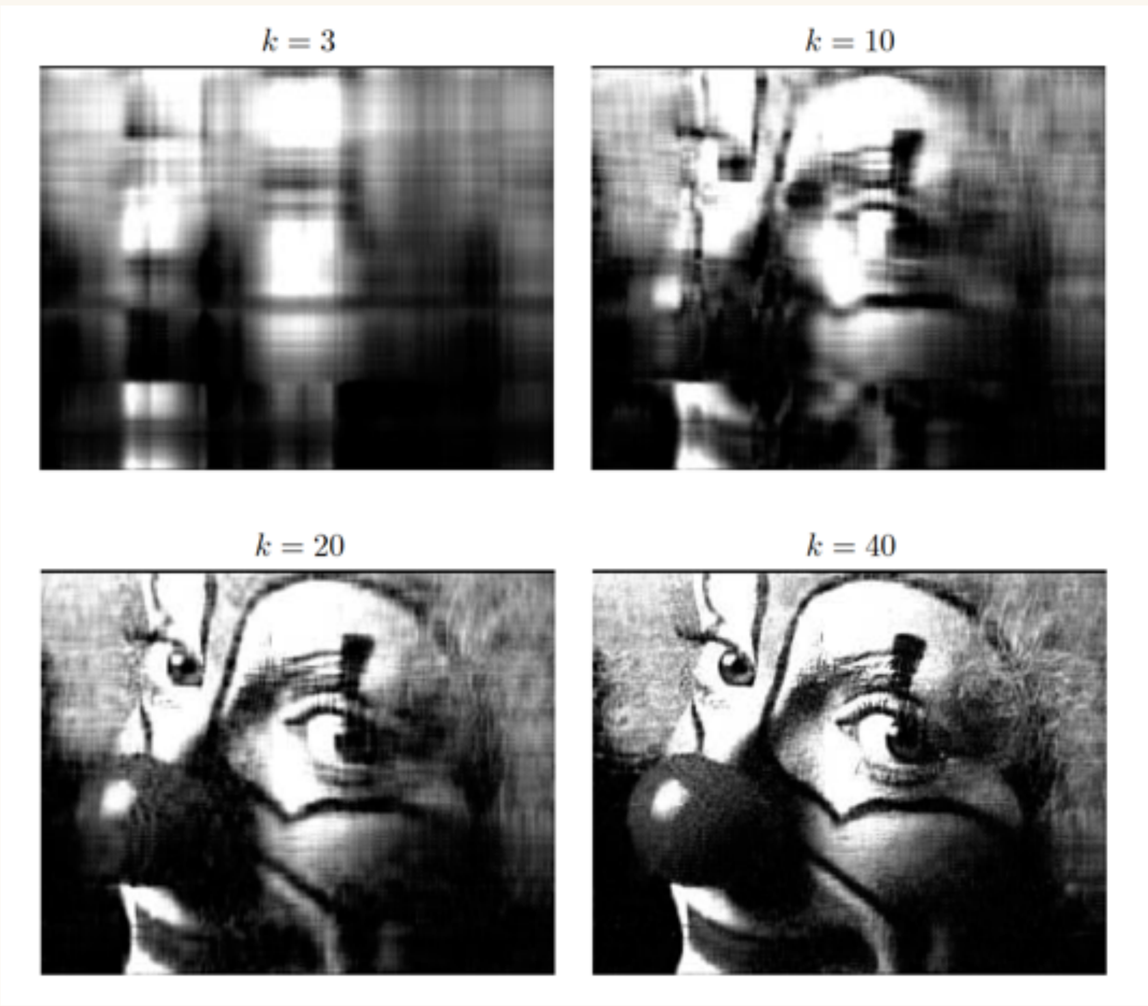


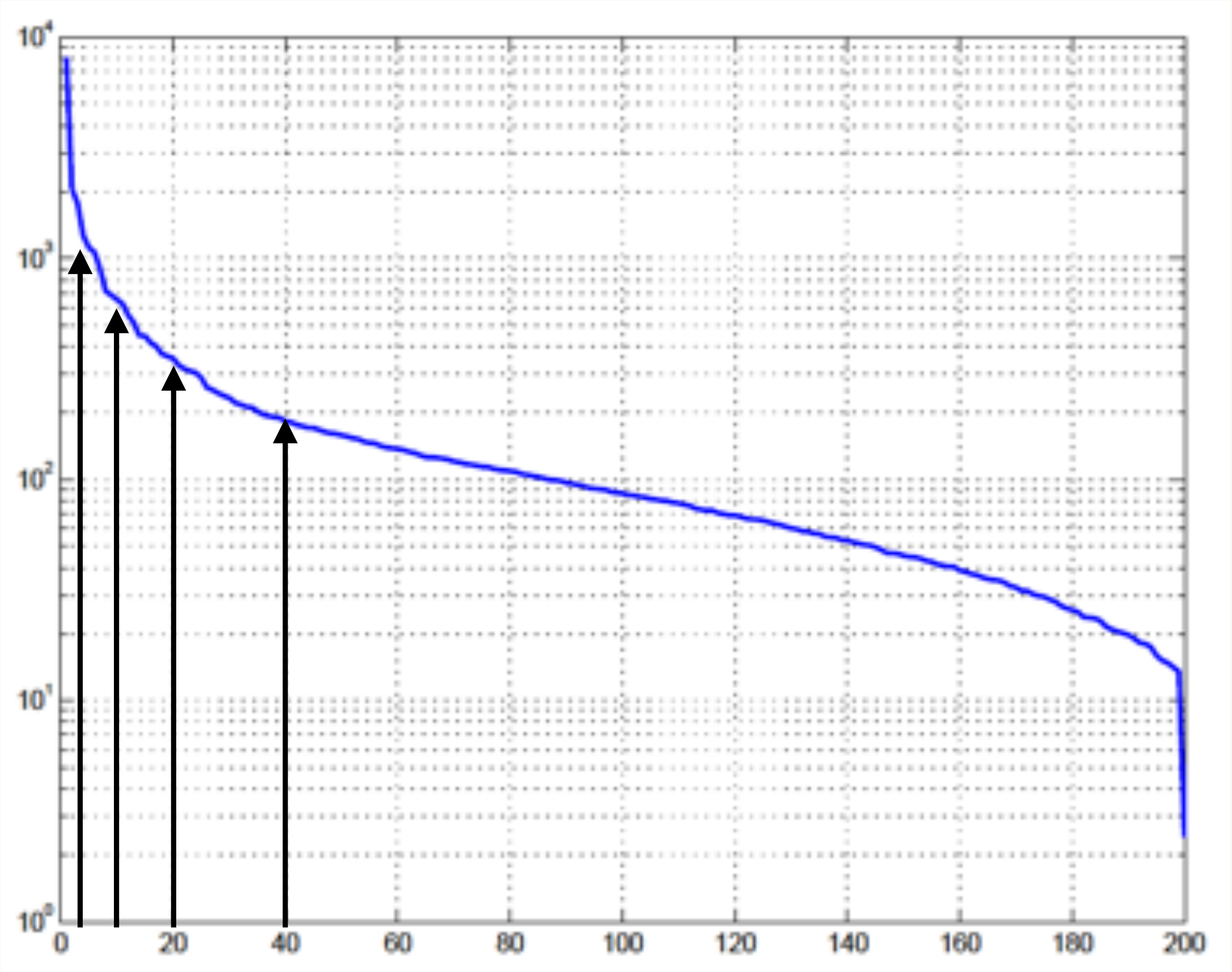
◇ より大きな特異値がより近似に重要 → (Frobenius norm)

→ 添字 k を打ち切って近似する

$$\mathrm{dim}(k) = \mathrm{dim}(a)\mathrm{dim}(b) \to D$$

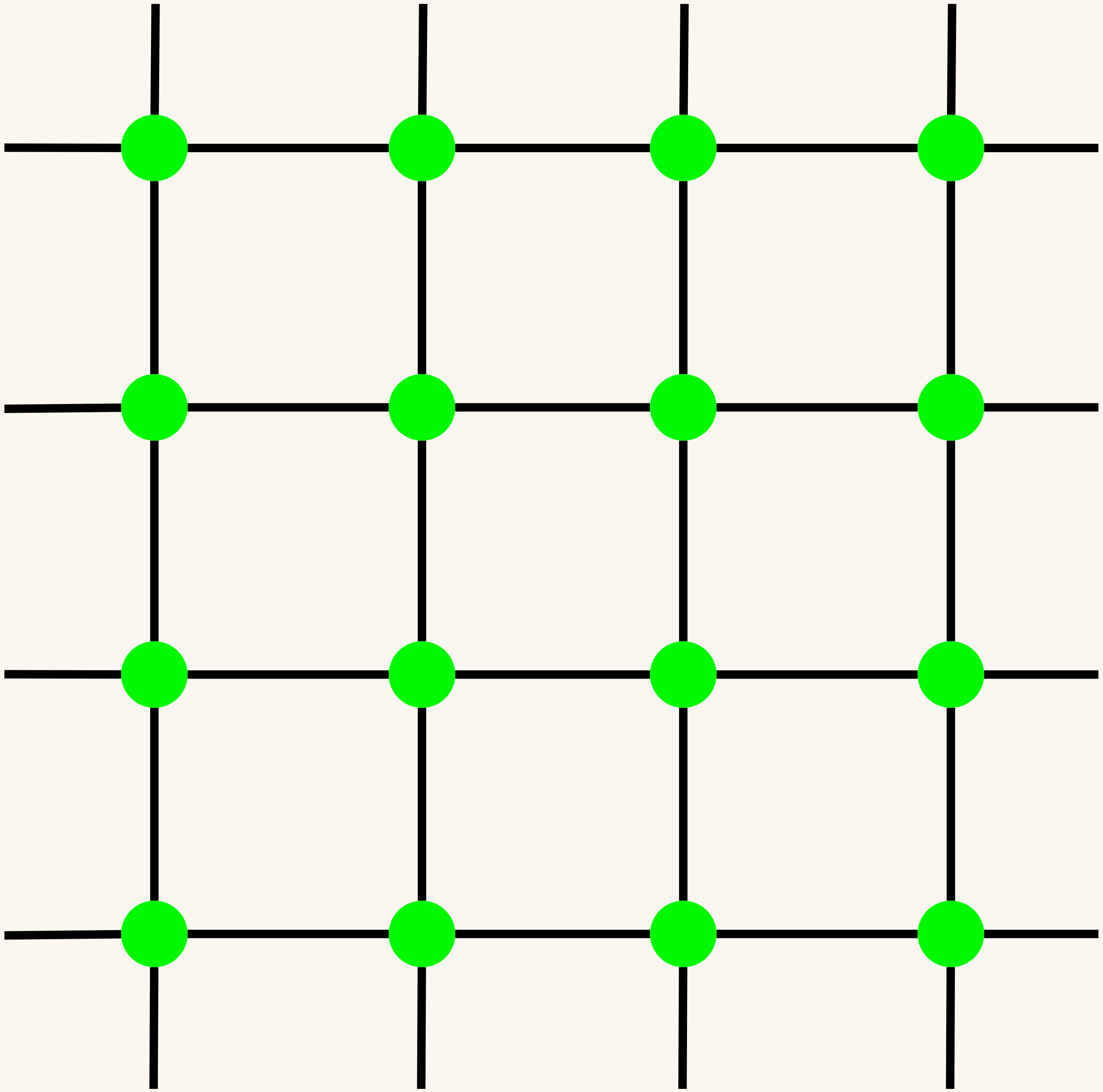
◉ SVDによる粗視化(e.g. 画像圧縮)

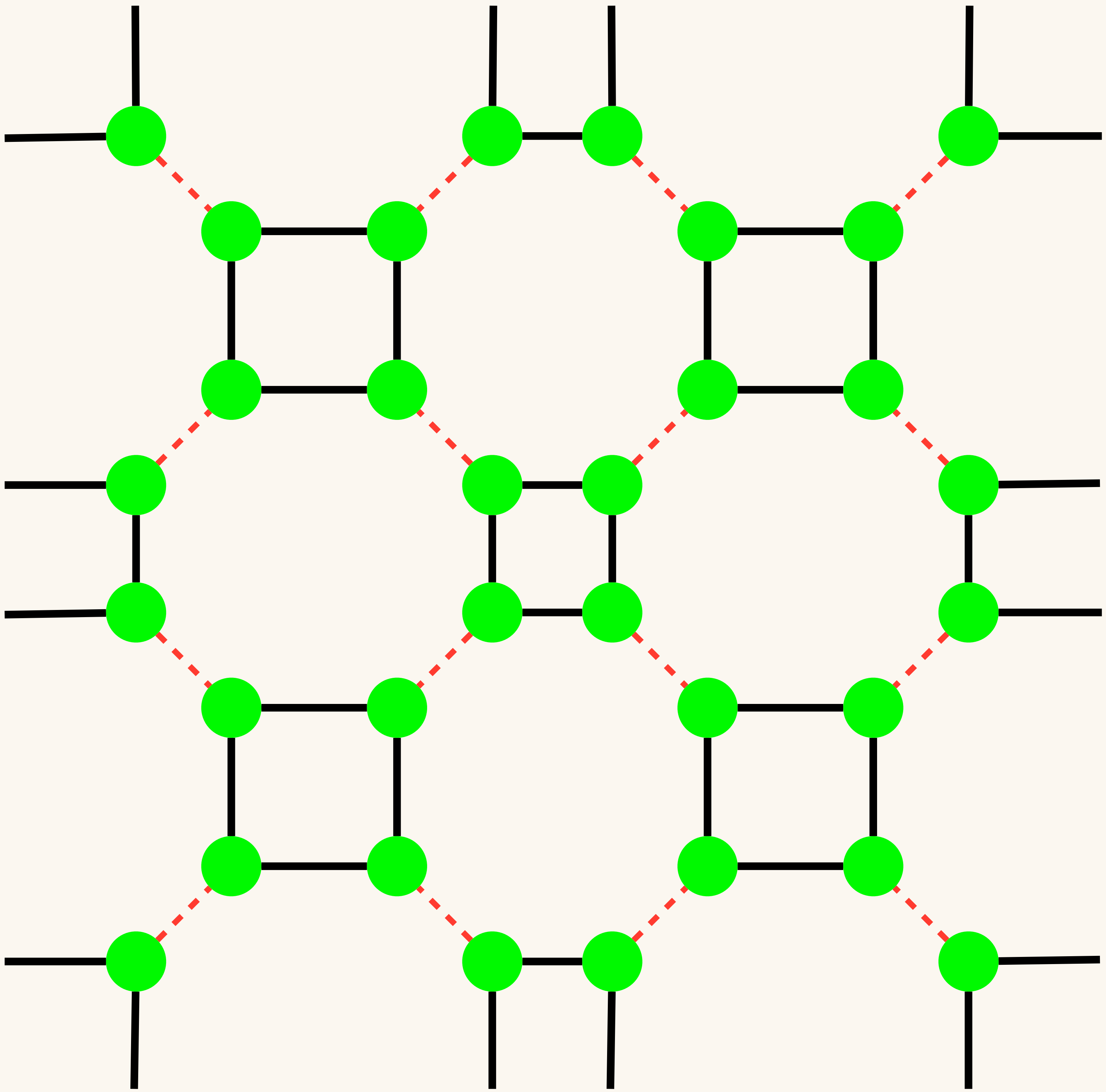


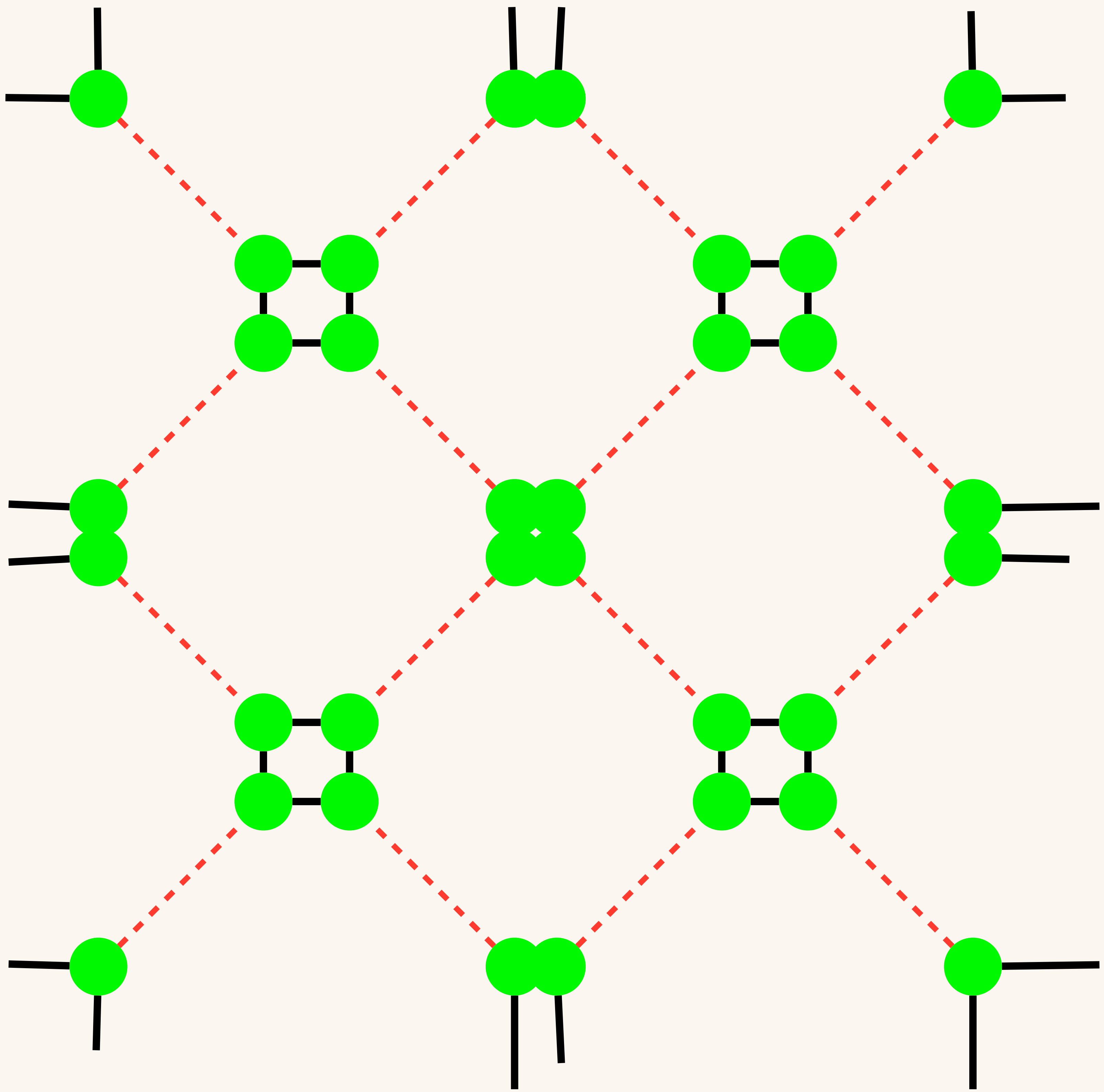


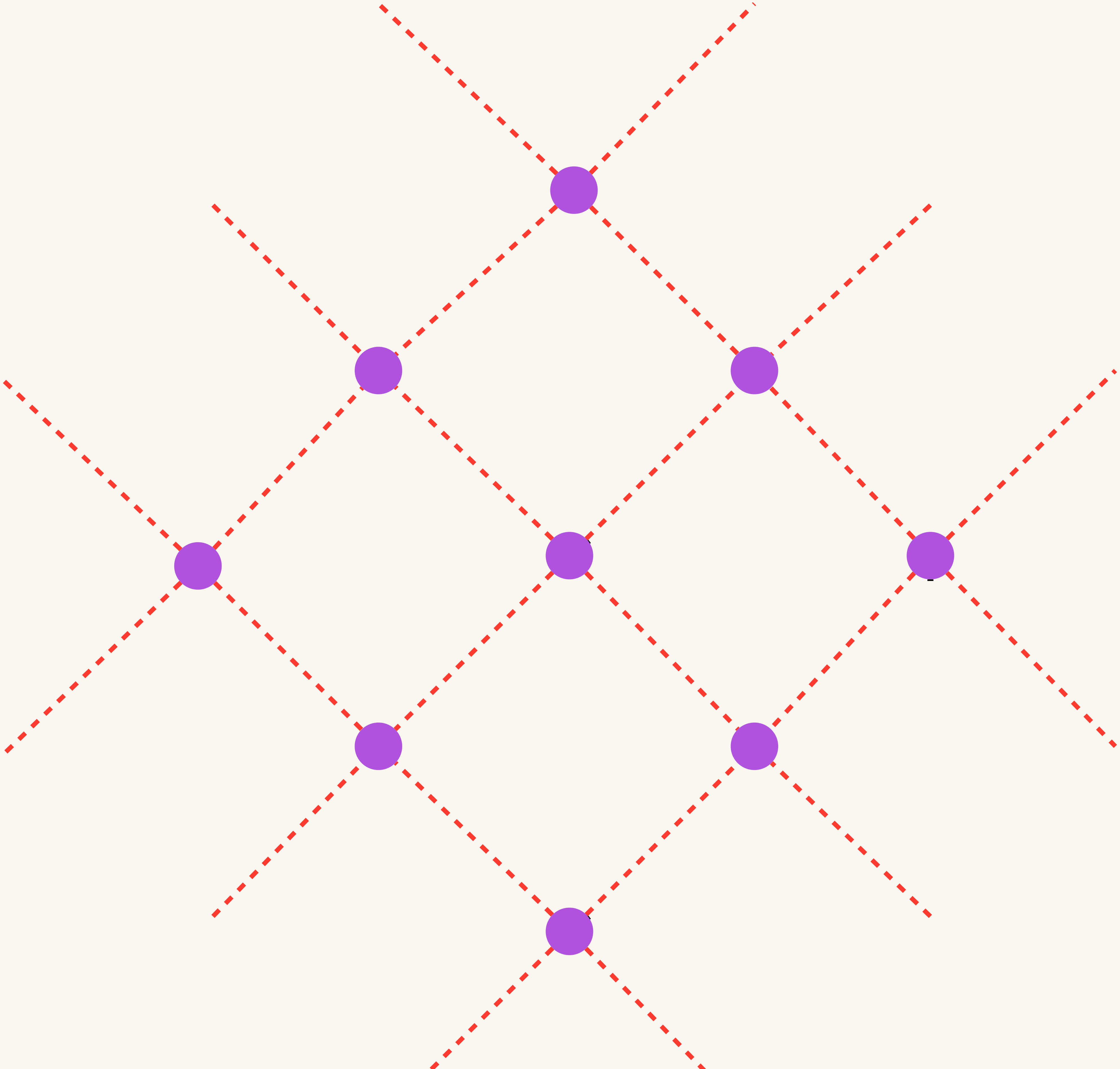
[http://www.na.scitec.kobe-u.ac.jp/~yamamoto/lectures/cse-introduction2009/cse-introduction090512.PPT]

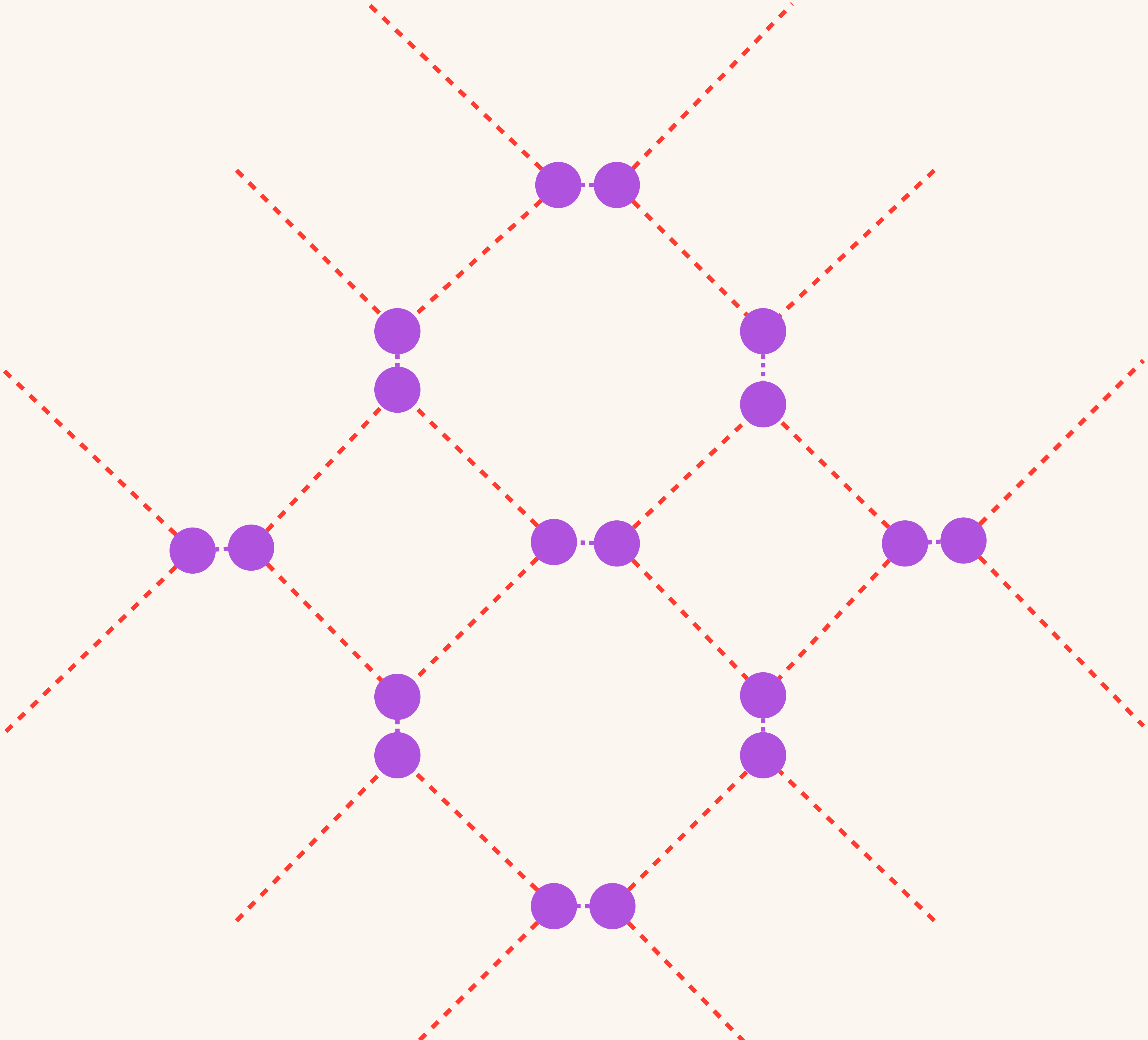
◉ SVDによる粗視化(e.g. Ising)

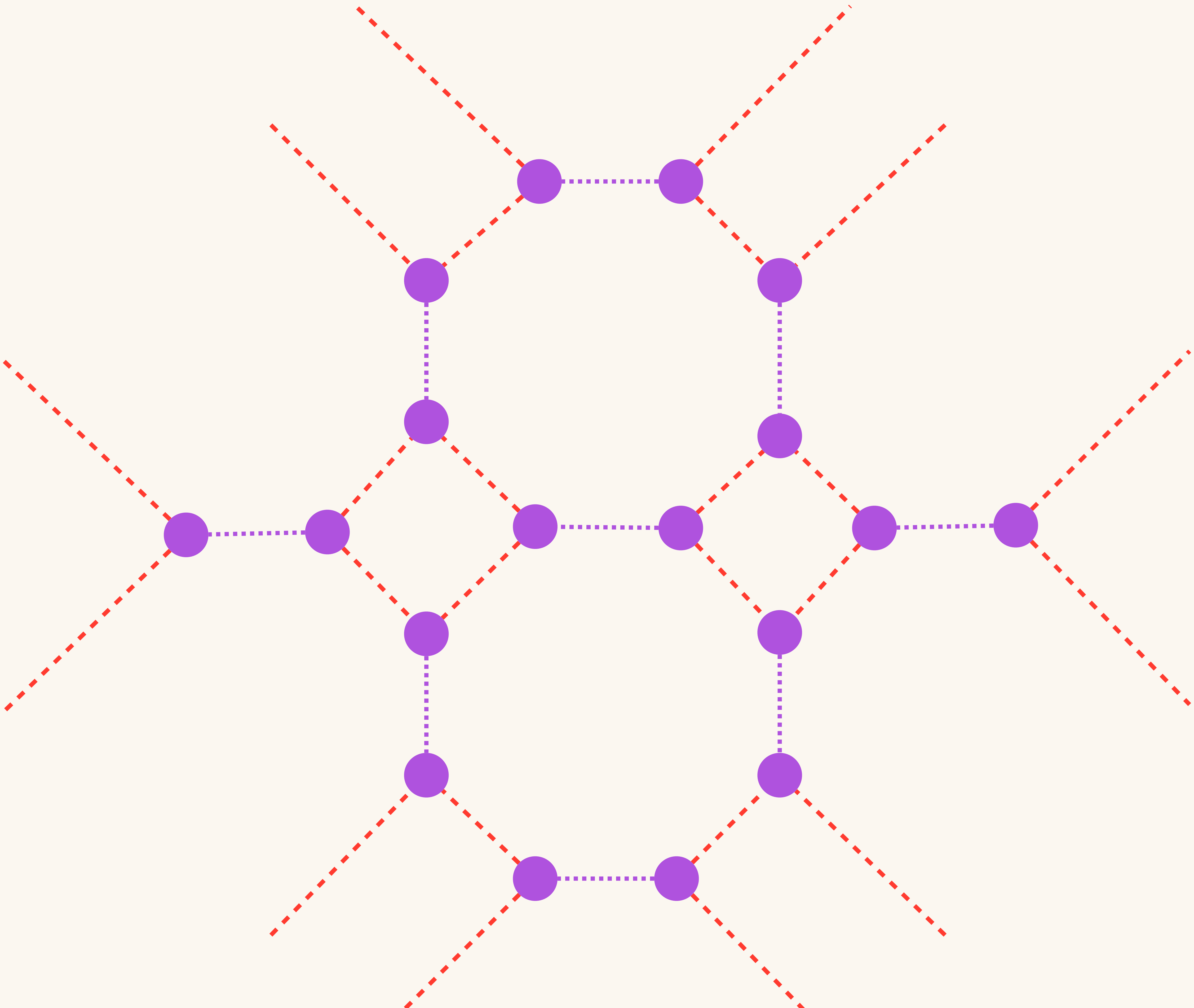


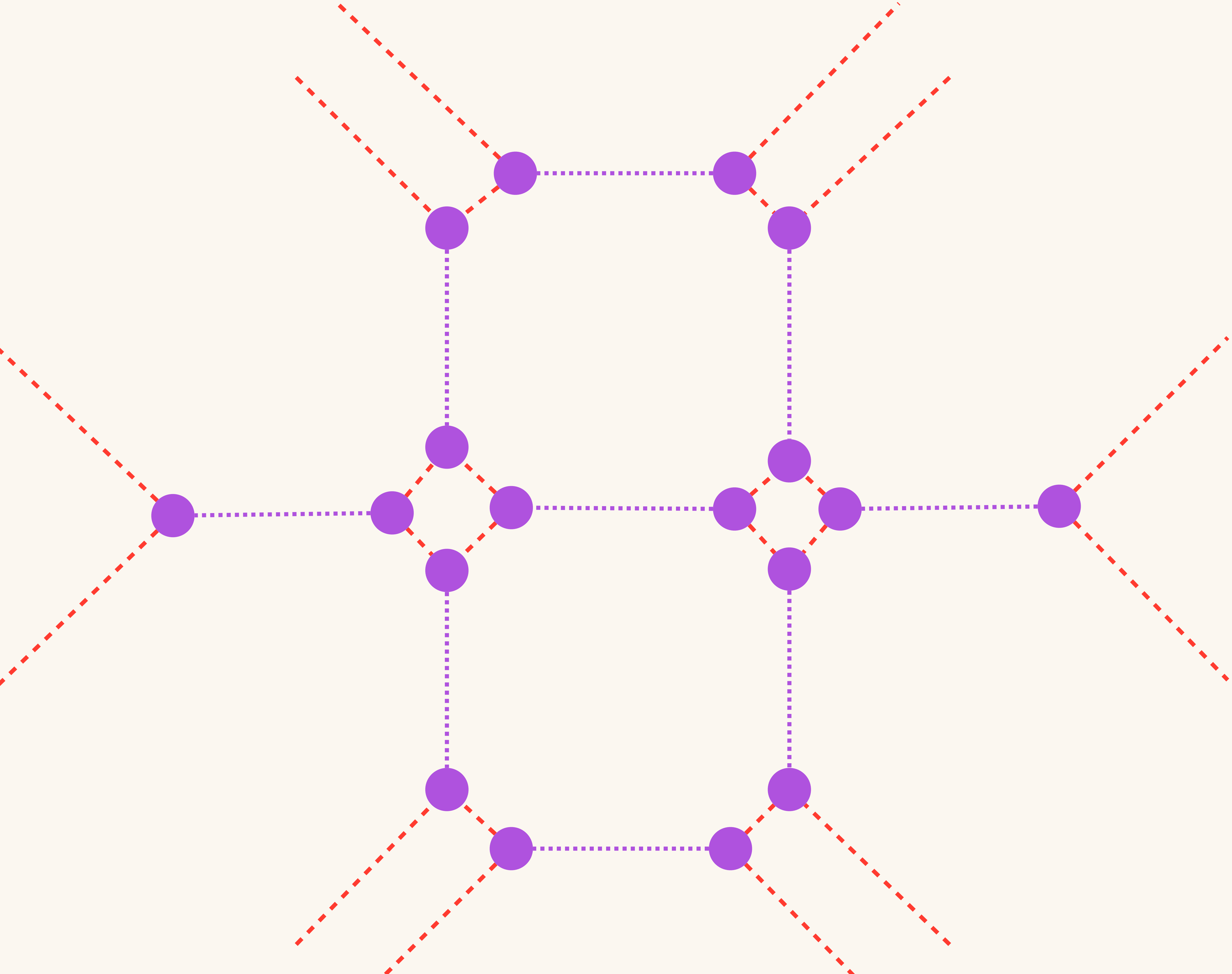


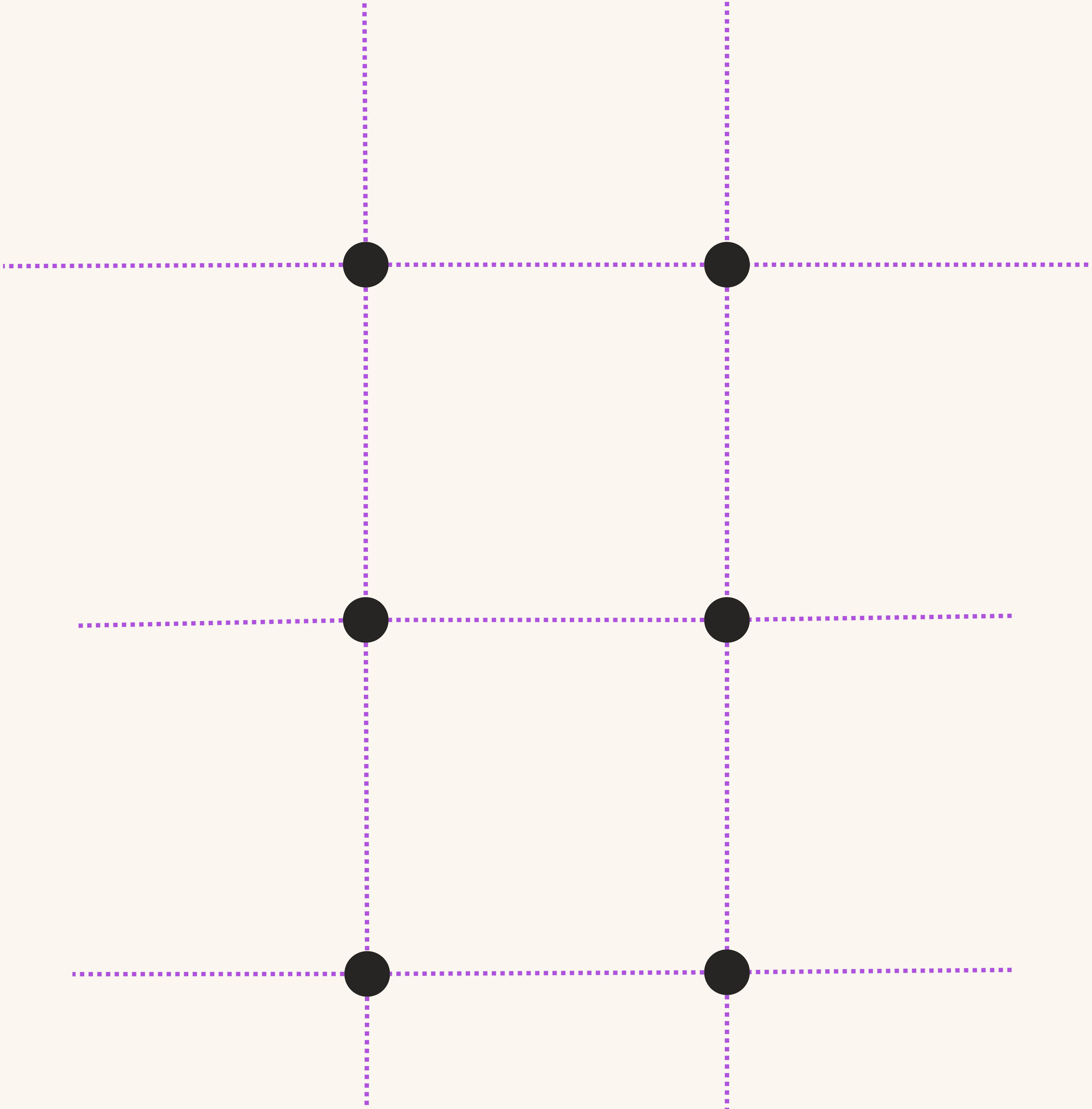






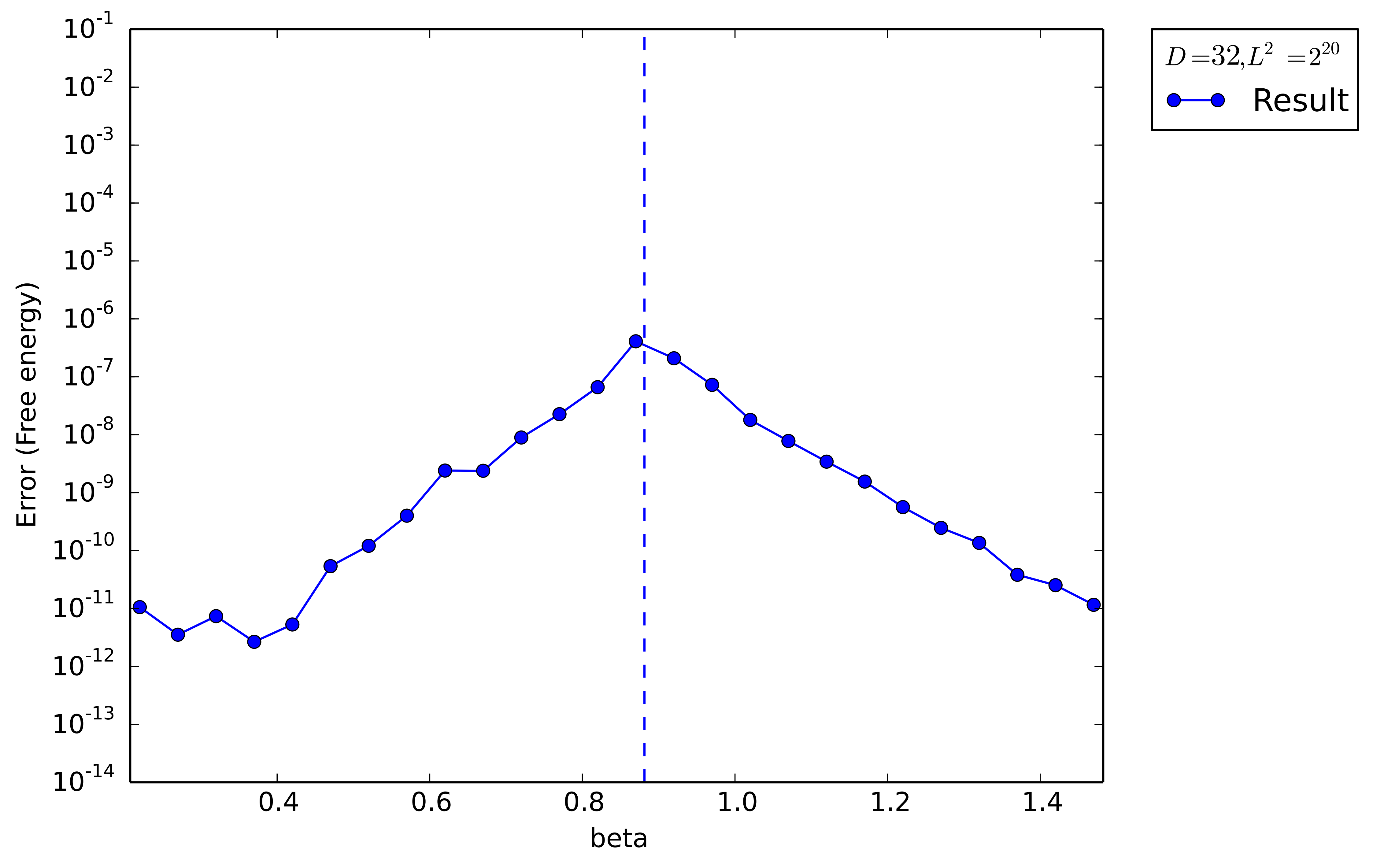






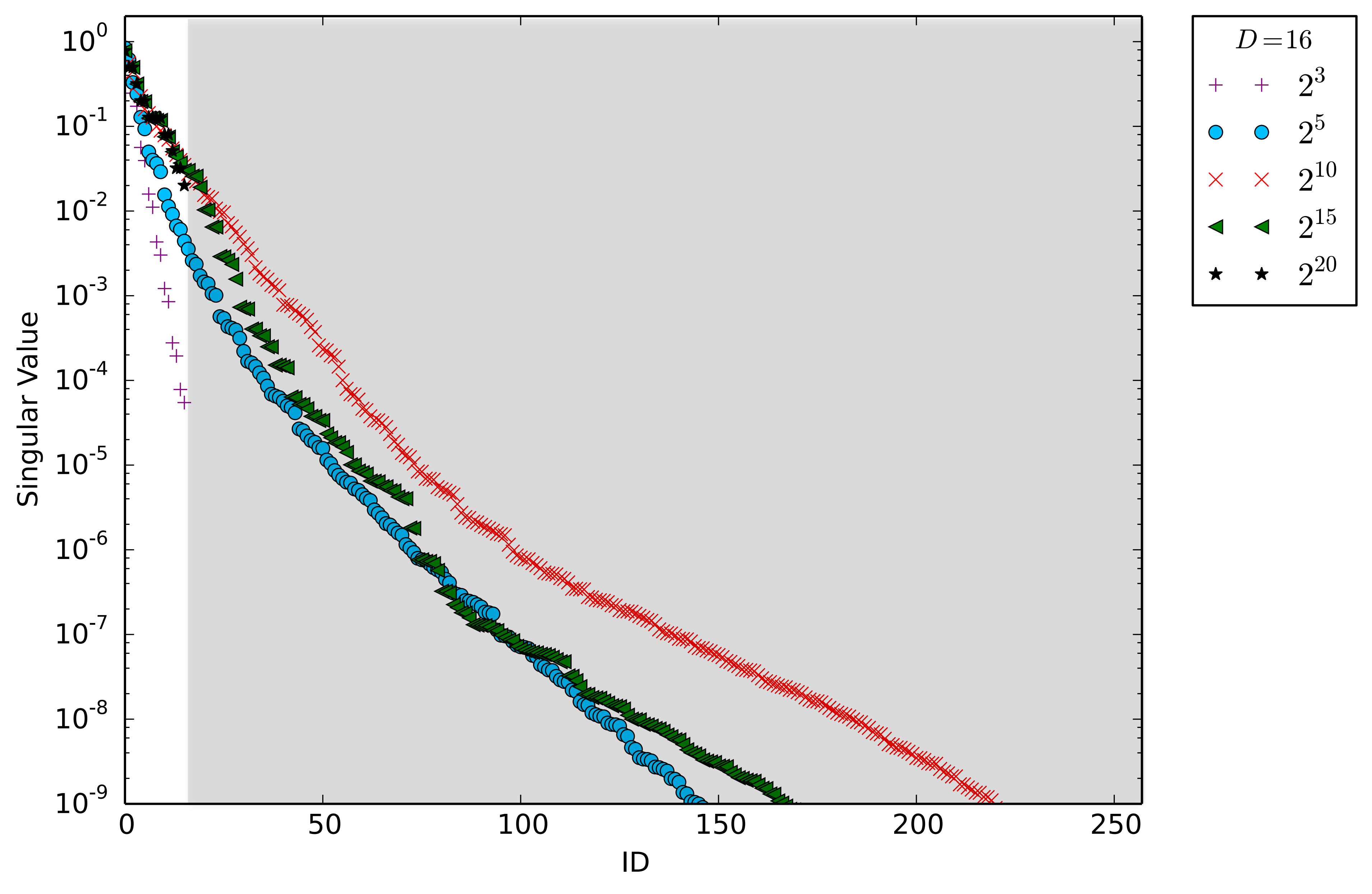
◉ SVDによる粗視化(e.g. Ising)

◇ 厳密解からのずれ(Free energy)



◉ 特異値の階層性

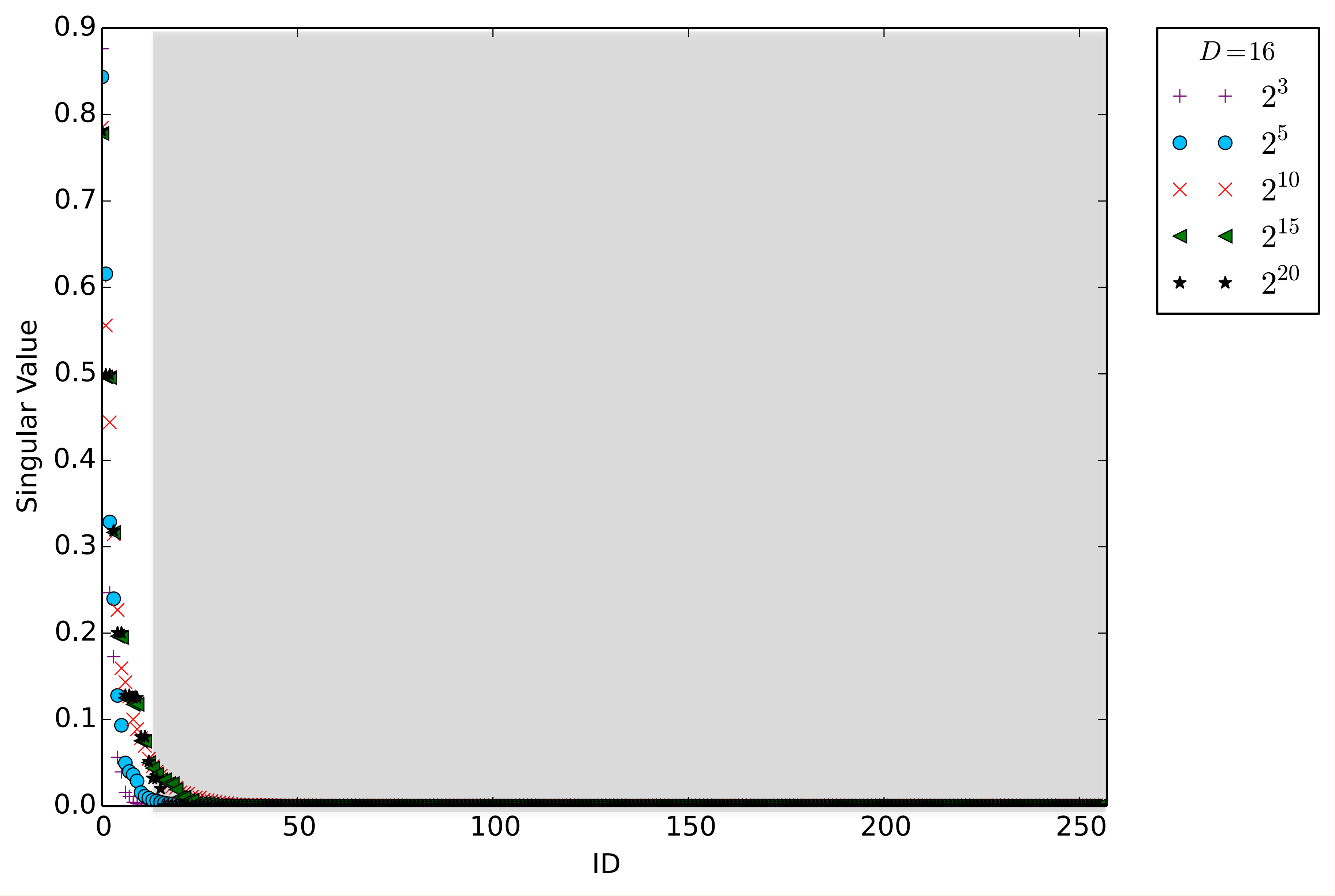
◇ なぜこの打ち切りがうまくいくのか?



→ 特異値は大きい順に並べると指数関数的に減少する

◉ 特異値の階層性

◇ なぜこの打ち切りがうまくいくのか?

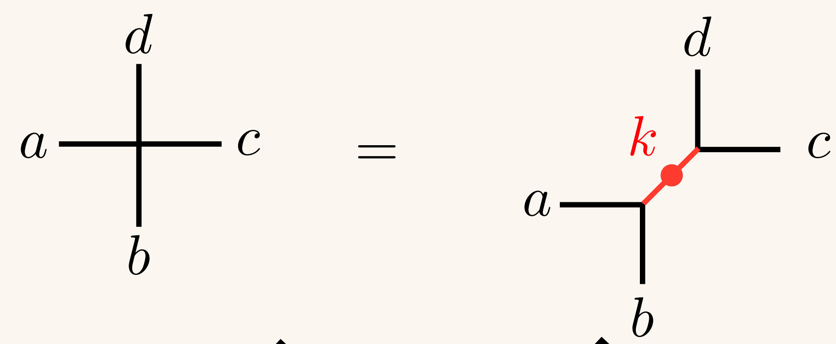


→ 特異値は大きい順に並べると指数関数的に減少する

◉ TRGの計算量

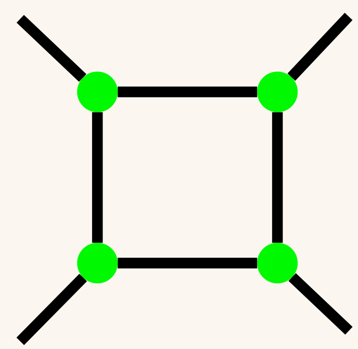
◇ 計算量

分解:



$O(D^6)$

縮約:



$O(D^6)$

$$2^{2V} \to O((\log V) \times D^6)$$

◇ 大きいボンドサイズDは難しい。

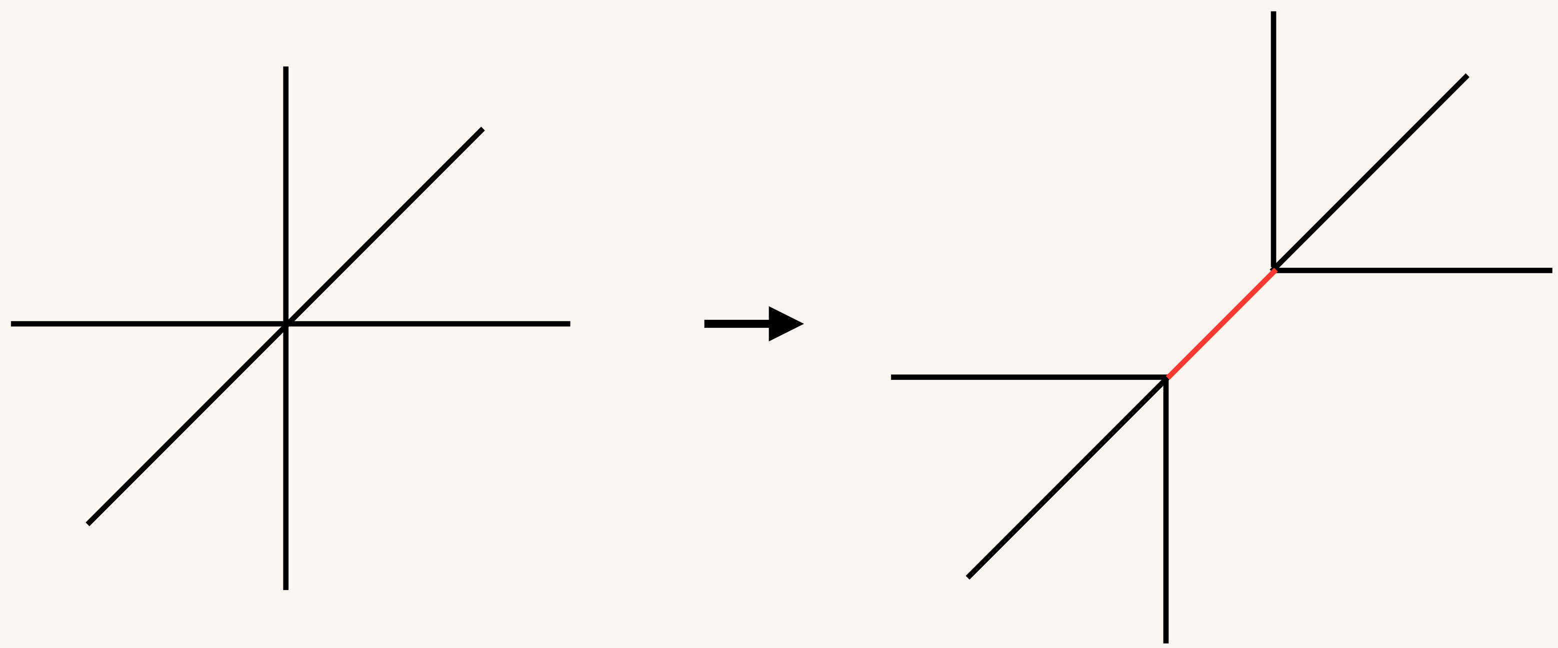
(高次元、複雑な相互作用)

→ 計算量削減が実務的には重要

◉ 高次元TRGにおける困難

◇ 単純なTRGの高次元への拡張は考えられないか?

→ 形式的にはできるが打ち切りも計算量も悪化



Cutoff:	$D^3 \to D$
Cost:	$O(D^{12})$

精度と速度の改善を考えたい。

Simple TRG,
Anisotropic TRG,
Bond-weighted TRG,
Core TRG,
CTMRG,
GILT,
HOTRG,
Randomized TRG,
SRG,
TNR,
Loop-TNR,
Triad TRG,
MDTRG,
ALL-mode TRG,
Branching TRG,
Boundary HOTRG
CTM-TRG
NNR-TNR

…etc.の組み合わせ

◉ テンソル繰り込み群の概観

◇ 色々あるが結局できることは何か?

近似

特異値分解　　or　　変分法

計算量削減

低ランク近似 (追加分解 or 打ち切りSVD or 境界条件)

精度改善

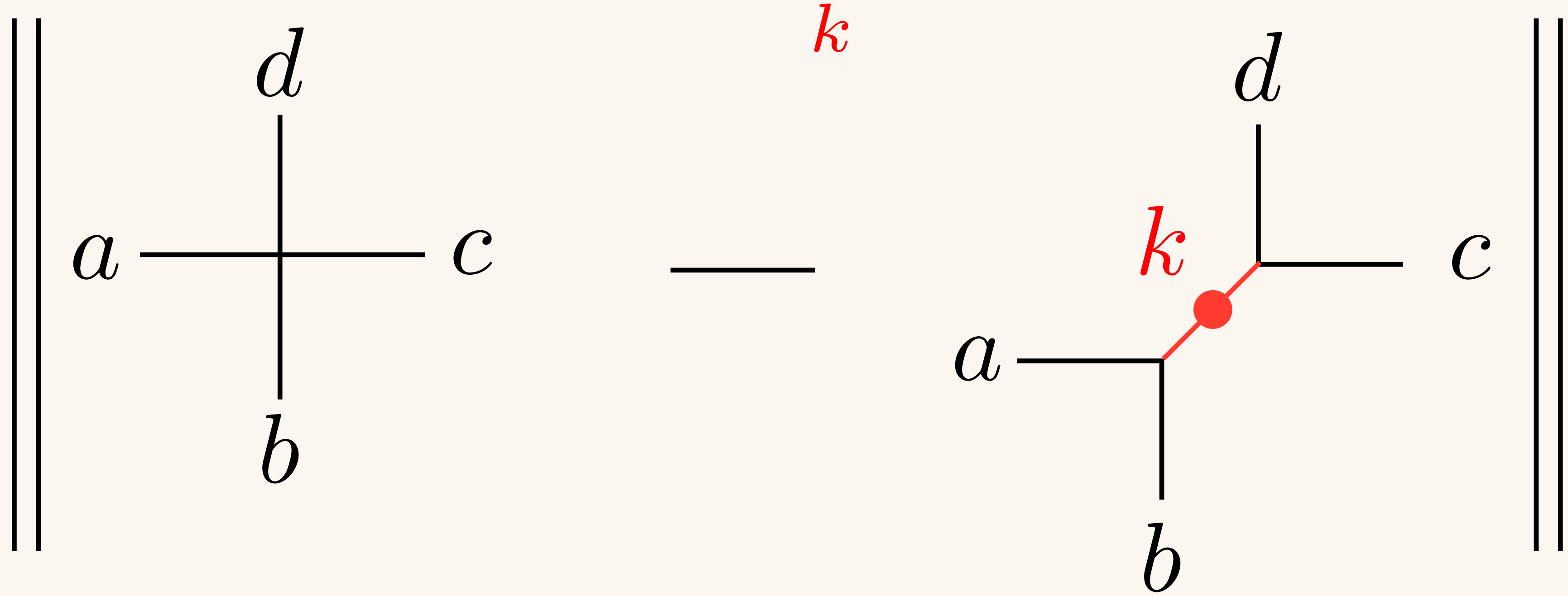
近似範囲の拡大, 大自由度による最適化,Disentangler

+ 近似範囲の違い。

→ 基本的には全ての手法がこれらの組み合わせで理解できる

◉ 変分法

$$T_{abcd} = \sum_{k}^{D} A_{ab}{}^{k} \lambda^{k} B_{cd}{}^{k}$$



◇ このコスト関数を逐次的に最小化させる手法

→ 添字 k を最初から小さく限定して最適化する

$$\mathrm{dim}(k) = \mathrm{dim}(a)\mathrm{dim}(b) \to D$$

◉ 乱拓特異値分解(R-SVD)

→ SVDの近似法として一般性がある

近似SVD

精度改善

計算量削減
打ち切りSVD

近似範囲
＋

→ 打ち切り特異値分解の手法。

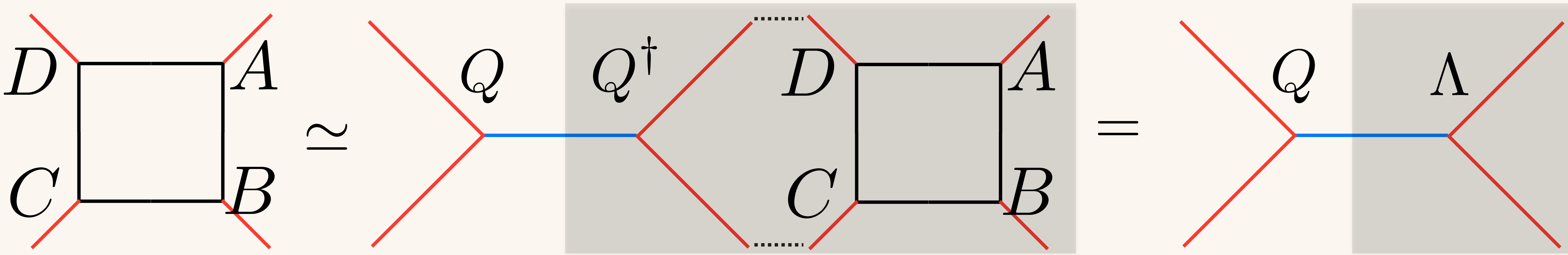
TRGに適用することで計算量を削減できる。

また、縮約の近似としても利用できる。

◉ 乱拓特異値分解(R-SVD)

[N. Halko, et al. arXiv:0909.4061]
[S. Morita, et al. arXiv:1712.01458]

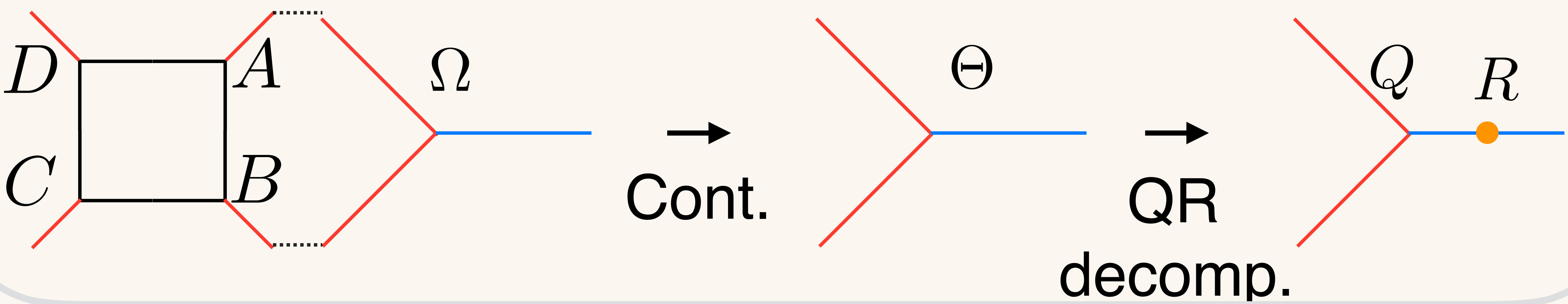
◇ 直交行列 Q による近似的な縮約法



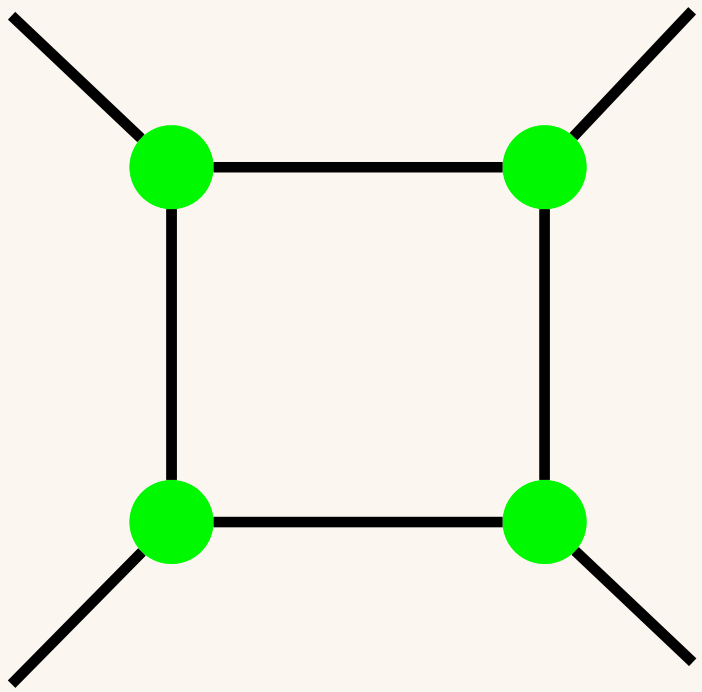
◇ $\Lambda \equiv Q^\dagger ABCD$ の特異値分解なら添字の数が減って早い

◇ Q の準備に乱数とQR分解を使う

◇ 乱数テンソル Ω でサンプリングして近似している

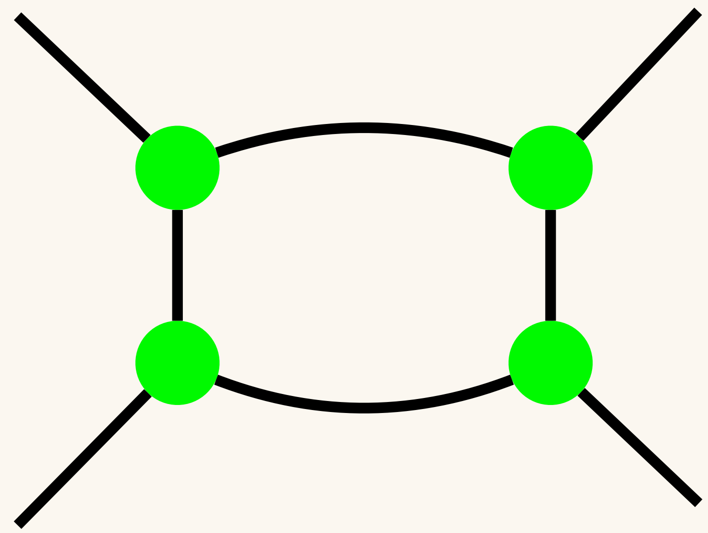


◉ Simple Contraction



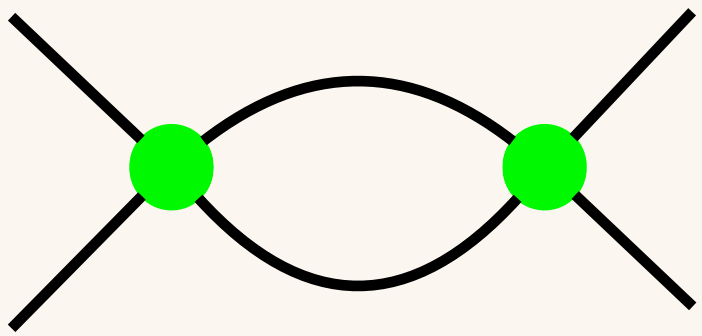
◇ Cost: $O(D^5) \to O(D^6)$

◉ Simple Contraction



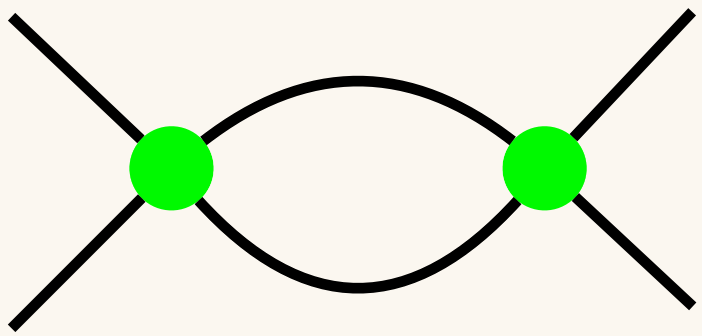
◇ Cost: $O(D^5) \to O(D^6)$

◉ Simple Contraction



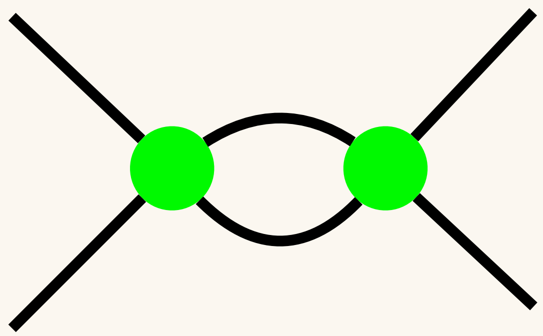
◇ Cost: $O(D^5) \to O(D^6)$

◉ Simple Contraction



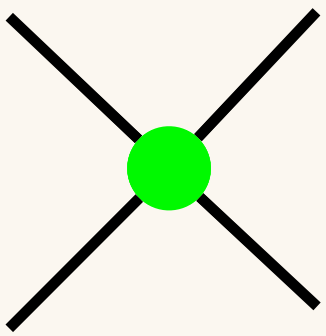
◇ Cost: $O(D^5) \rightarrow O(D^6)$

◉ Simple Contraction



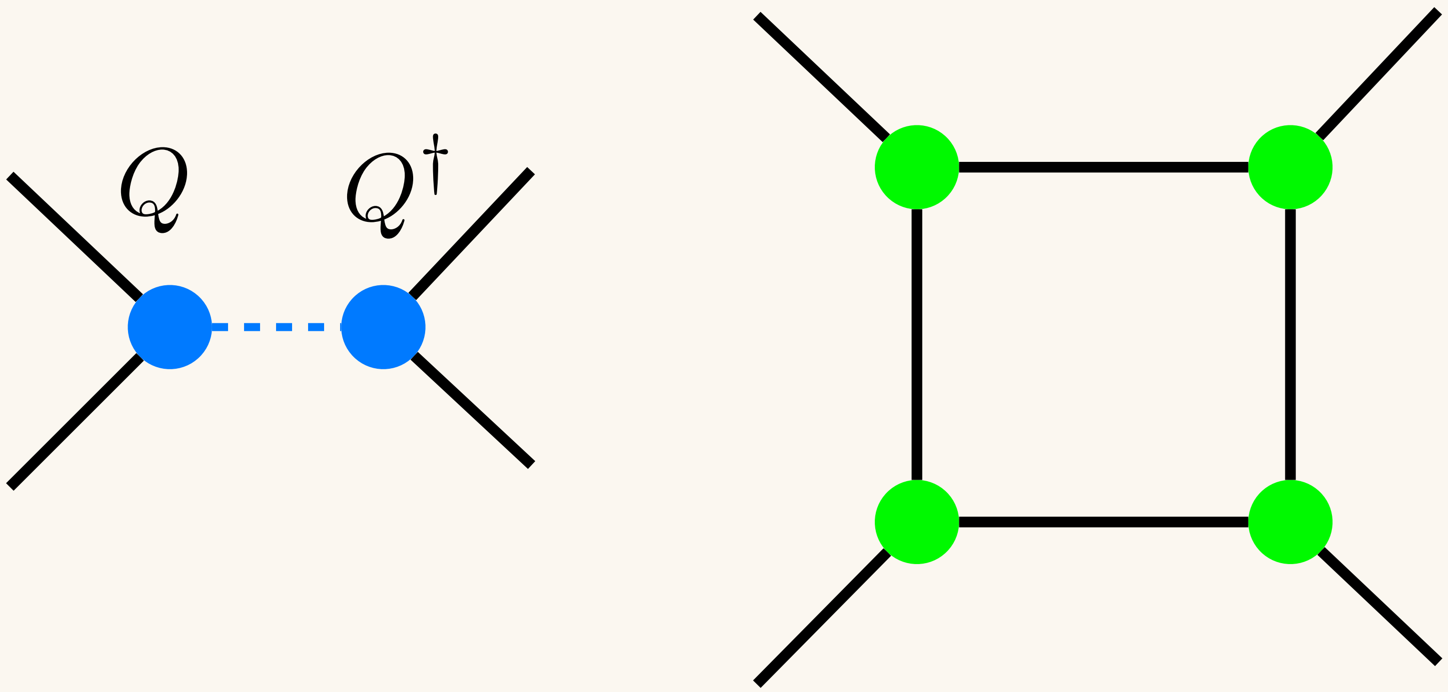
◇ Cost: $O(D^5) \rightarrow O(D^6)$

◉ Simple Contraction



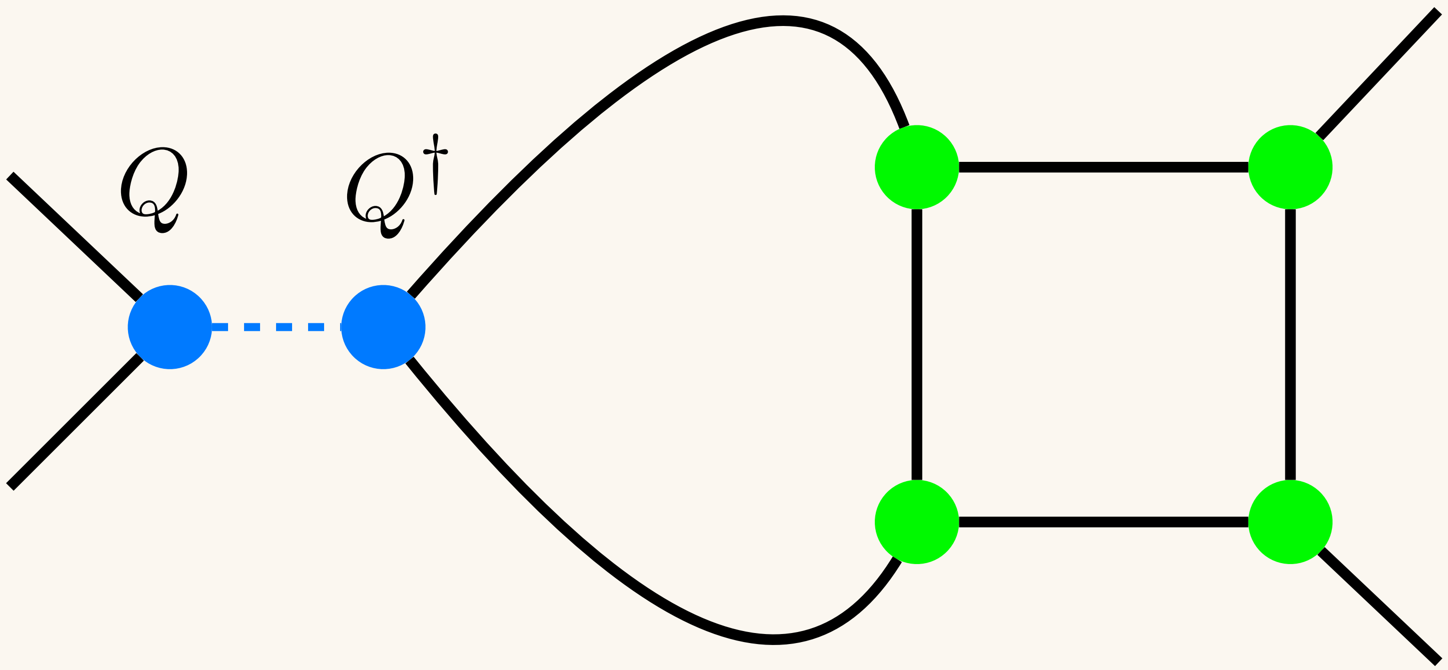
◇ Cost: $O(D^5) \rightarrow O(D^6)$

◉ Contraction by R-SVD



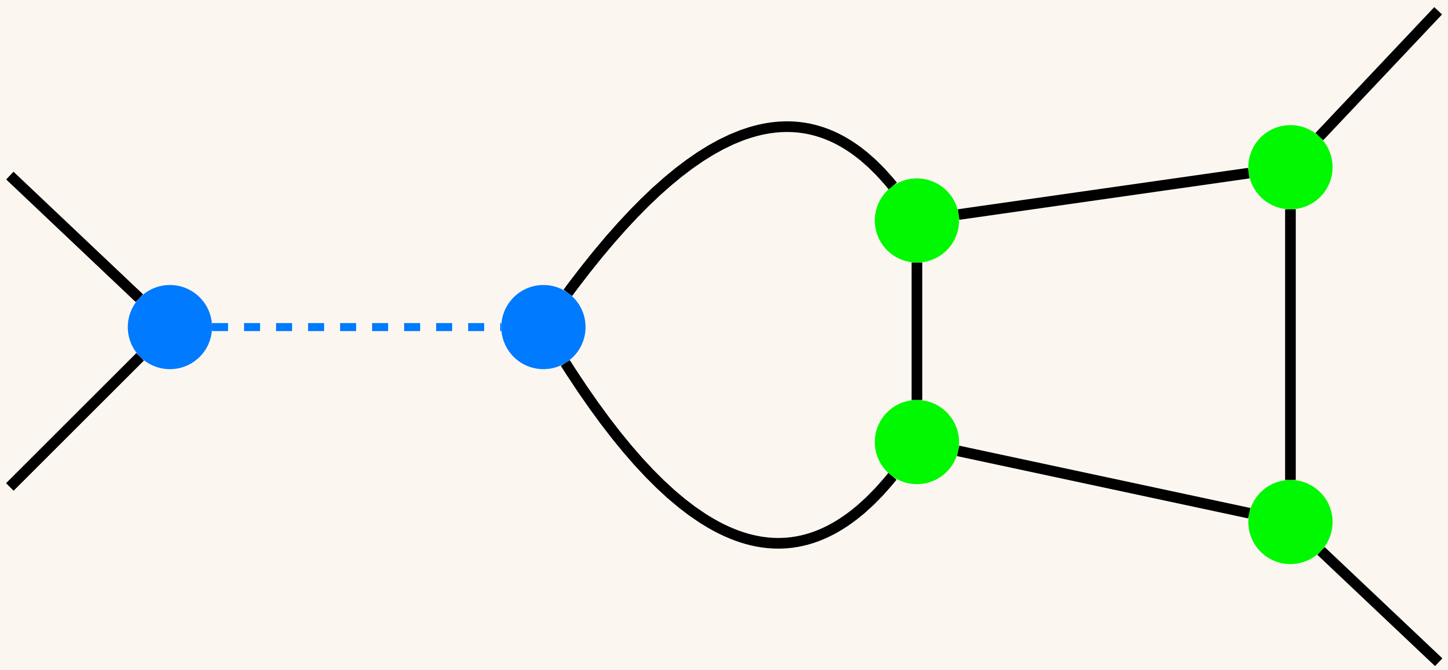
◇ Cost: $O(D^5) \to O(D^5) \to O(D^5)$

◉ Contraction by R-SVD



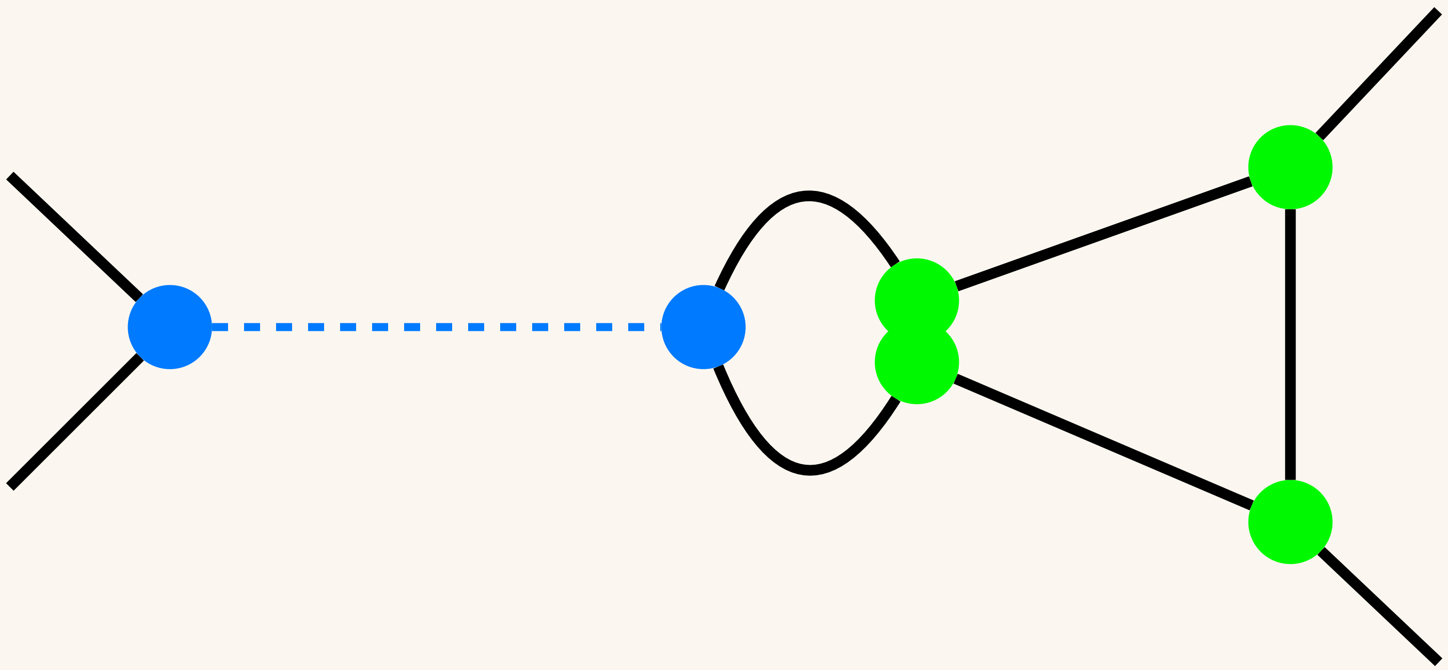
◇ Cost: $O(D^5) \to O(D^5) \to O(D^5)$

◉ Contraction by R-SVD



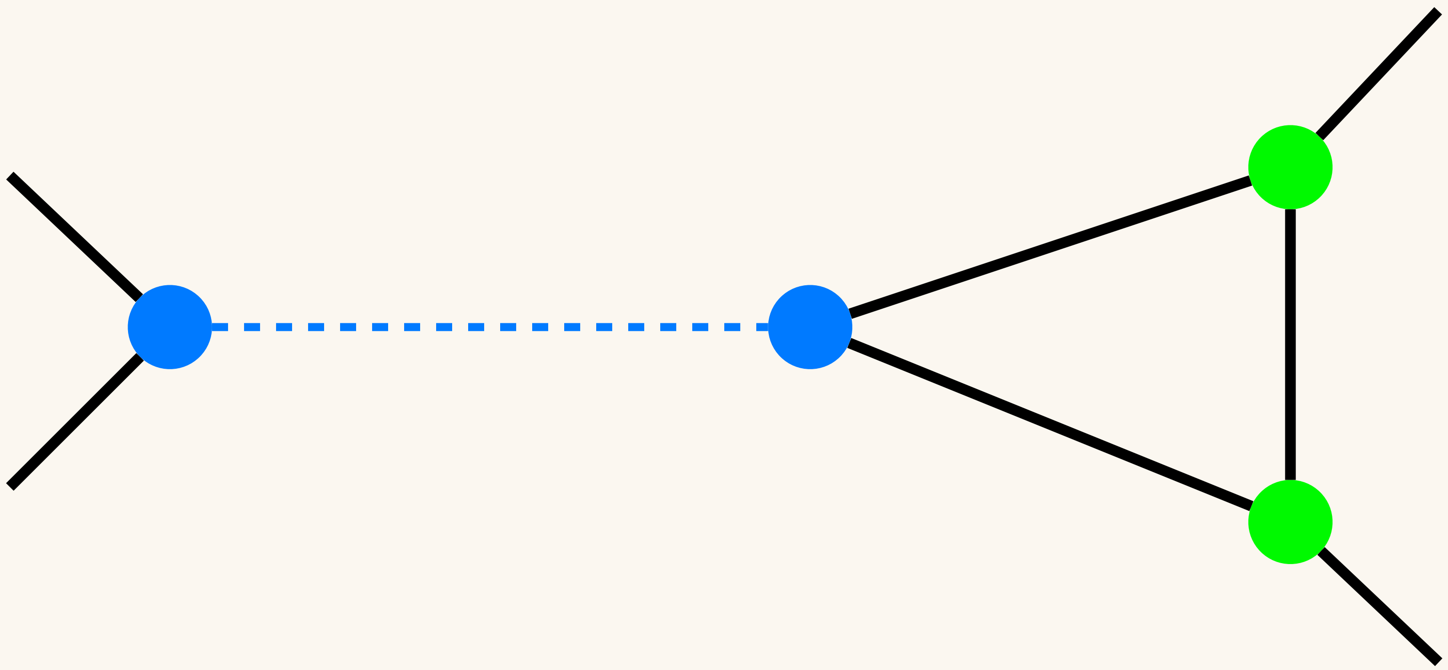
◇ Cost: $O(D^5) \rightarrow O(D^5) \rightarrow O(D^5)$

◉ Contraction by R-SVD



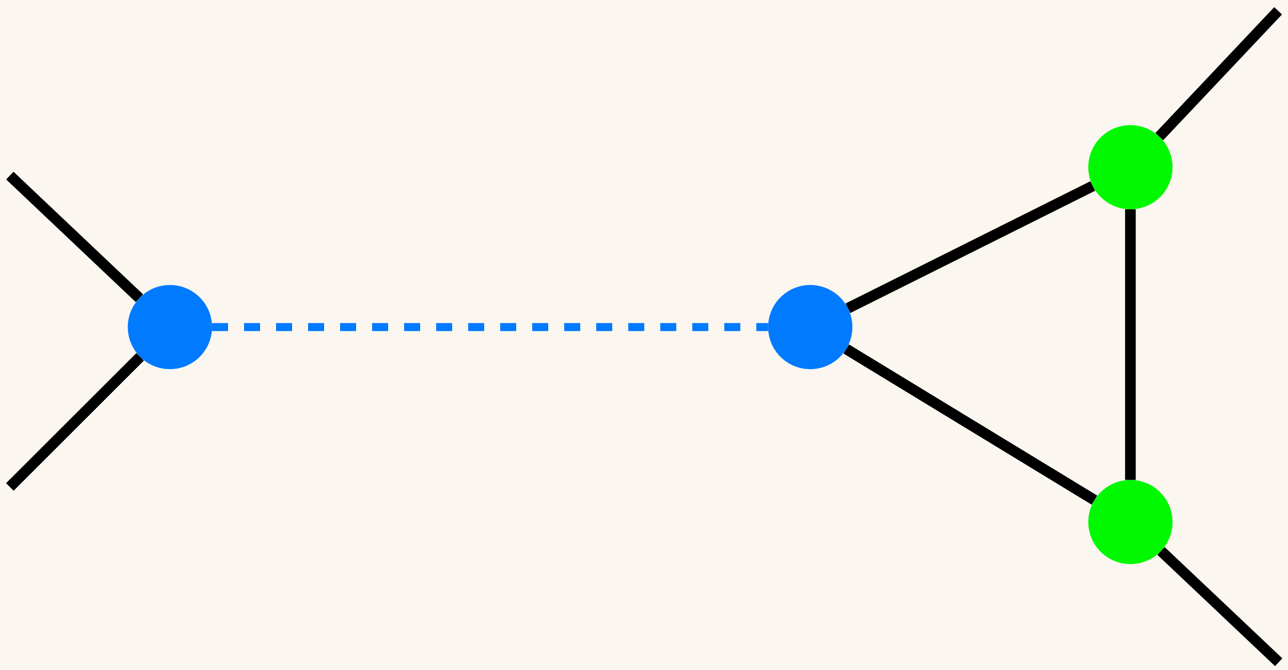
◇ Cost: $O(D^5) \to O(D^5) \to O(D^5)$

◉ Contraction by R-SVD



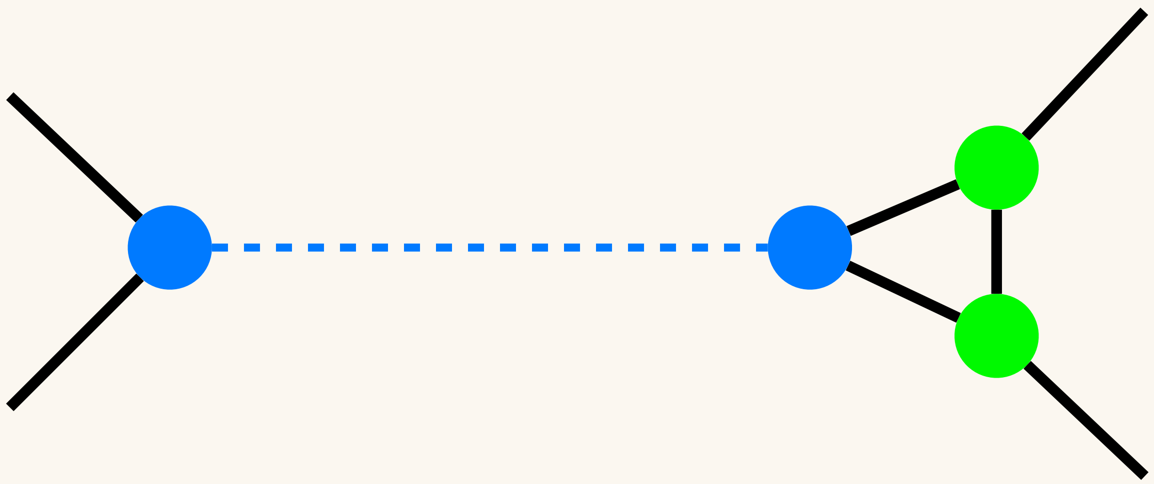
◇ Cost: $O(D^5) \to O(D^5) \to O(D^5)$

◉ Contraction by R-SVD



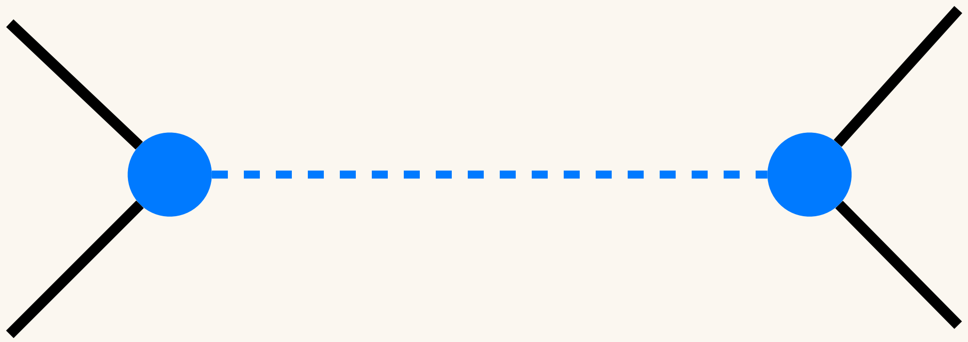
◇ Cost: $O(D^5) \rightarrow O(D^5) \rightarrow O(D^5)$

◉ Contraction by R-SVD



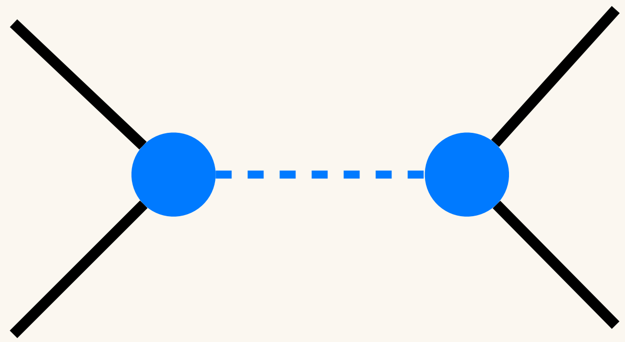
◇ Cost: $O(D^5) \rightarrow O(D^5) \rightarrow O(D^5)$

◉ Contraction by R-SVD



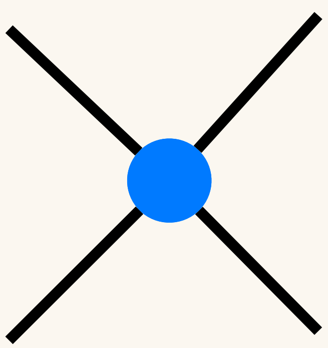
◇ Cost: $O(D^5) \to O(D^5) \to O(D^5)$

◉ Contraction by R-SVD



◇ Cost: $O(D^5) \to O(D^5) \to O(D^5)$

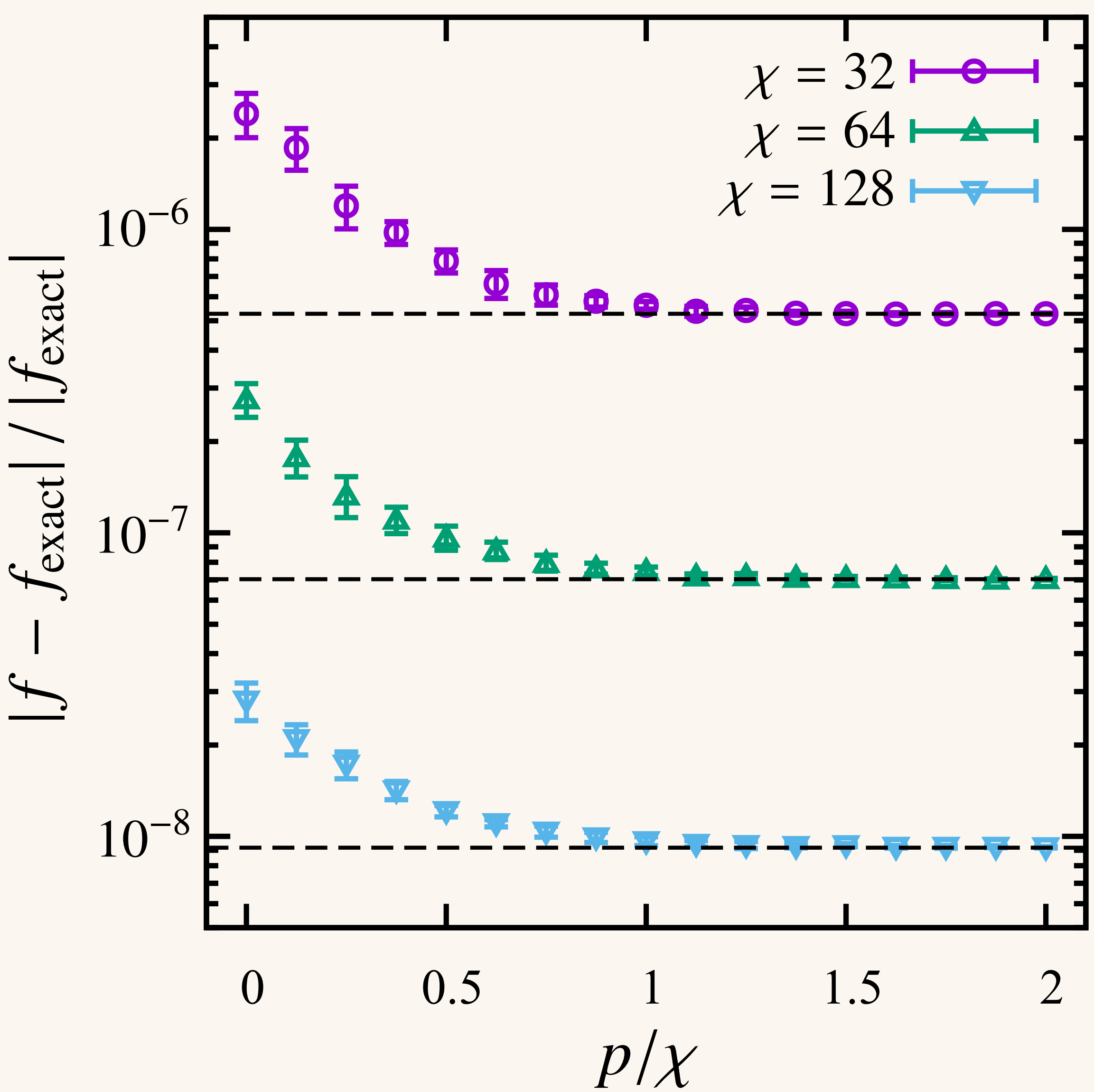
◉ Contraction by R-SVD

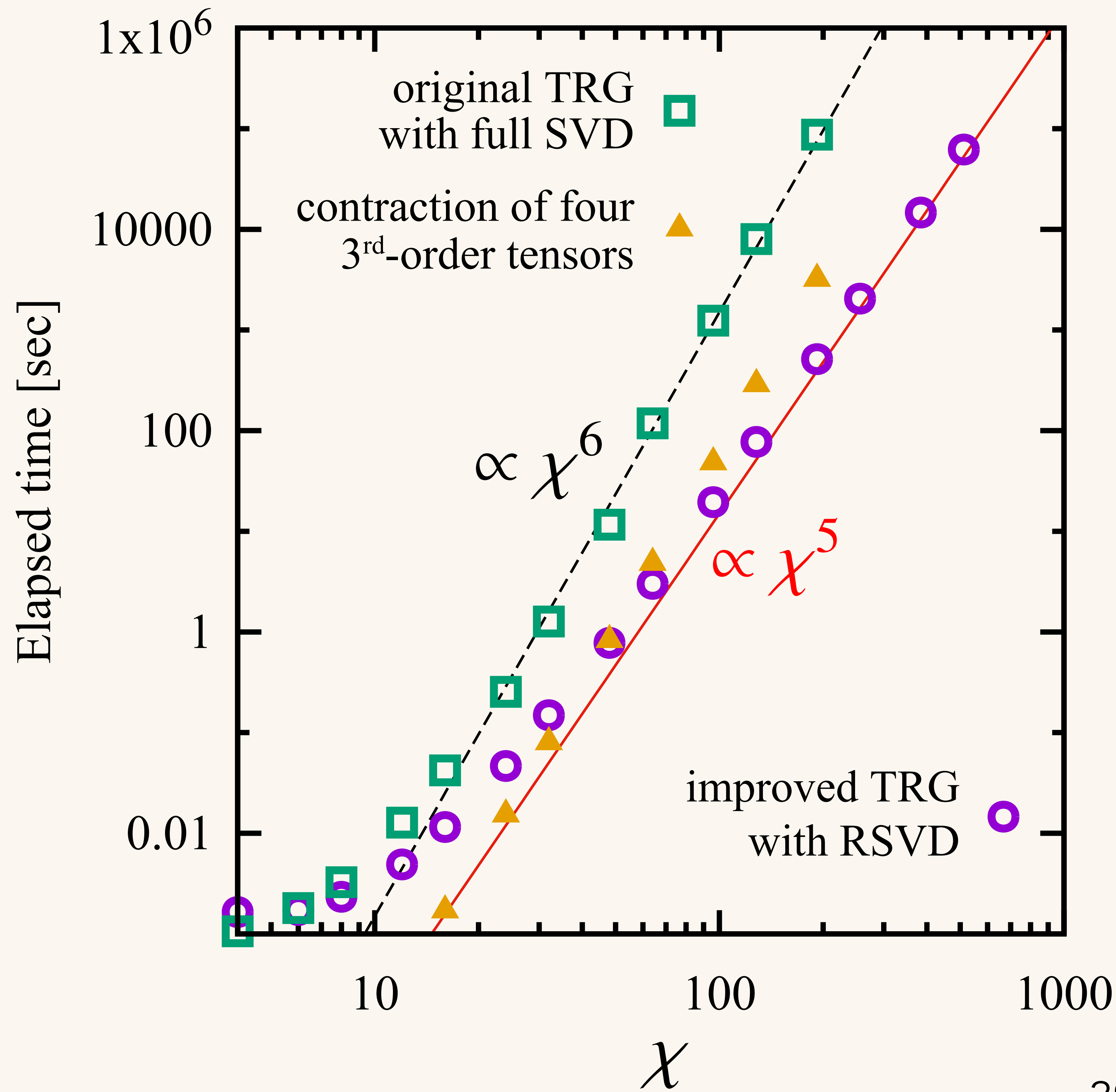


◇ Cost: $O(D^5) \to O(D^5) \to O(D^5)$

◉ Numerical costs for randomized TRG

◇ Cost reduced: $O(D^6) \to O(D^5)$





[S. Morita, R. Igarashi et al. arXiv:1712.01458]

◉ Higher-Order TRG (HOTRG)

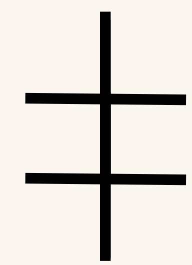
→ Isometryの明示的な導入と高次元への拡張

近似
SVD(Isometry)

精度改善
近似範囲

計算量削減

近似範囲

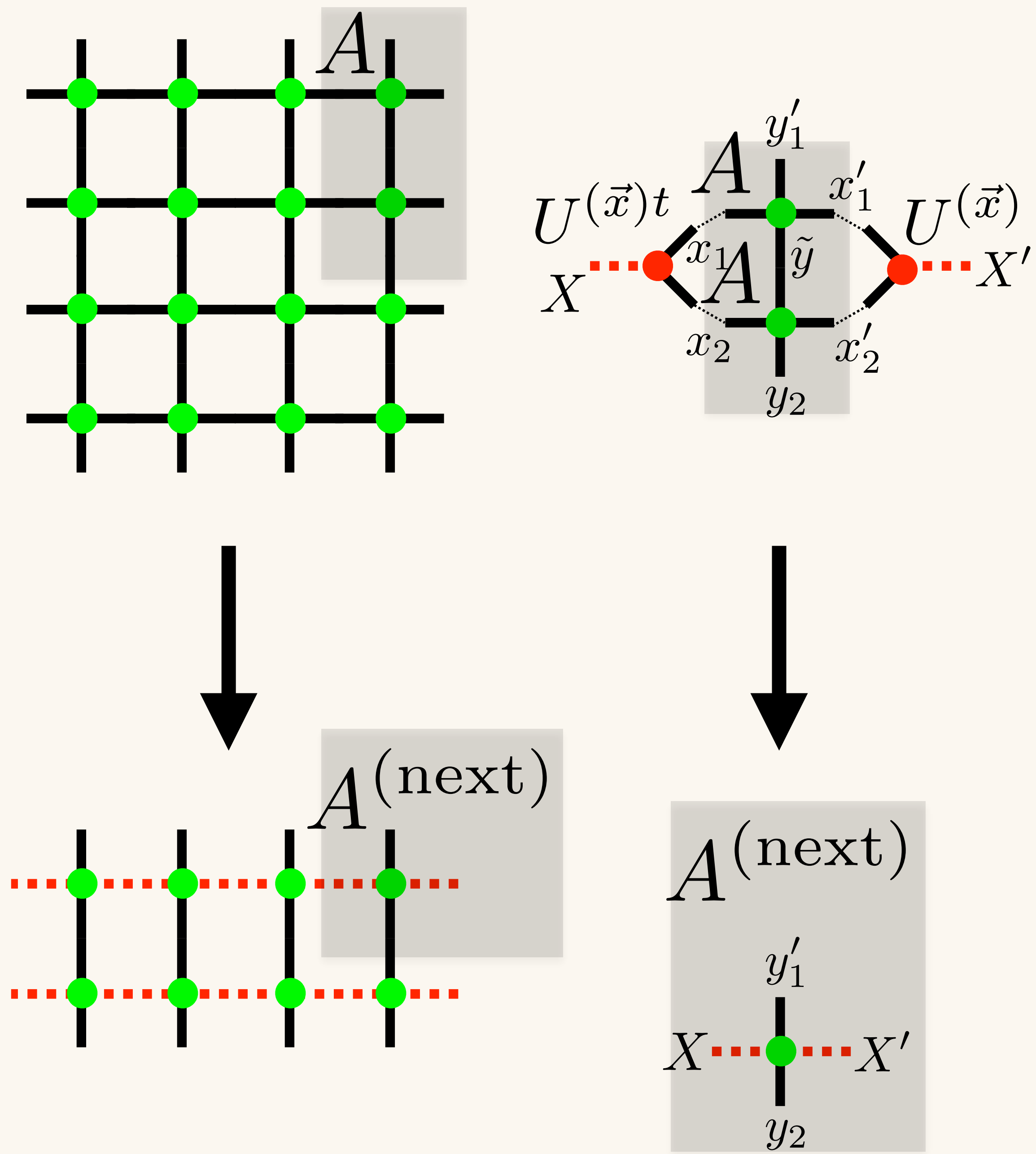


→ 近似範囲が一つのテンソルではない分、
計算量はTRGより増えるが精度は上がりうる。
Isometryで粗視化を表現。高次元への拡張が単純に。

◉ Higher-Order TRG (HOTRG)

[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

◇ 射影テンソルUを用いた近似的縮約



$$\Gamma^{(AA)} = AA \to A^{(\mathrm{next})}$$

→$U^{(\vec{x})}$は$\Gamma\Gamma^t$のSVDから得る

$$[\Gamma\Gamma^t]_{[x_1 x_2][x_1^t x_2^t]} = \sum_{k=1}^{D^2} U^{(x)}_{[x_1 x_2]k} \lambda_k U^{(x)}_{[x_1^t x_2^t]k}$$

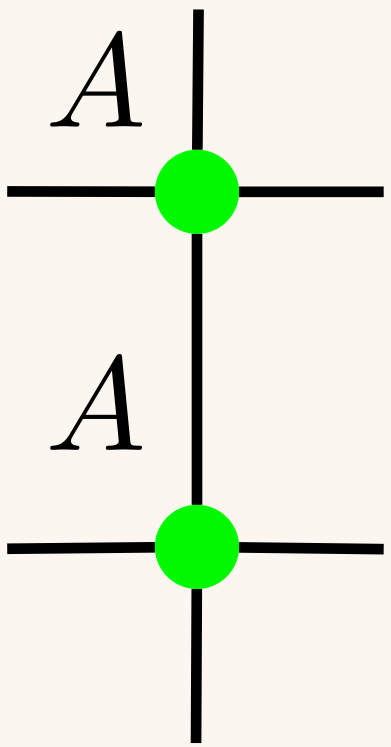
SVD打ち切り: $D^2 \to D$

射影テンソルの計算量:$O(D^6)$

$$U^t AAU = A^{(\mathrm{next})}$$

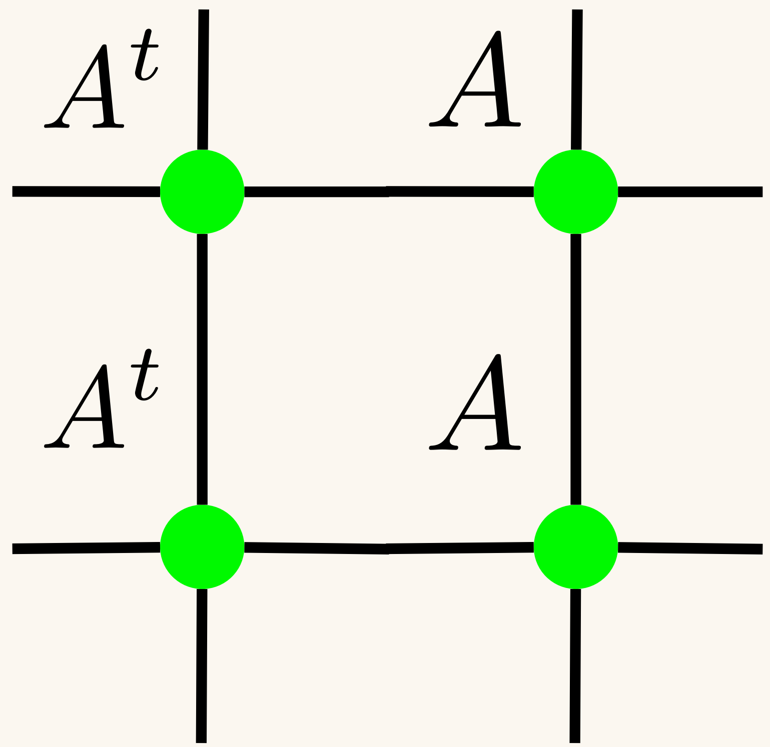
縮約の計算量: $O(D^7)$

◉ HOTRG: Isometry step



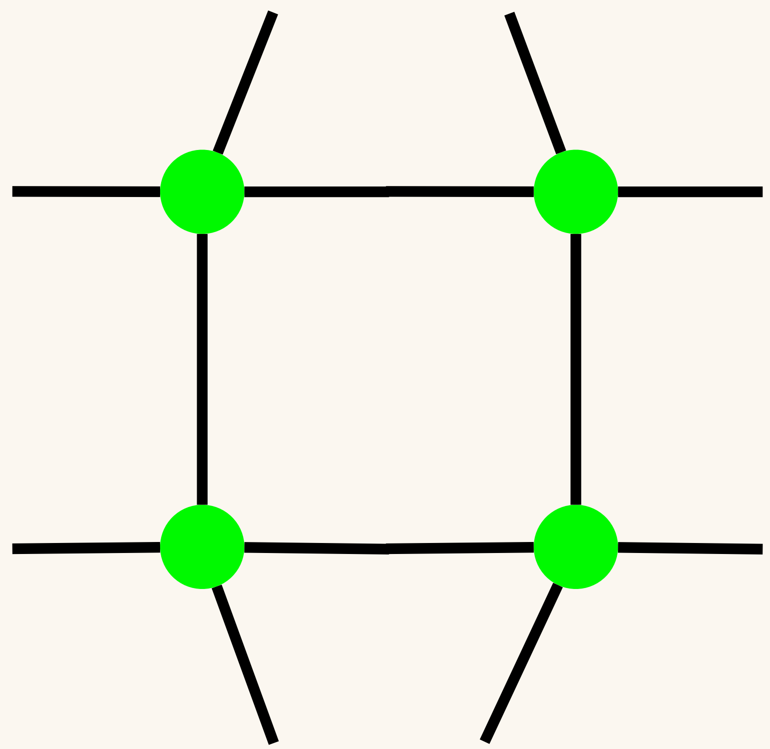
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



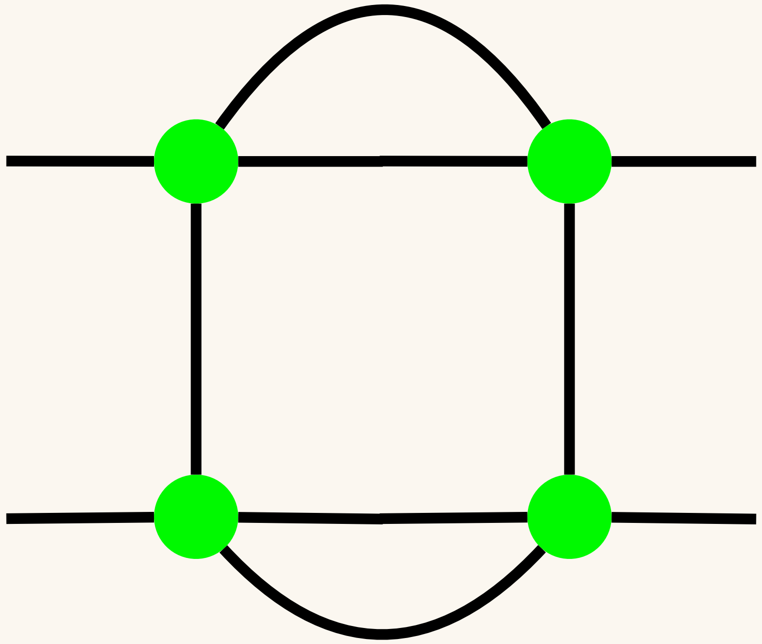
◇ Cost: $O(D^6) \rightarrow O(D^6) \rightarrow O(D^6)$

◉ HOTRG: Isometry step



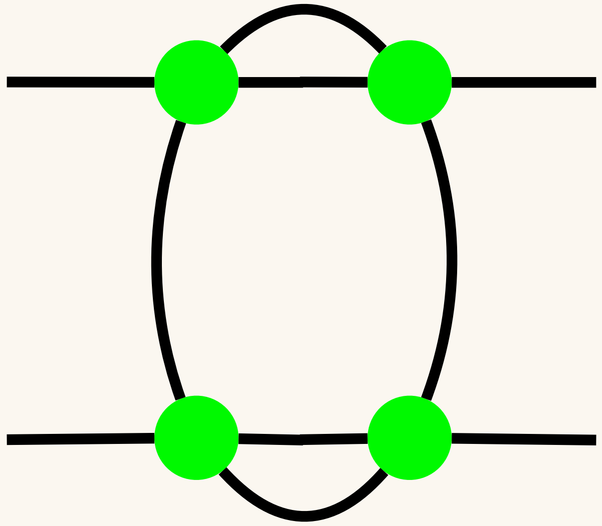
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



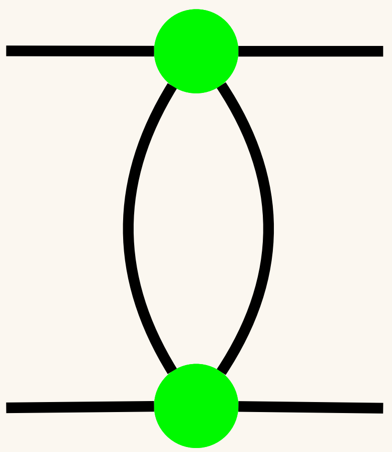
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



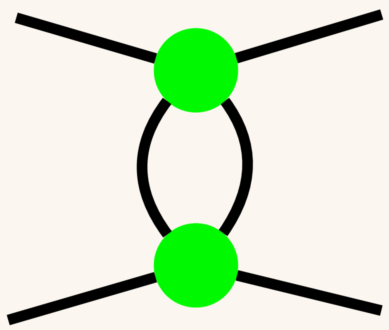
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



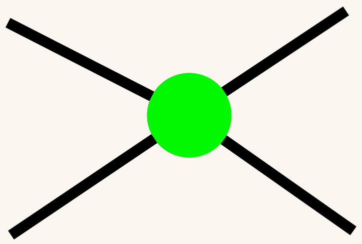
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



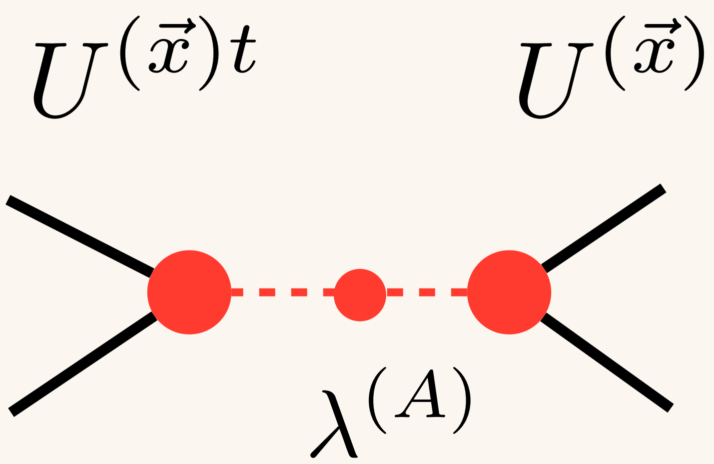
◇ Cost: $O(D^6) \rightarrow O(D^6) \rightarrow O(D^6)$

◉ HOTRG: Isometry step



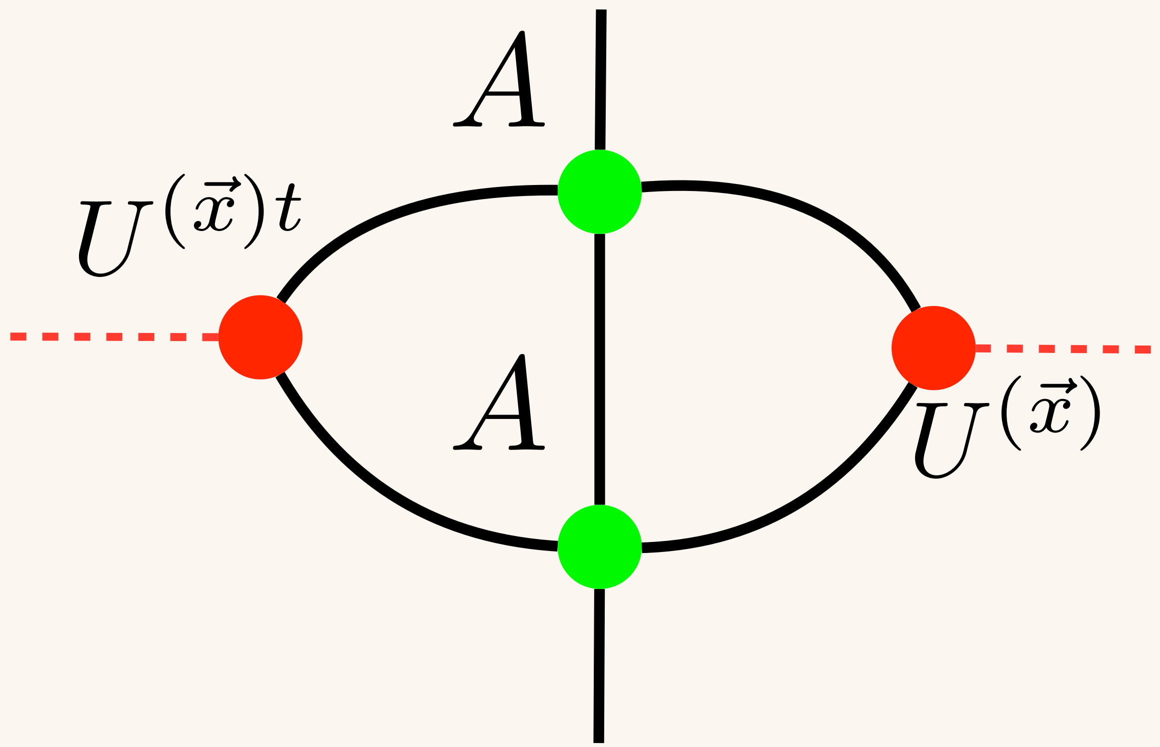
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



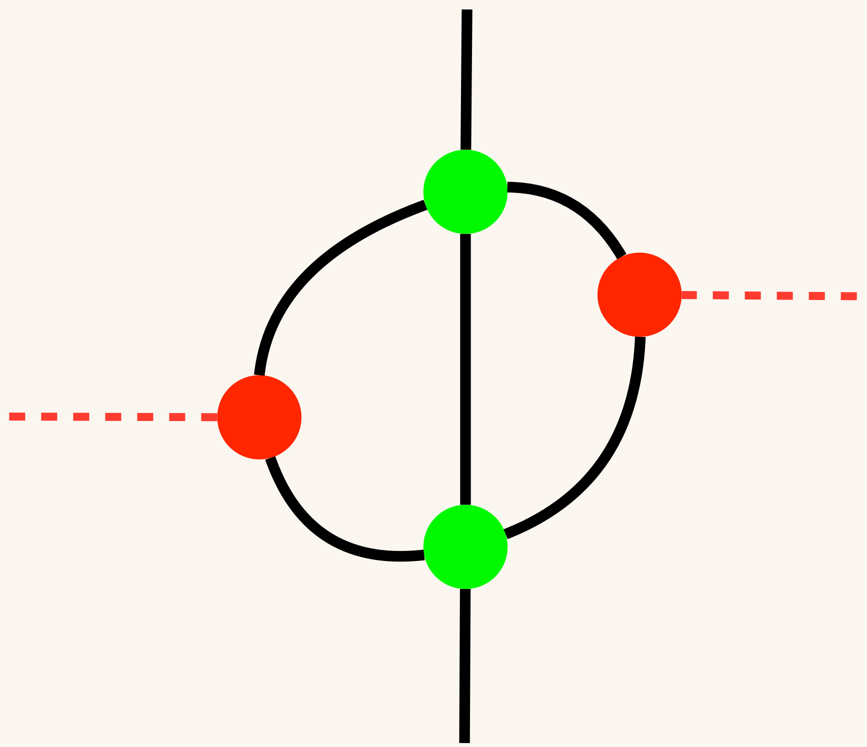
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Contraction step



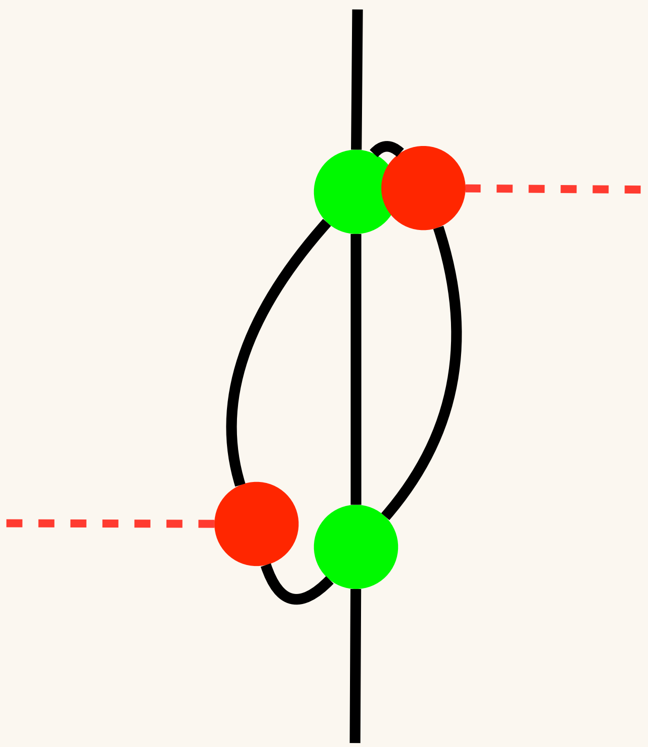
◇ Cost: $O(D^6) \to O(D^7)$

◉ HOTRG: Contraction step



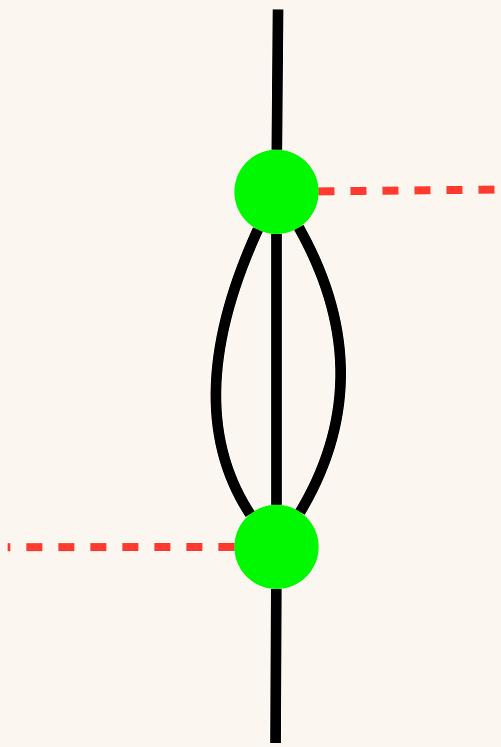
◇ Cost: $O(D^6) \to O(D^7)$

◉ HOTRG: Contraction step



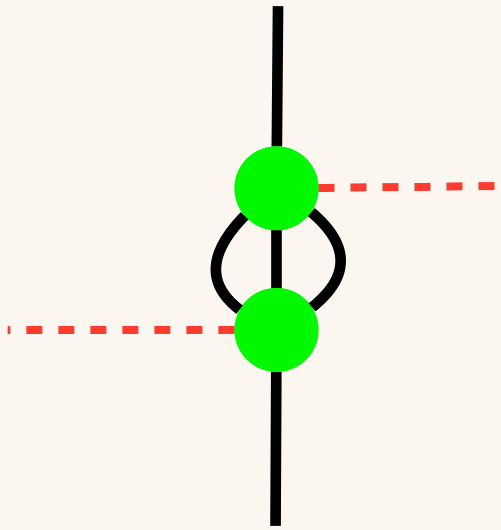
◇ Cost: $O(D^6) \to O(D^7)$

◉ HOTRG: Contraction step



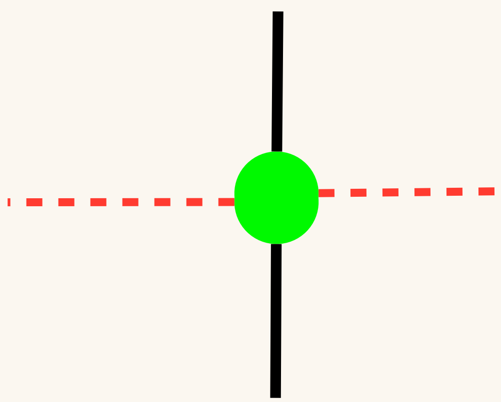
◇ Cost: $O(D^6) \to O(D^7)$

◉ HOTRG: Contraction step



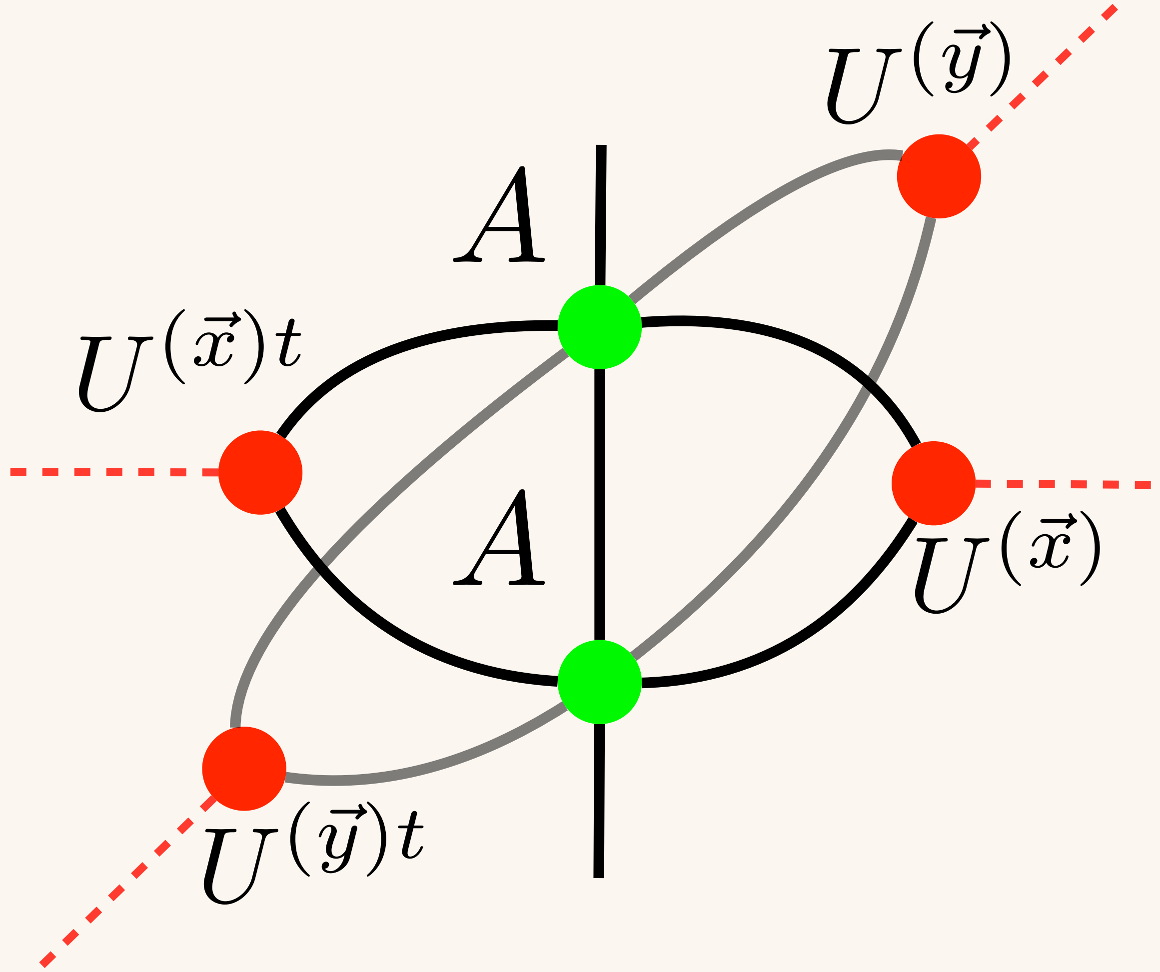
◇ Cost: $O(D^6) \to O(D^7)$

◉ HOTRG: Contraction step



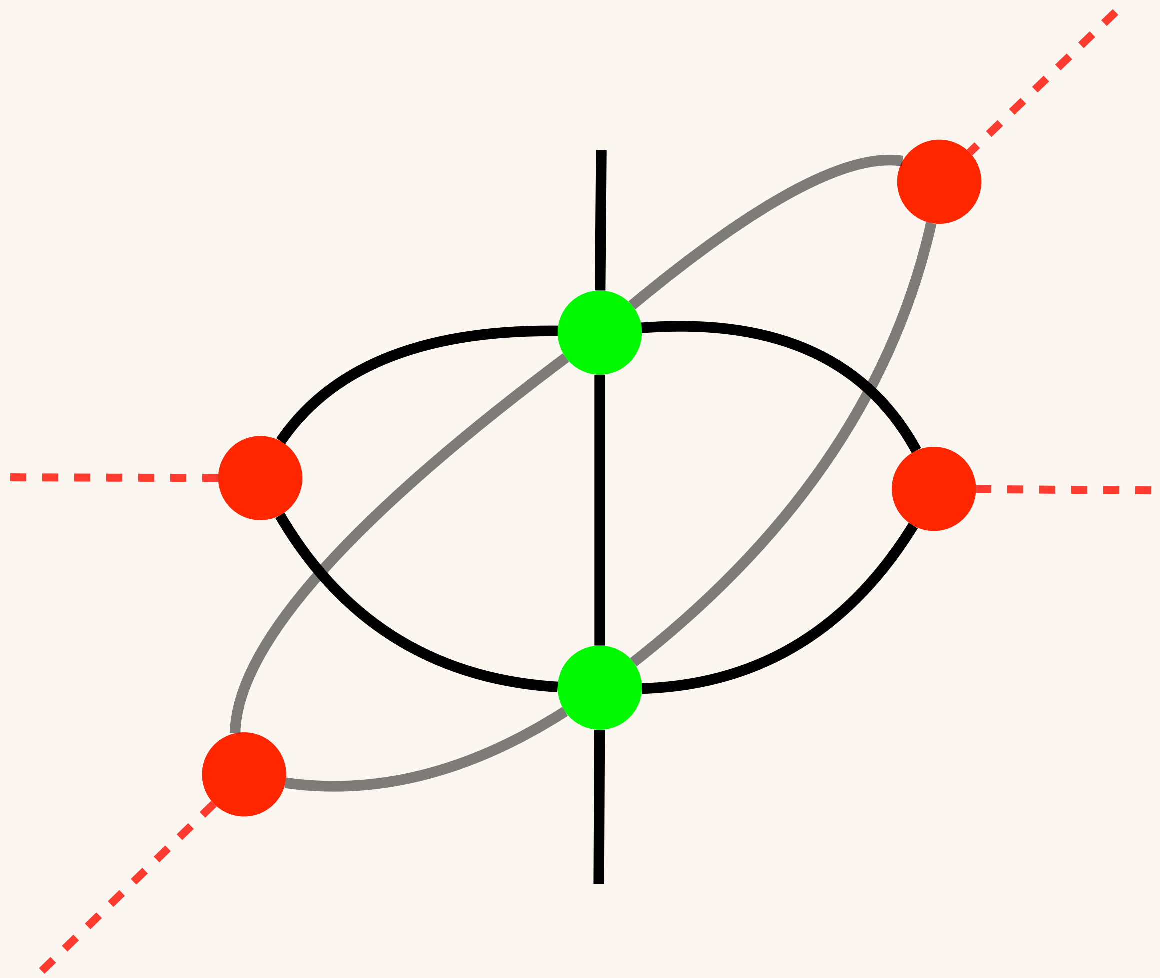
◇ Cost: $O(D^6) \to O(D^7)$

◉ HOTRG: Contraction step



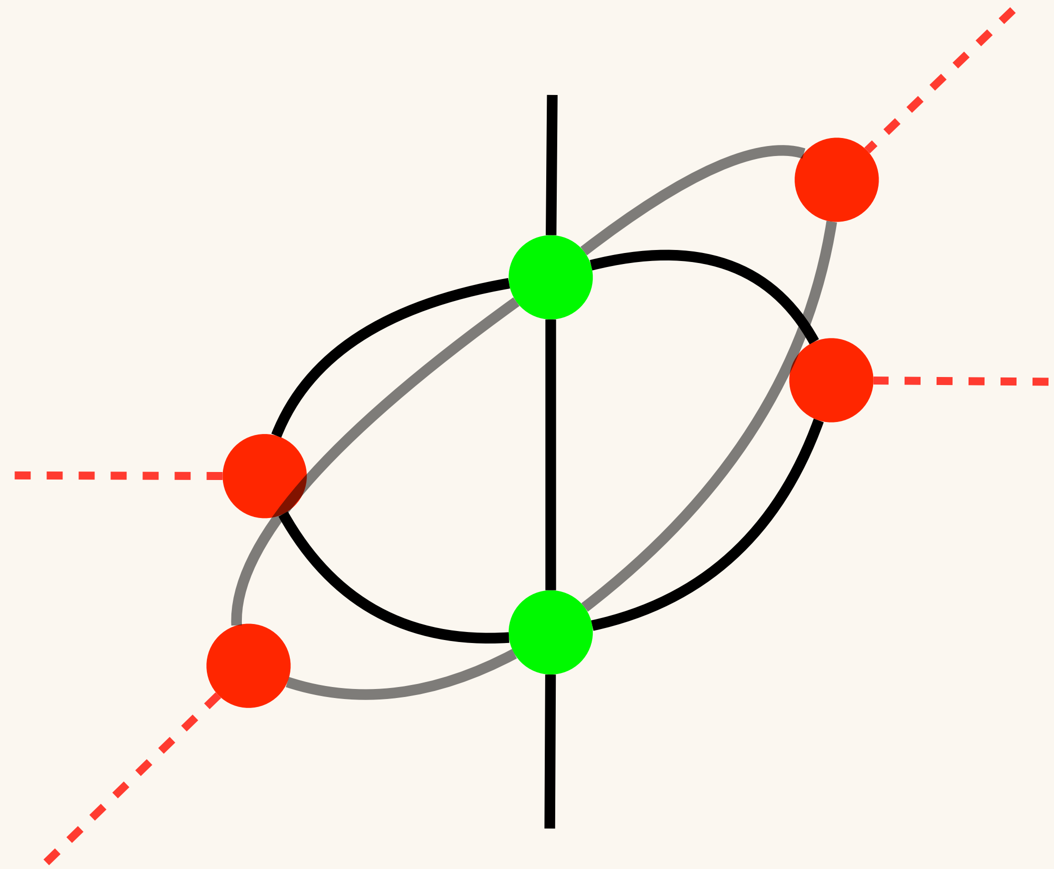
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



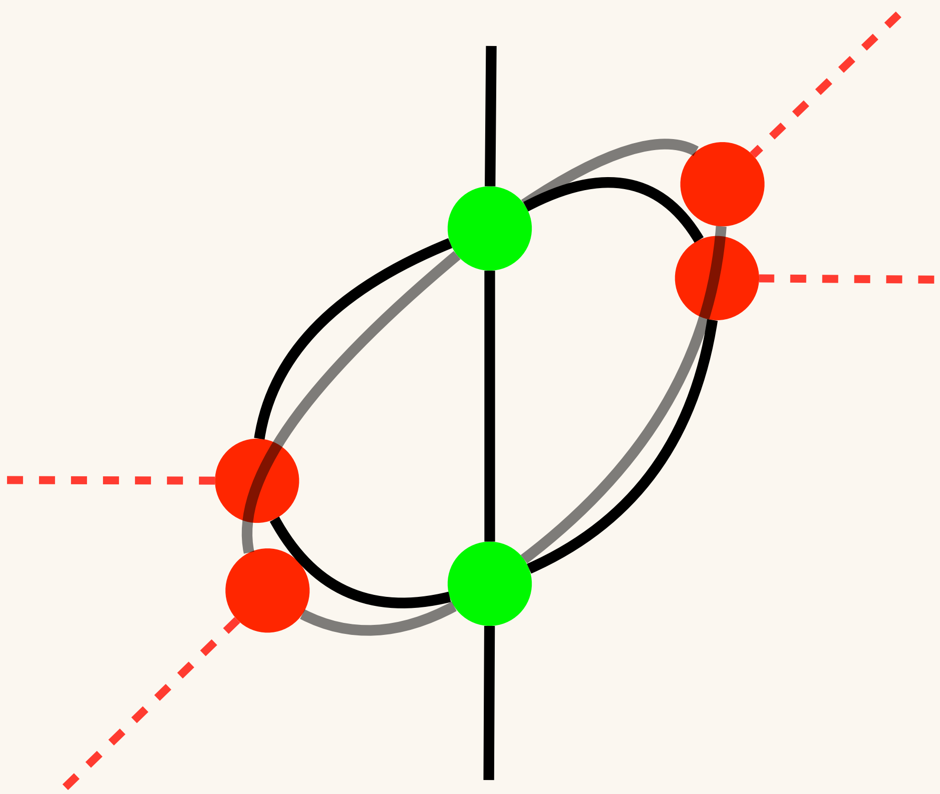
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



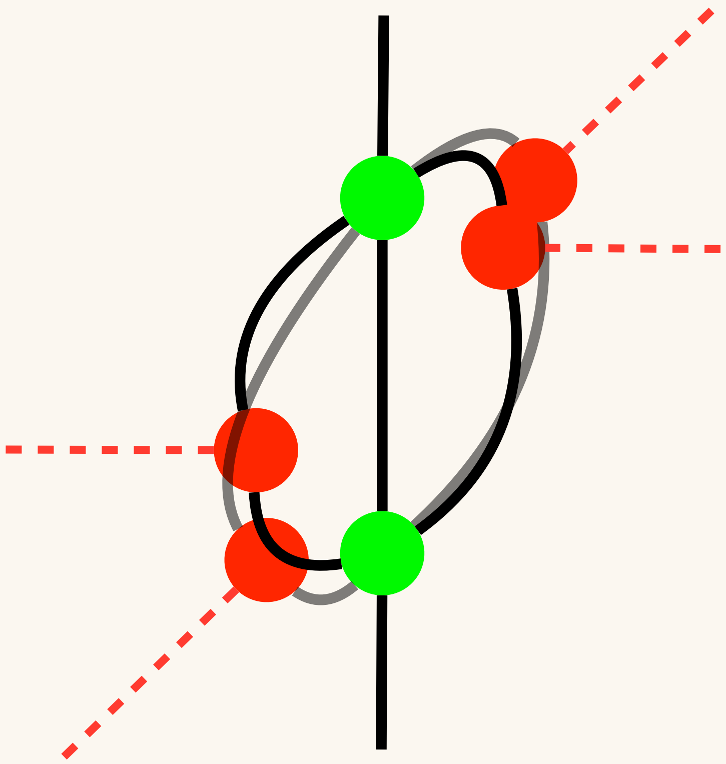
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



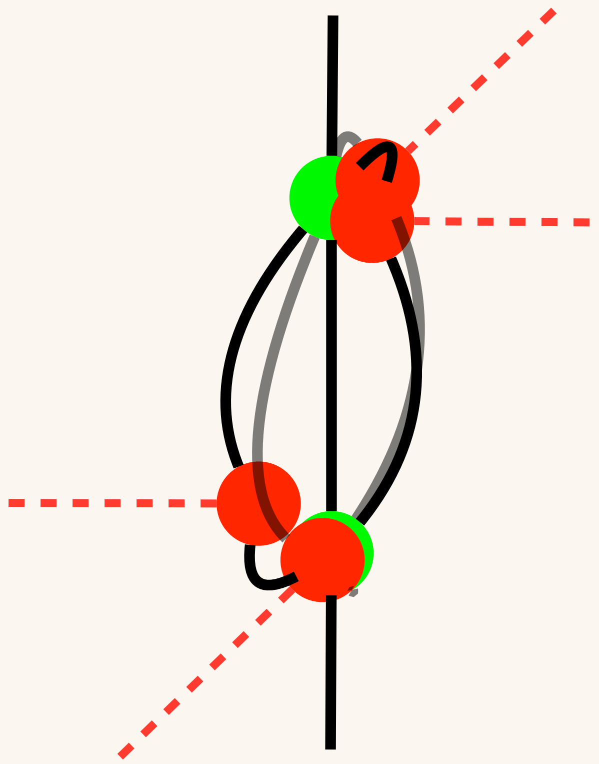
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



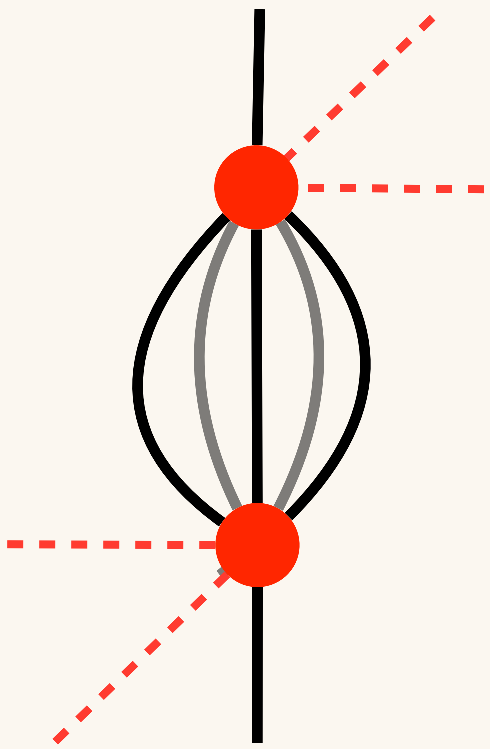
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



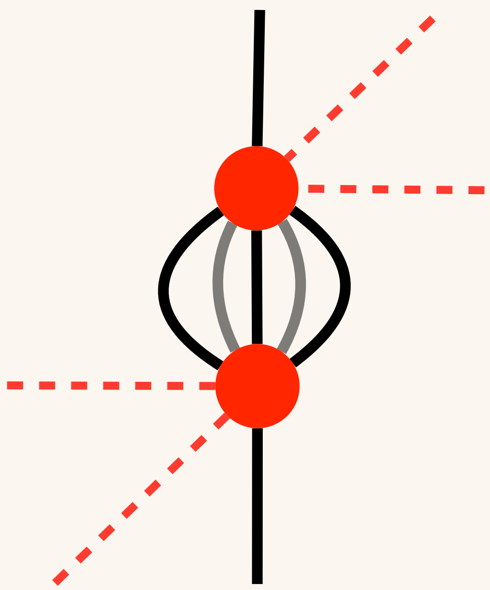
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



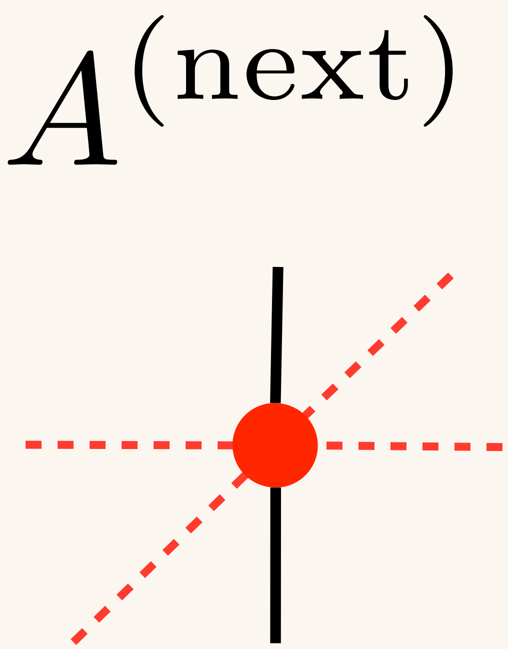
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step

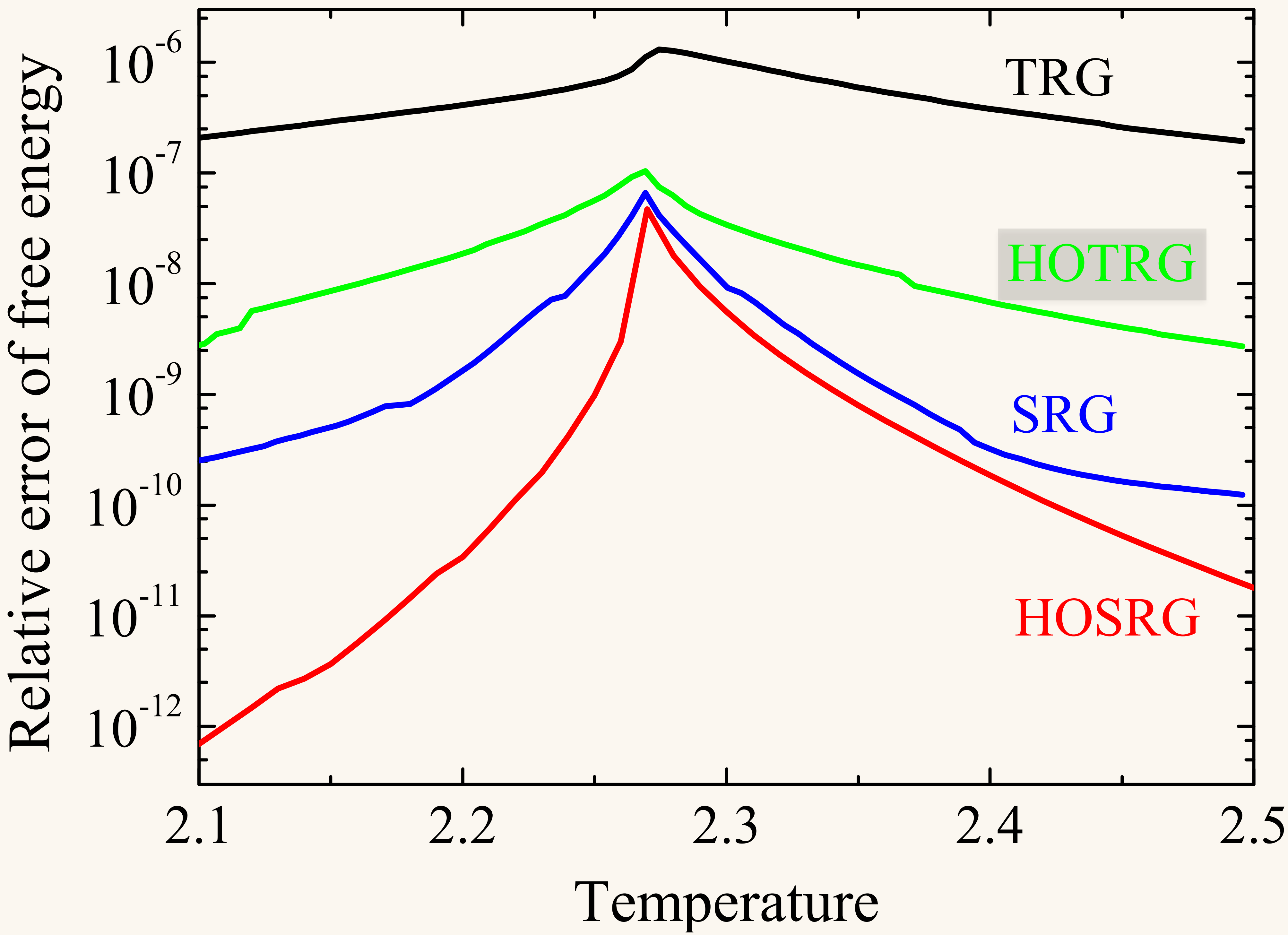


◇ Cost: $O(D^9) \rightarrow O(D^{11})$

◉ Higher-Order TRG (HOTRG)

[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

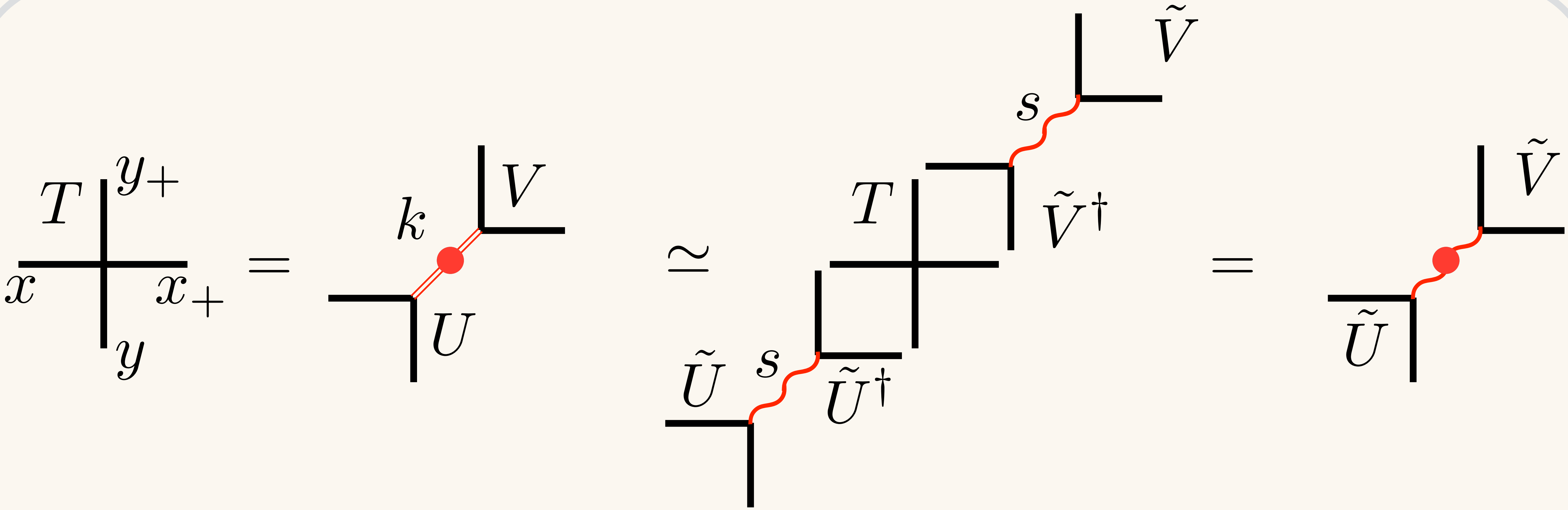
◇ Ising模型



◉ Isometry rep. of simple TRG

◇ 全てのTRGをIsometryで統一的に表記できる。

◇ 単純なTRGのIsometryを使った説明



→ 周りくどいものの、全てのSVDを用いた近似をIsometryで考えられるのはシンプル。

(SVDの打ち切りはIsometry演算と等価)

◉ Anisotropic TRG (ATRG)

→ 分解で計算量削減

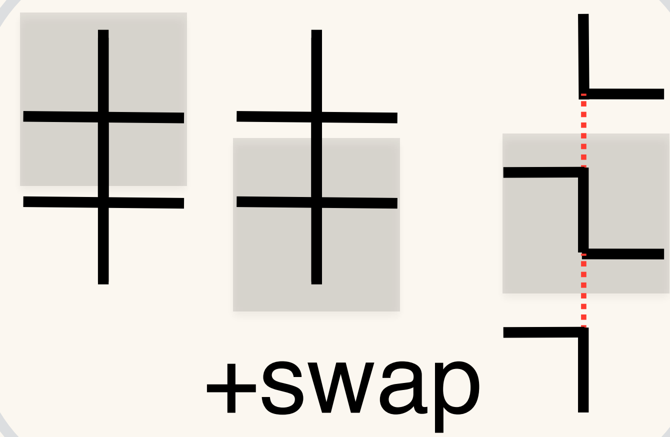
近似
SVD

精度改善

計算量削減
追加分解

打ち切りSVD

近似範囲



→ 全て局所的な縮約と分解の組み合わせで構成可能。

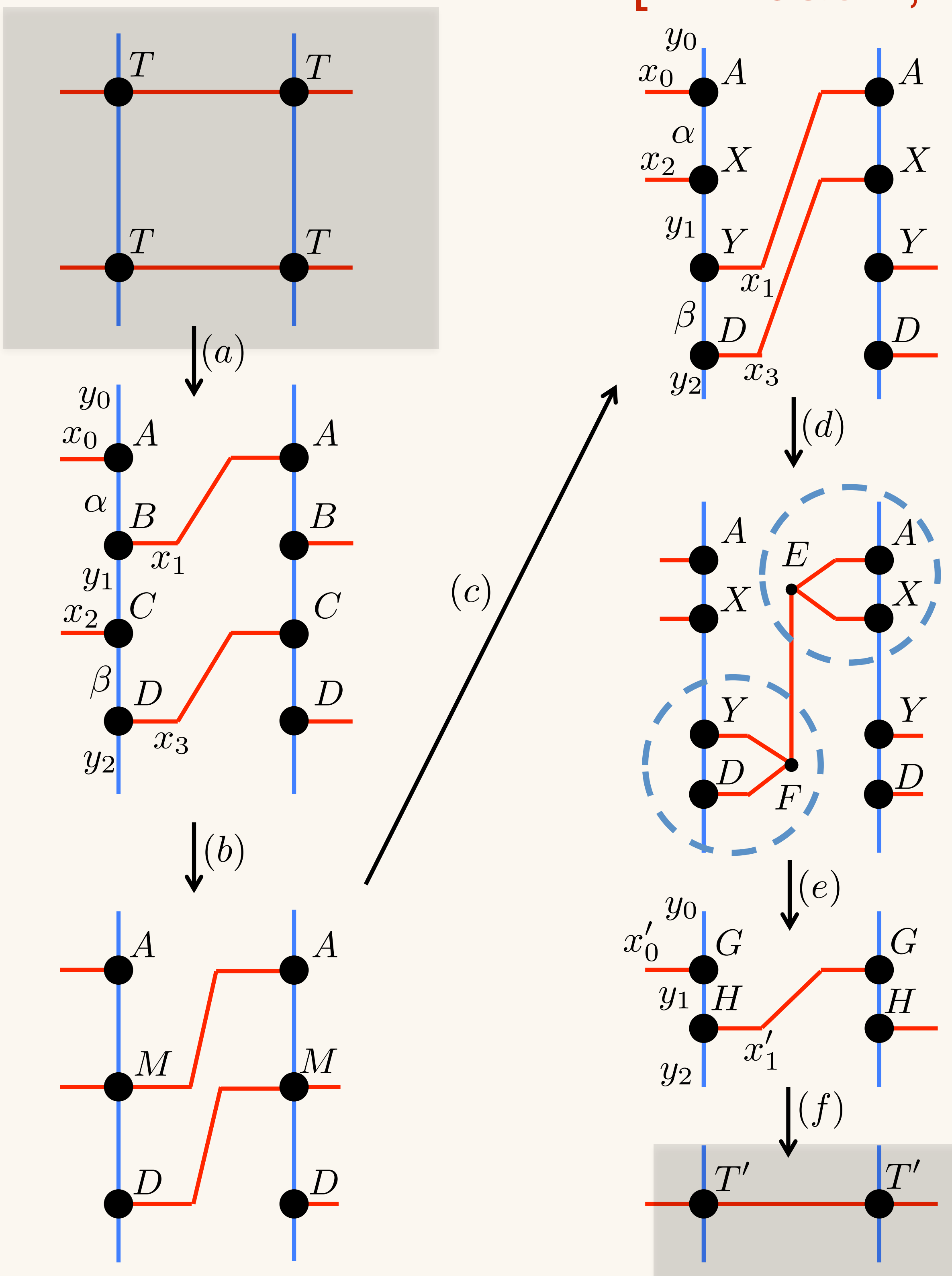
組み合わせにすることで低階数テンソルの計算にする。

近似範囲はHOTRGと似ているが、

分解のたびに注目している範囲は違う。

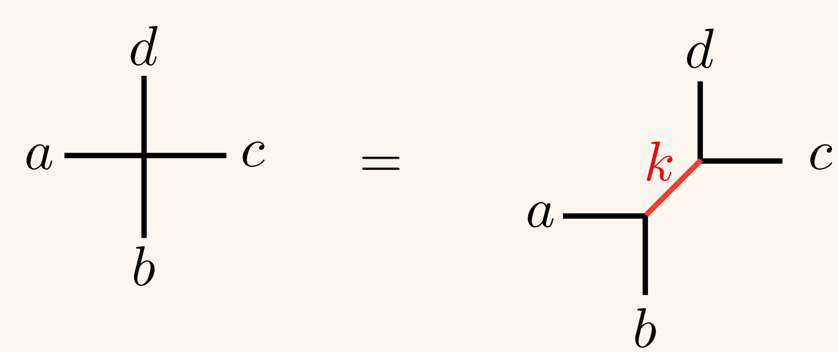
◉ Anisotropic TRG (ATRG)

[D. Adachi, T. Okubo, and S. Todo. arXiv:1906.02007]

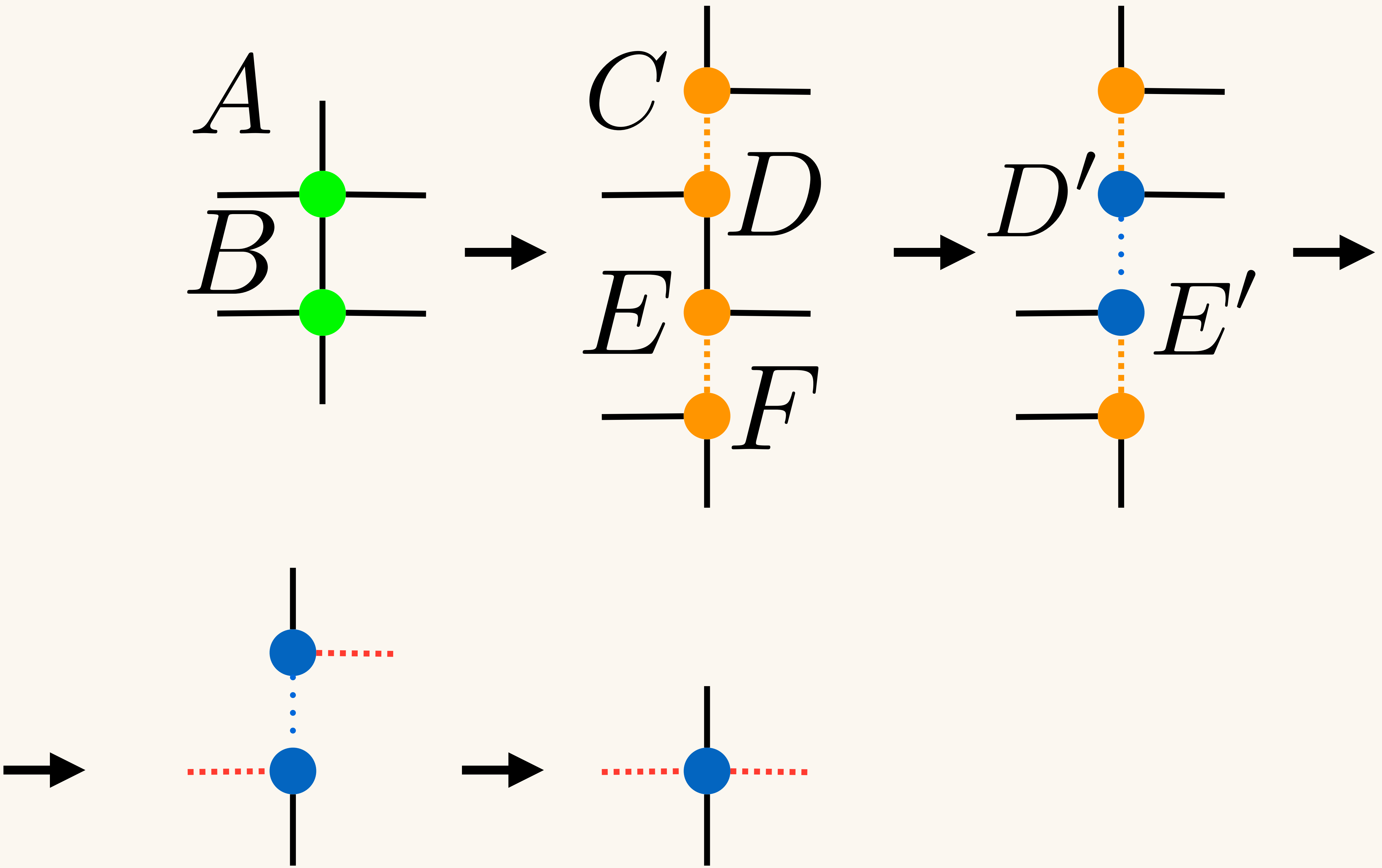


◇ 追加の分解でテンソルのランクを落とす

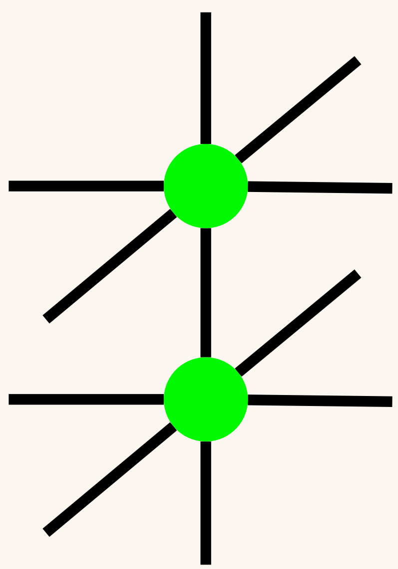
$$O(D^{4\mathrm{dim}-1}) \to O(D^{2\mathrm{dim}+1})$$



◉ ATRG



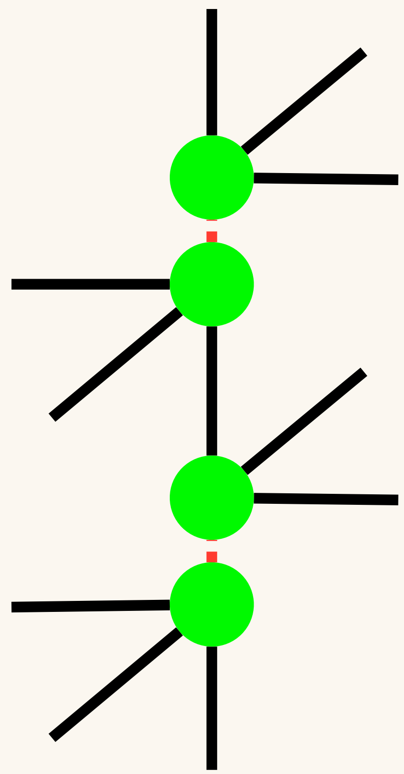
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

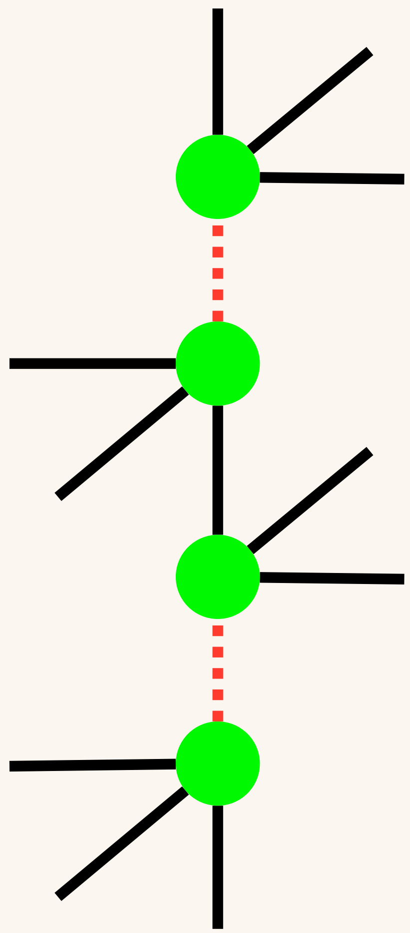
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

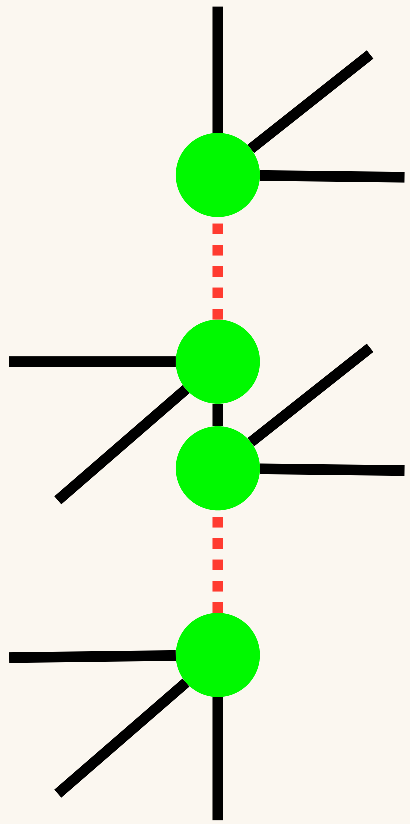
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

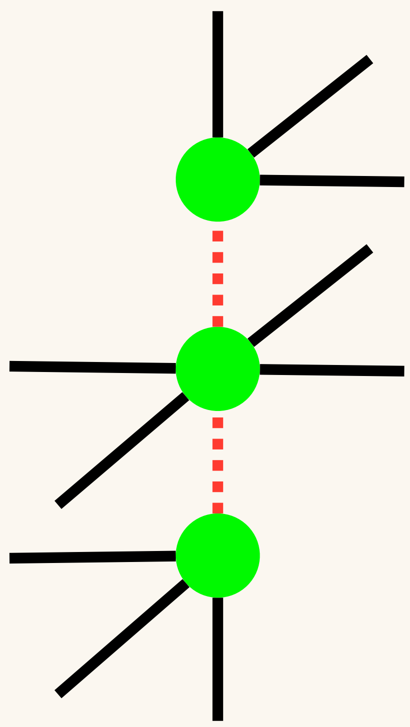
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

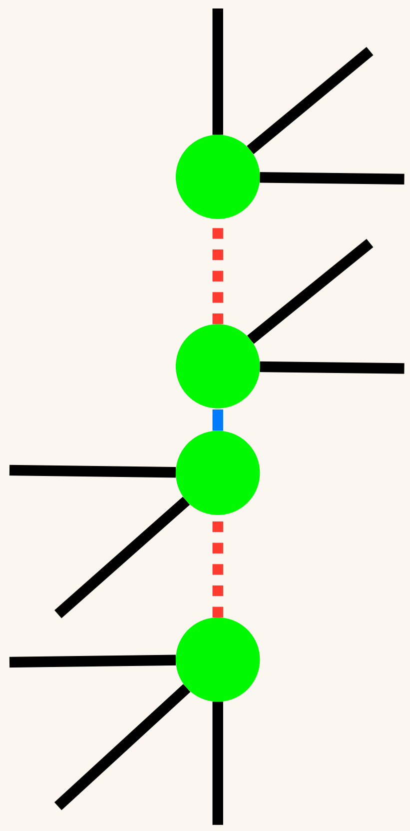
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

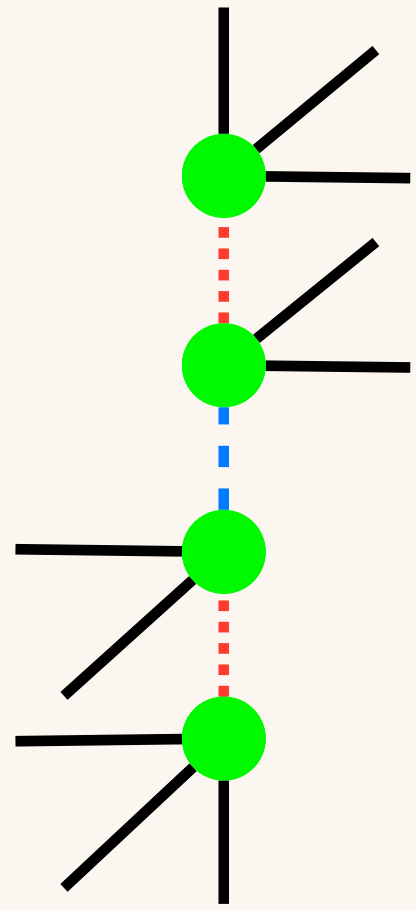
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

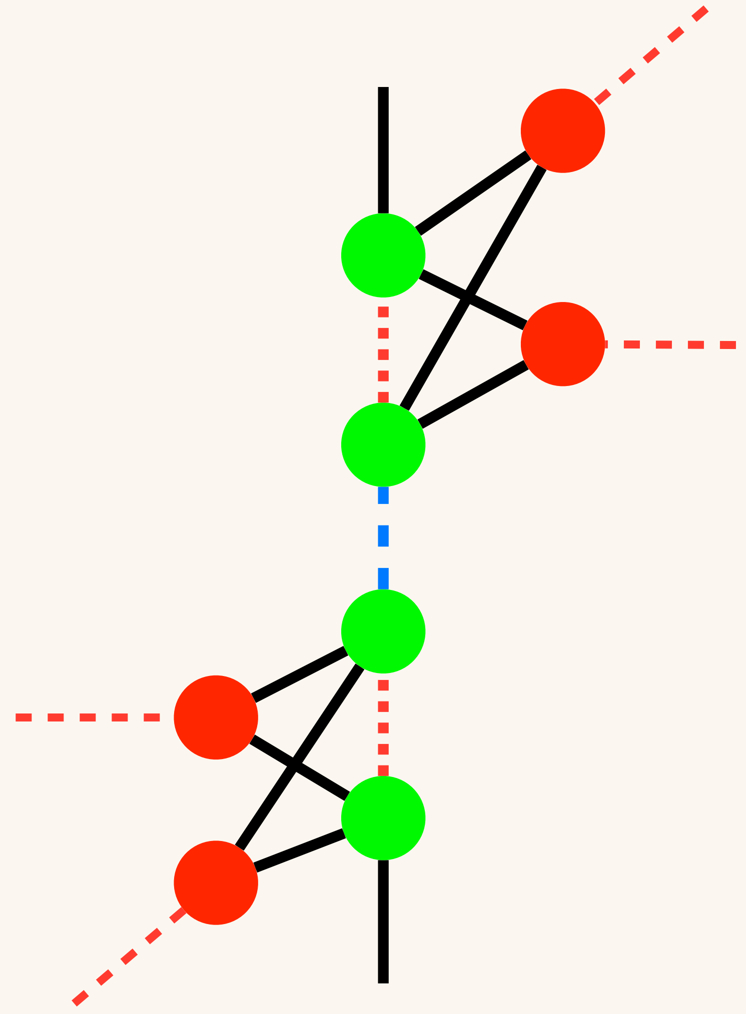
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

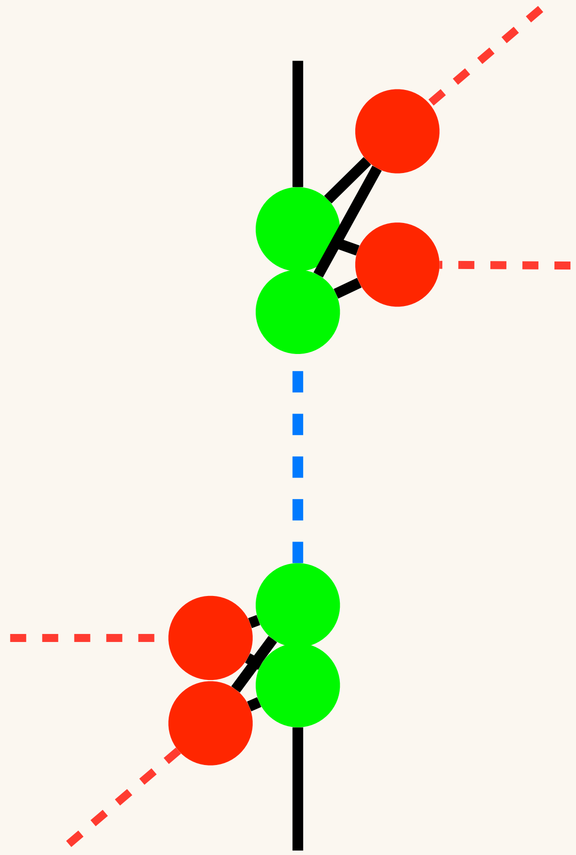
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

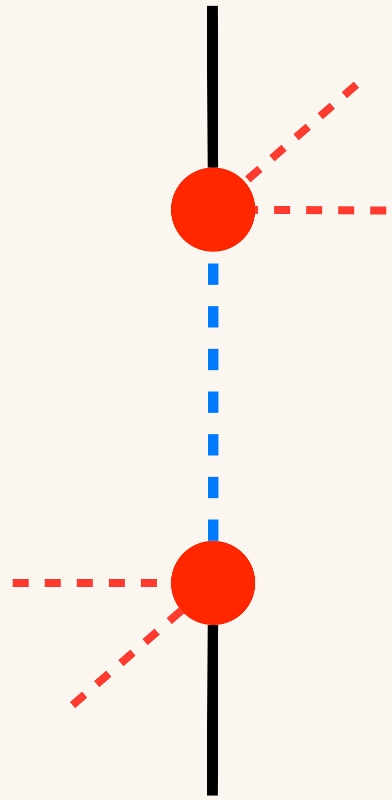
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

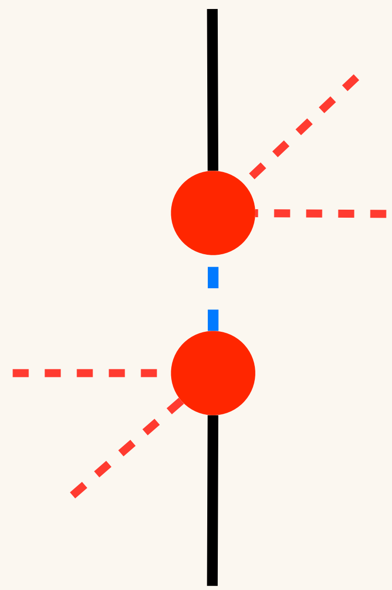
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

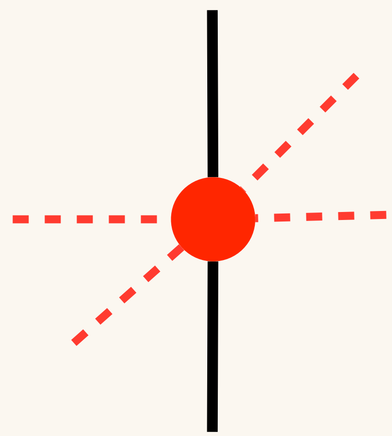
◉ ATRG



→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

◉ ATRG

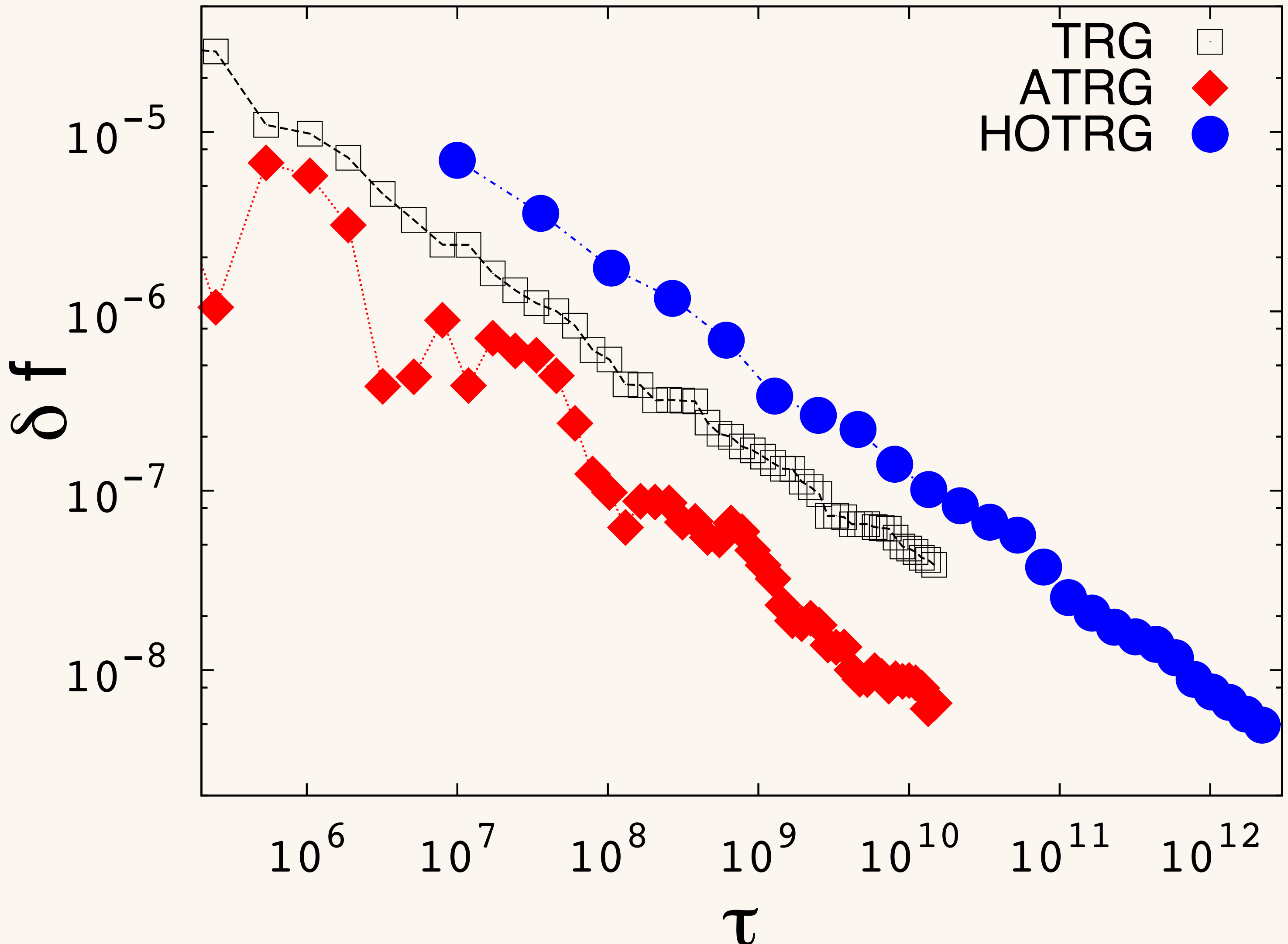


→ 分解や縮約が必ず隣り合ったものとで行われてる。

(全体のIsometryを準備しなくても計算できる)

◉ Numerical costs for ATRG

[D. Adachi, T. Okubo, and S. Todo. arXiv:1906.02007]



$$\tau = \begin{cases} D^5 & \text{for TRG and ATRG} \\ D^7 & \text{for HOTRG} \end{cases}$$

→ 計算量のスケール仕方が削減できている。

追加の分解における打ち切りで同じDでの精度は落ちる。

◉ Triad TRG

[D. Kadoh and K.N. arXiv:1912.02414]

→ 分解で計算量削減

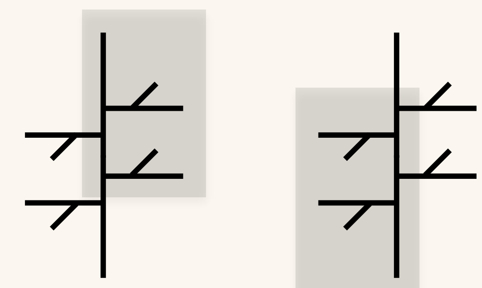
近似
SVD(Isometry)

精度改善

計算量削減
追加分解

打ち切りSVD

近似範囲

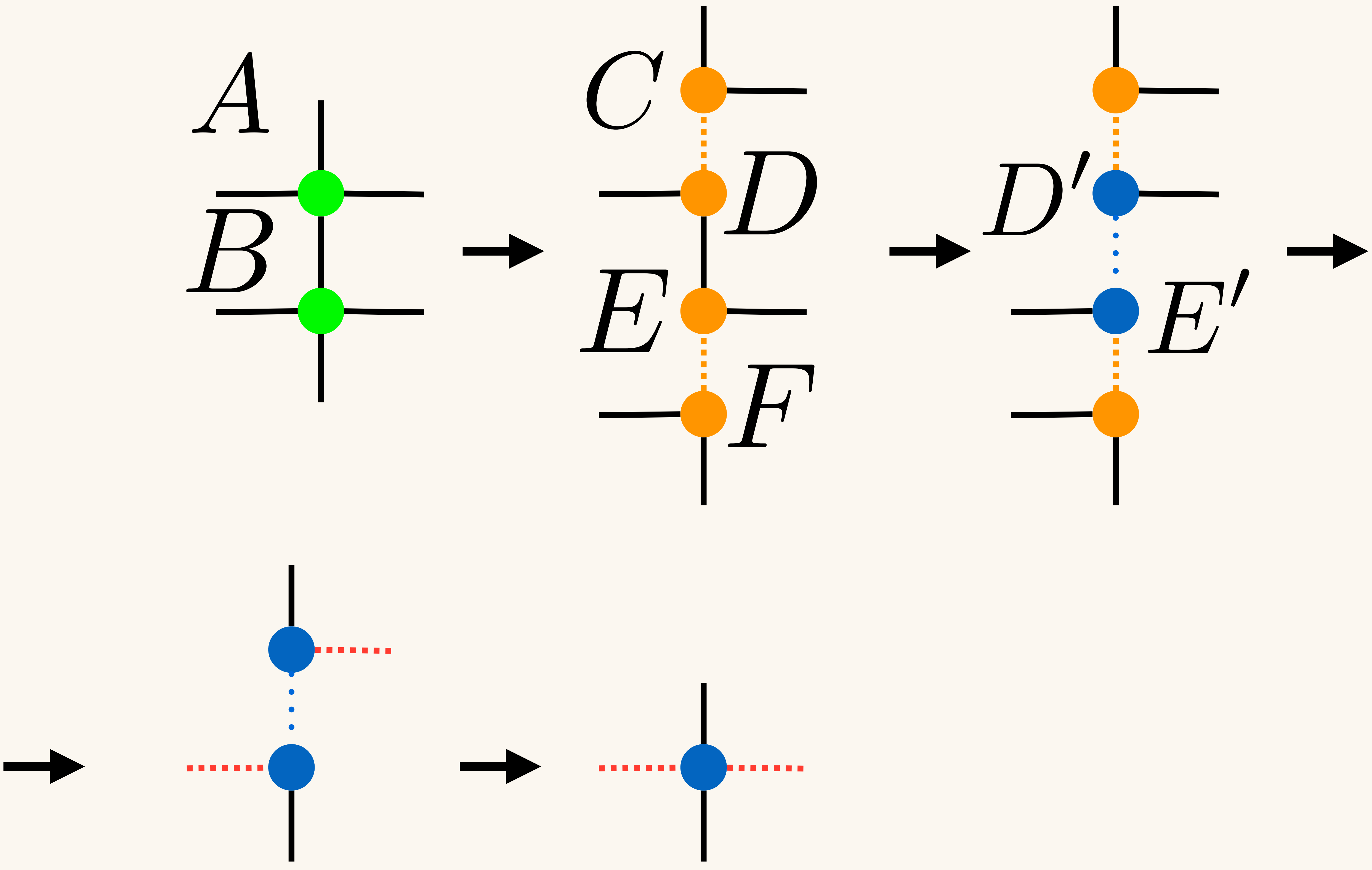


+打ち切り縮約

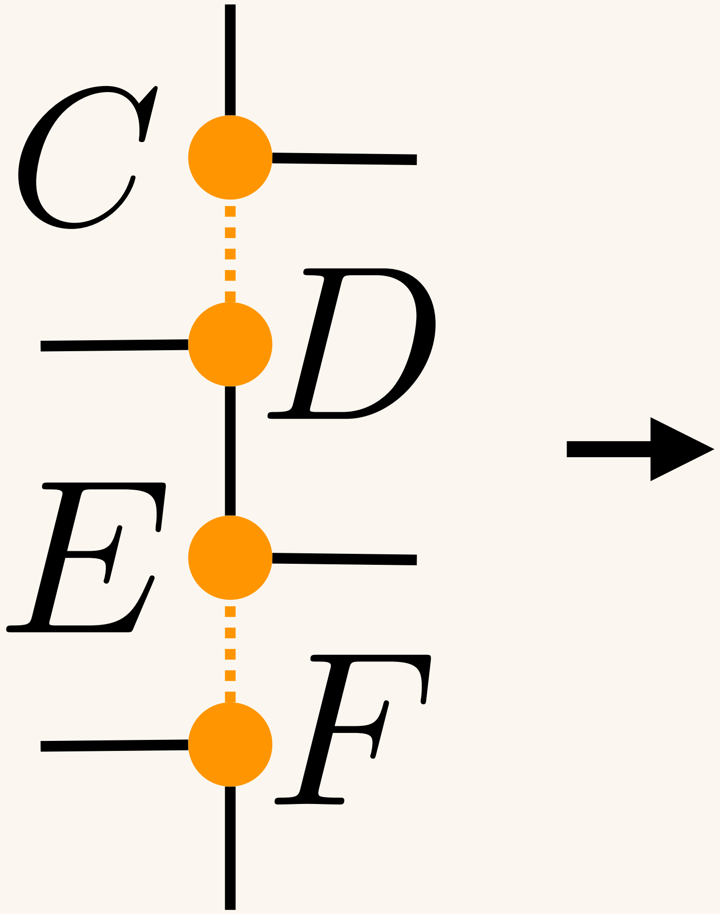
→ HOTRGをTriad表現を基本として、

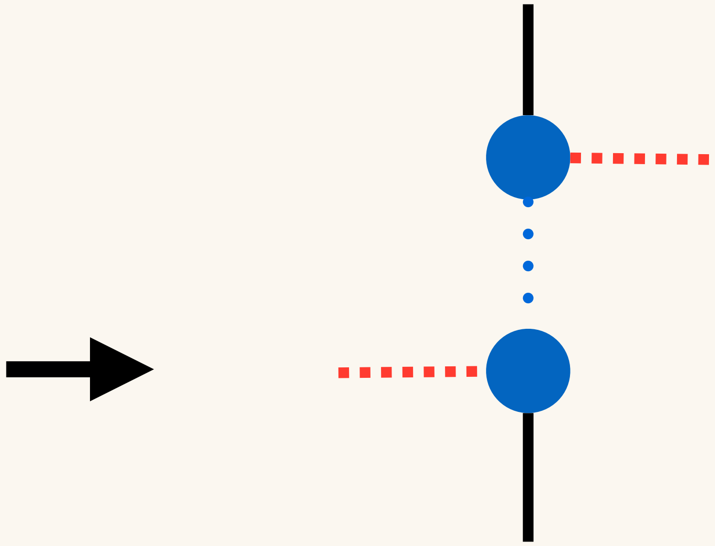
一部を除いて(swapしない)、分解、縮約を局所的に行う

ATRG



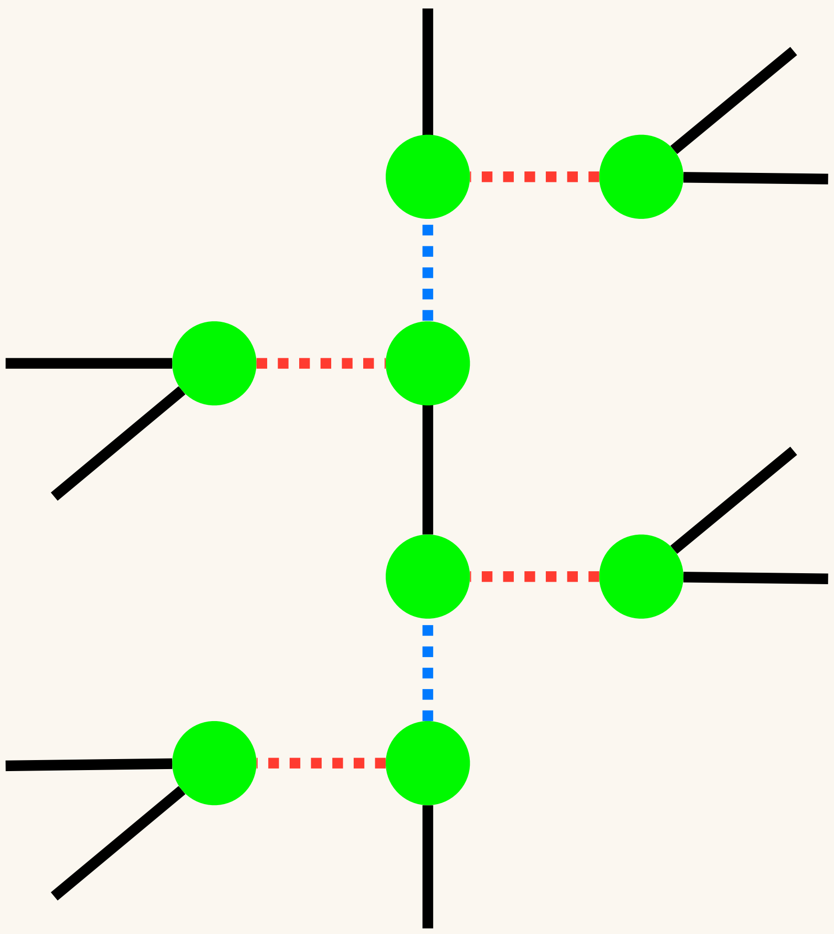
◉ Triad TRG





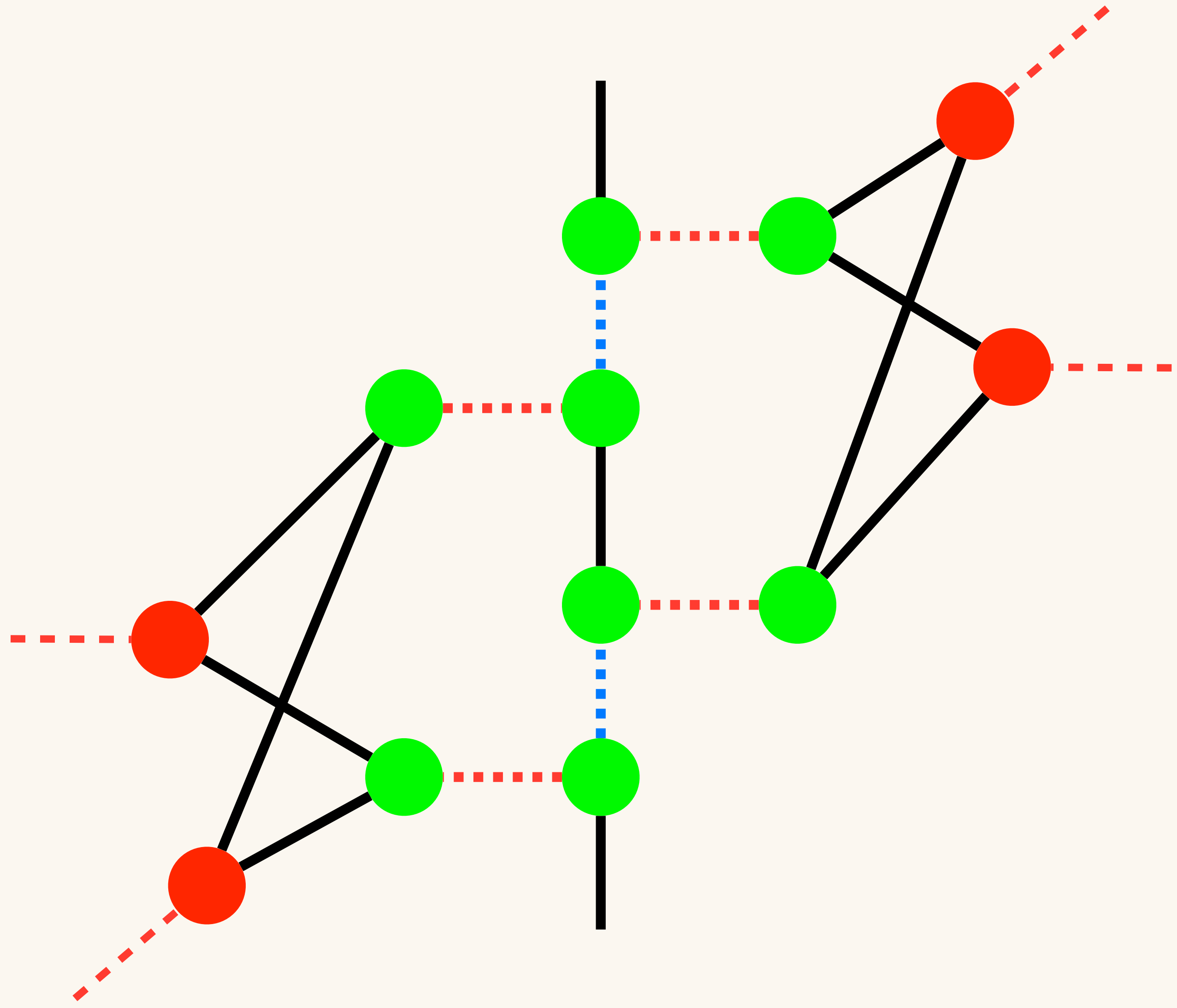
→ 2次元の場合はATRGの単純化(swapなし)にも見える。

◉ Triad TRG

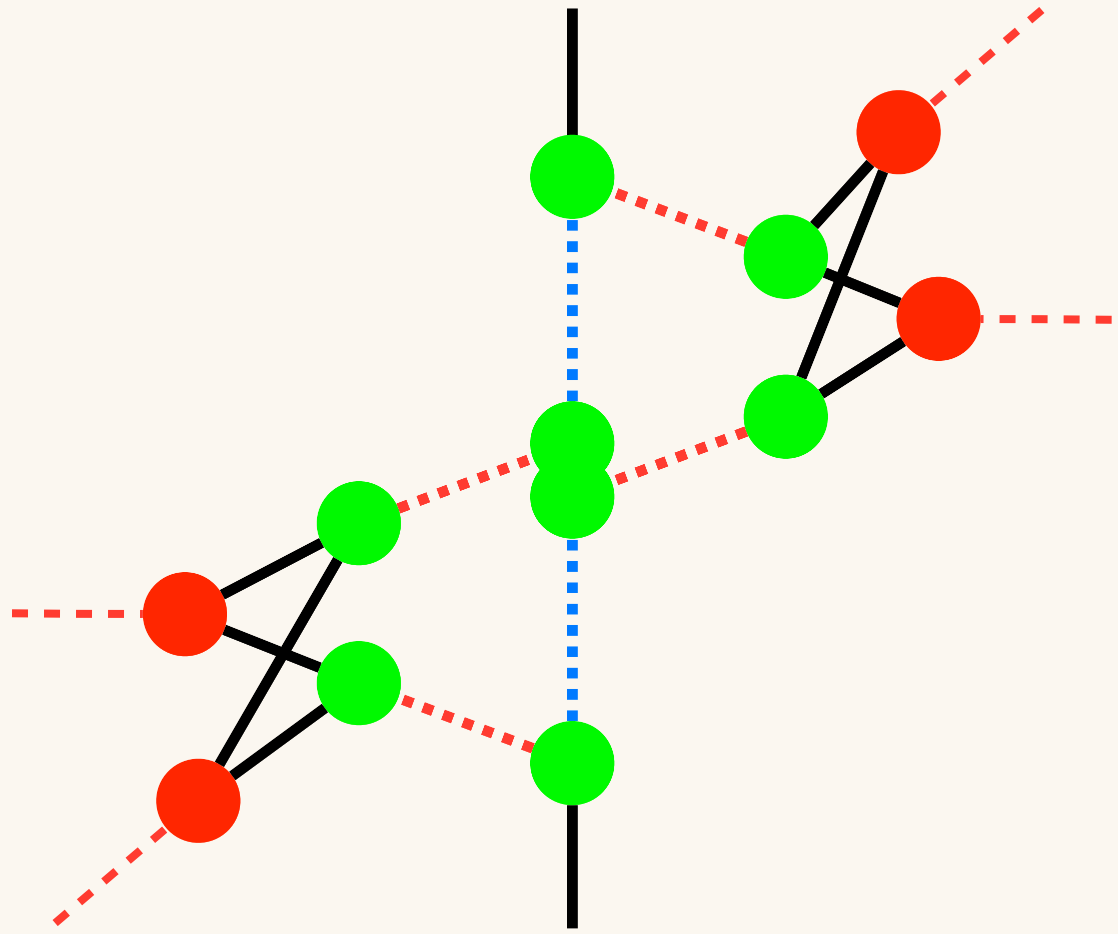


→ 3次元の場合は複雑。

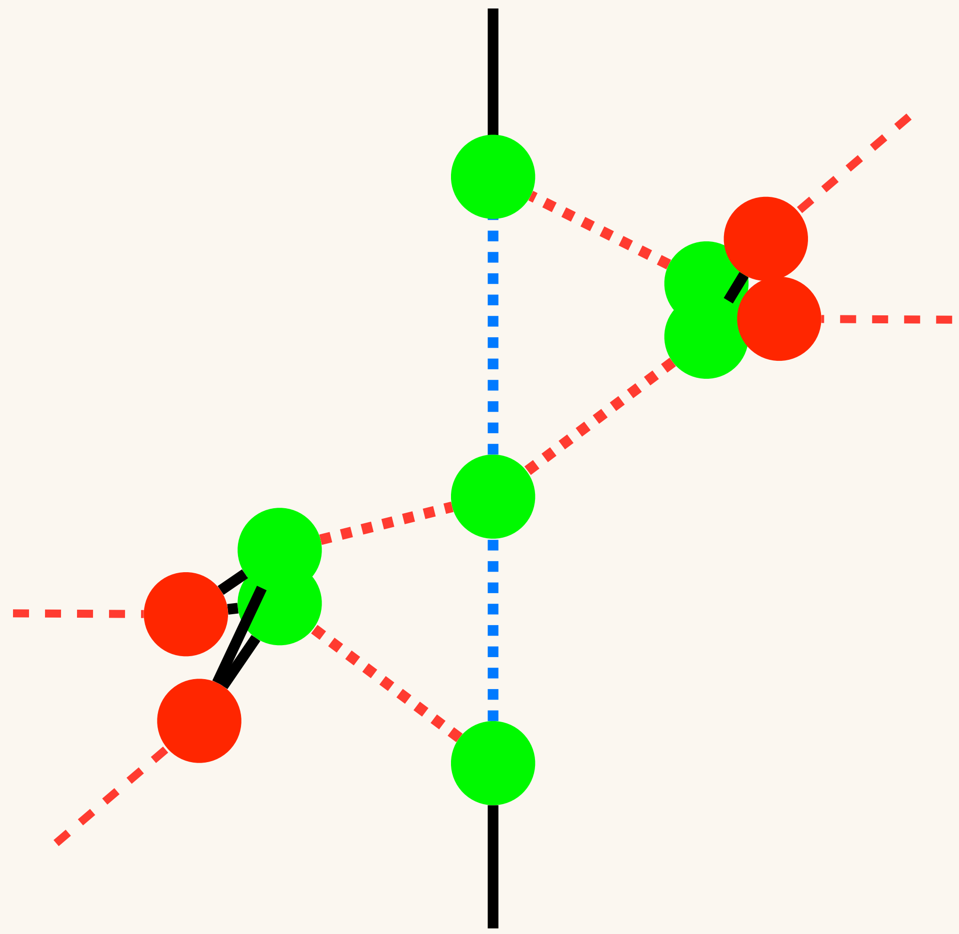
◉ Triad TRG



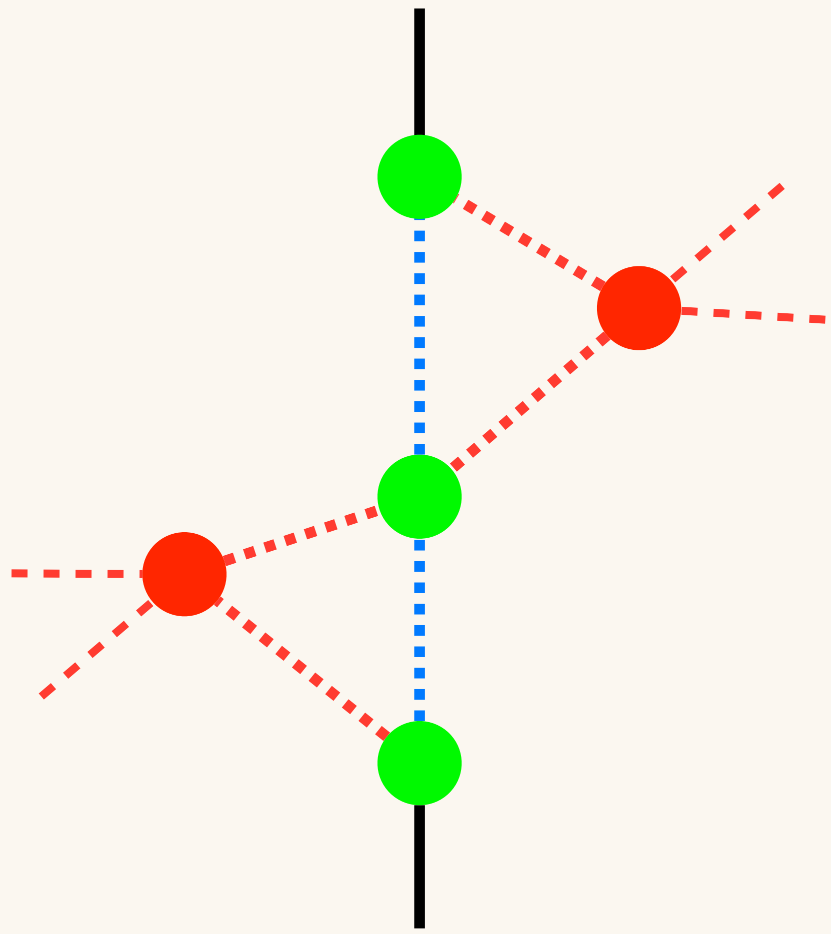
◉ Triad TRG



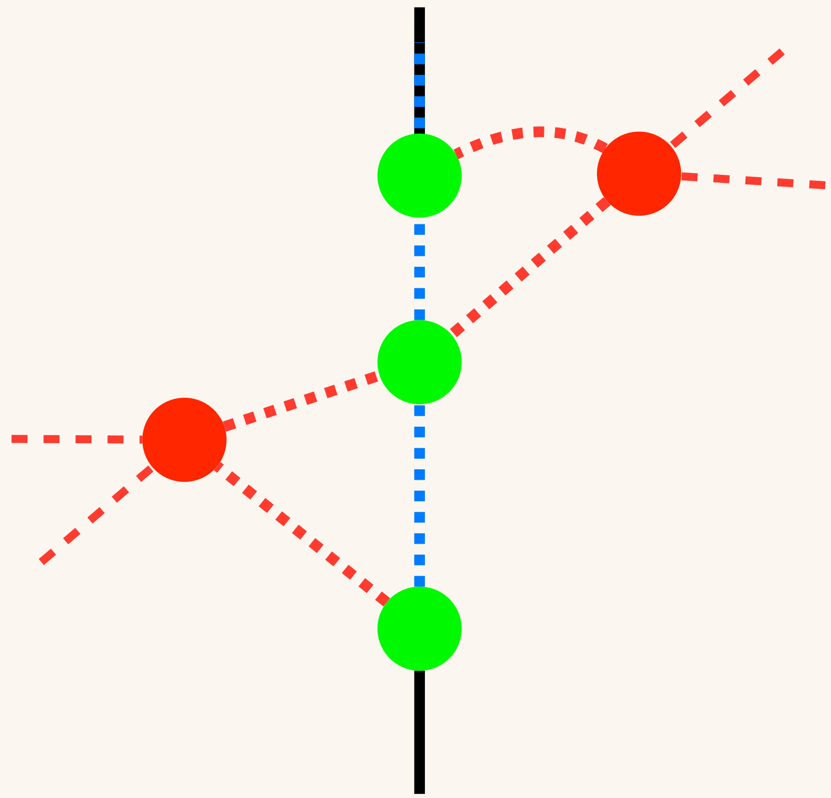
◉ Triad TRG



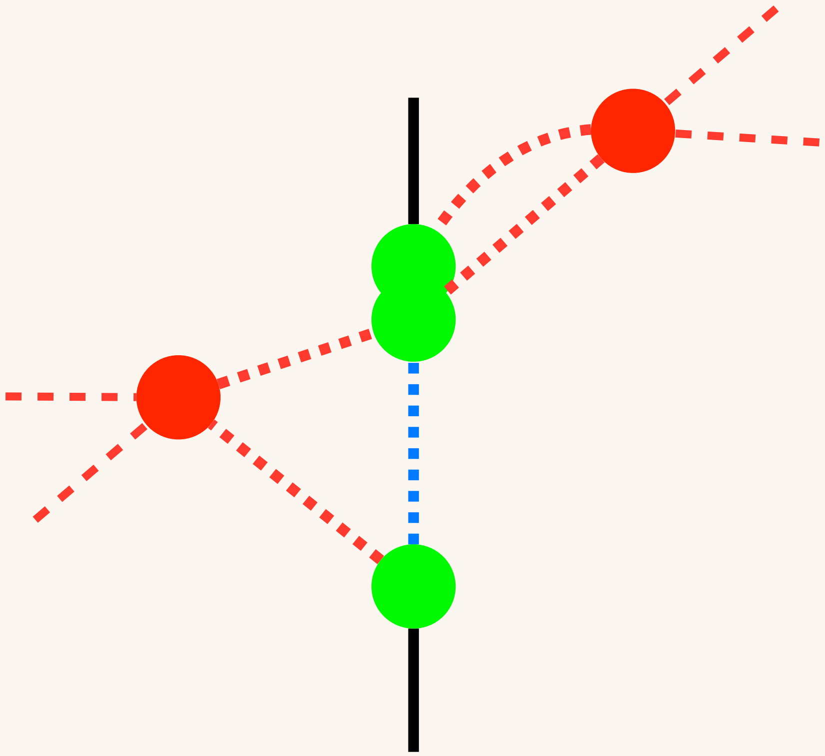
◉ Triad TRG



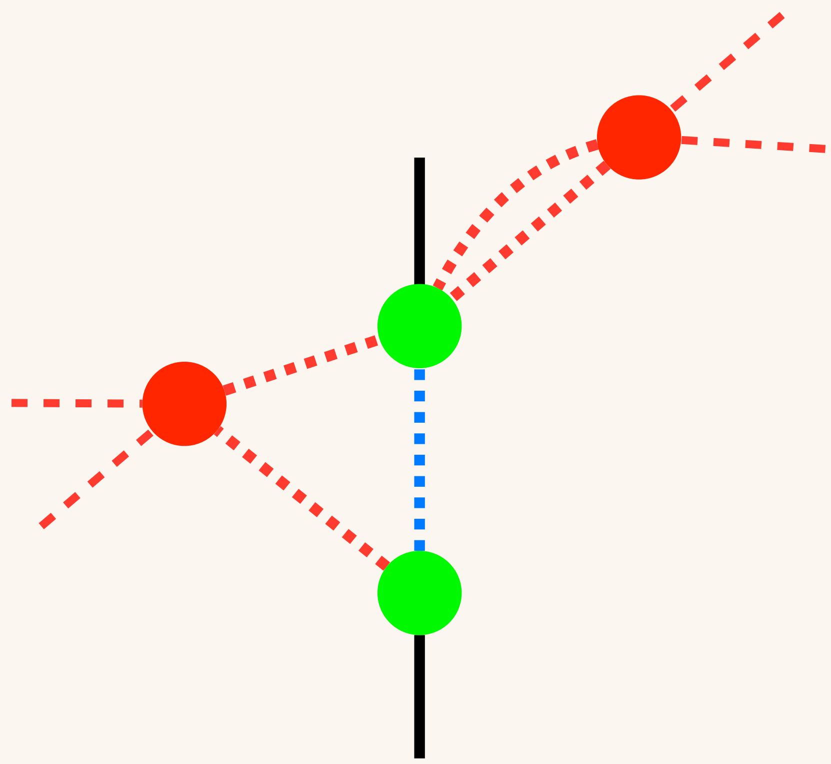
◉ Triad TRG



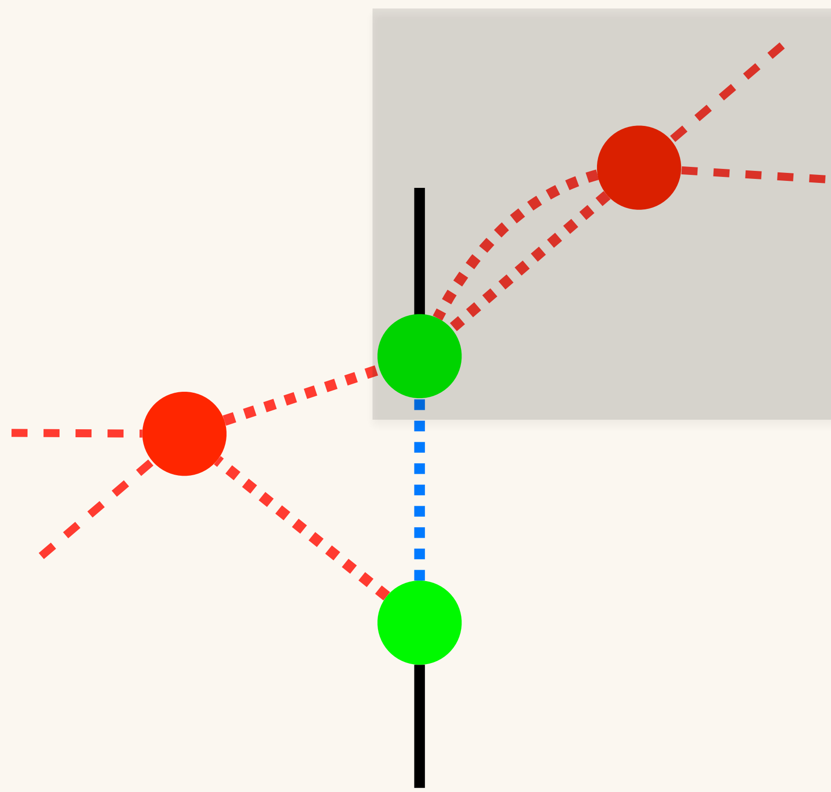
Triad TRG



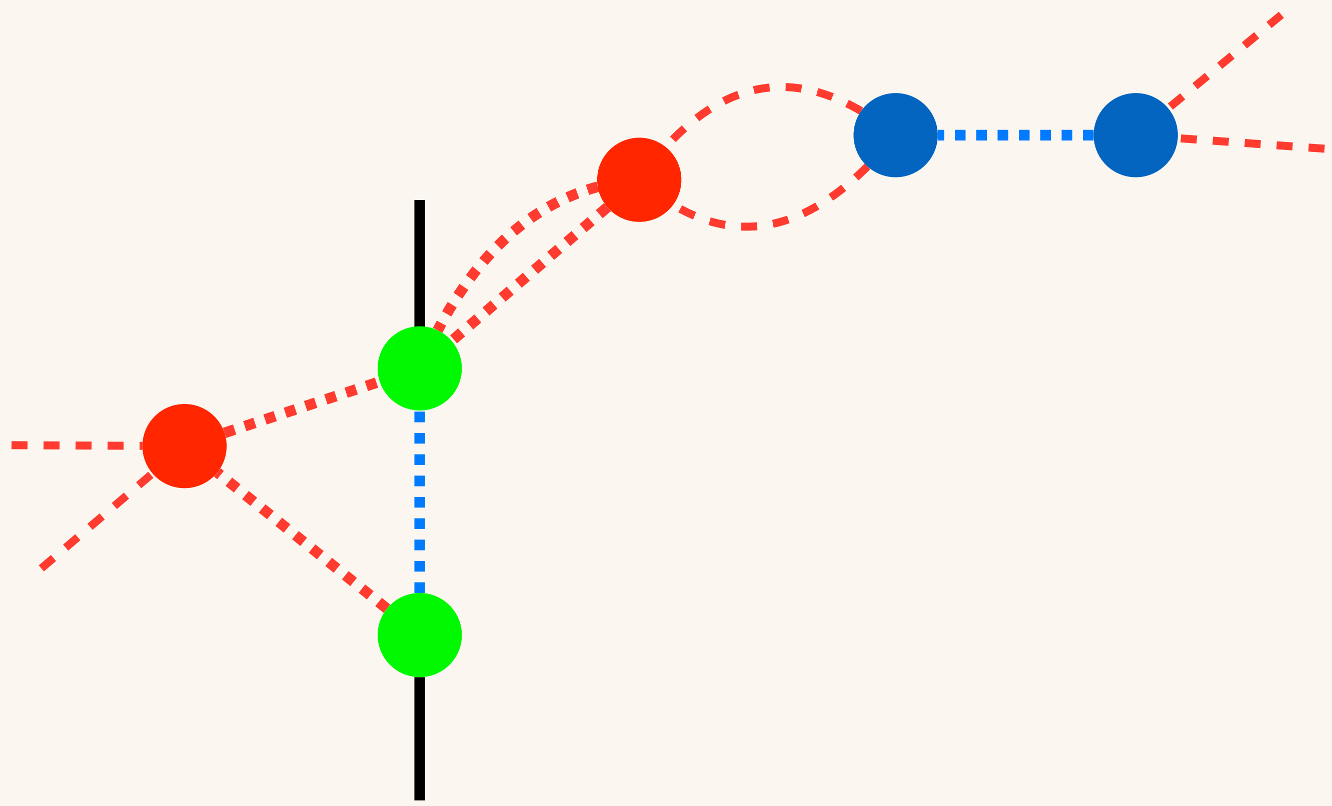
Triad TRG



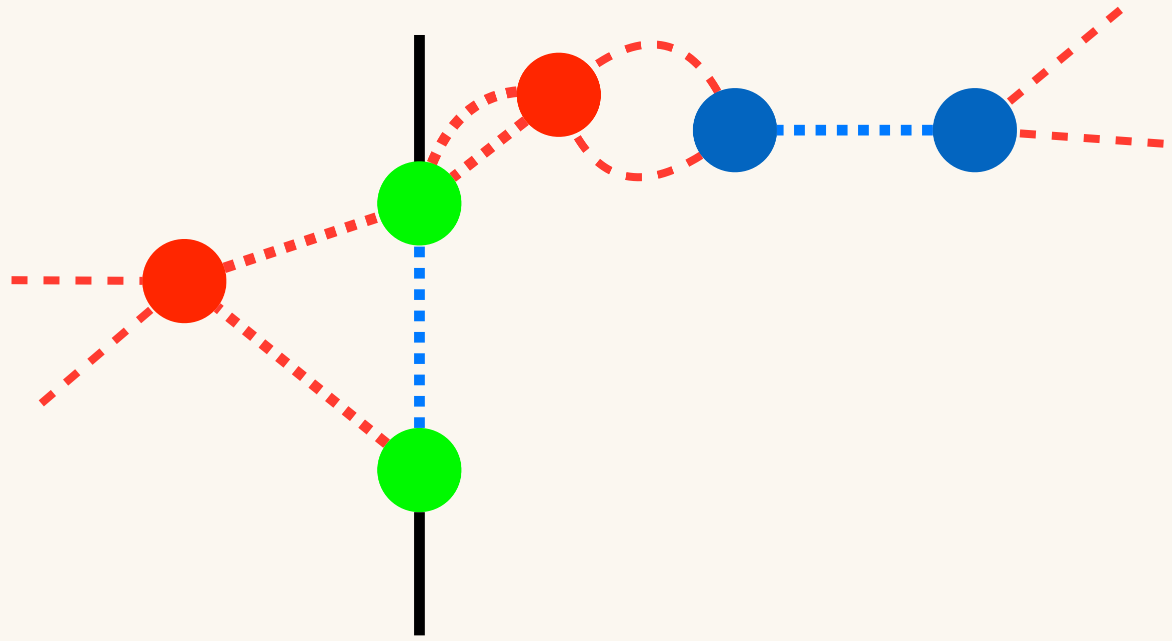
◉ Triad TRG



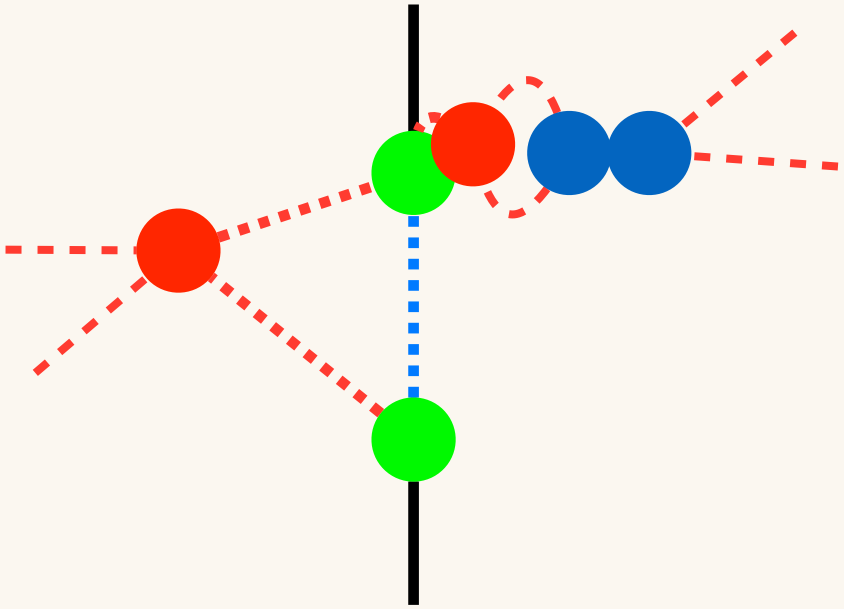
◉ Triad TRG



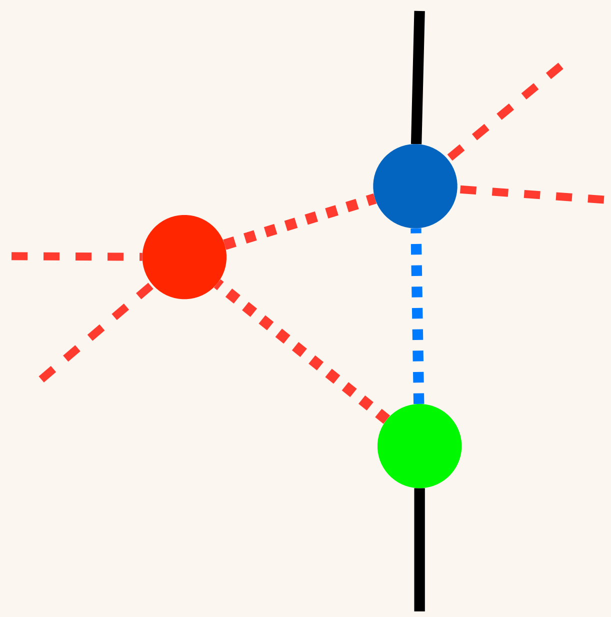
◉ Triad TRG



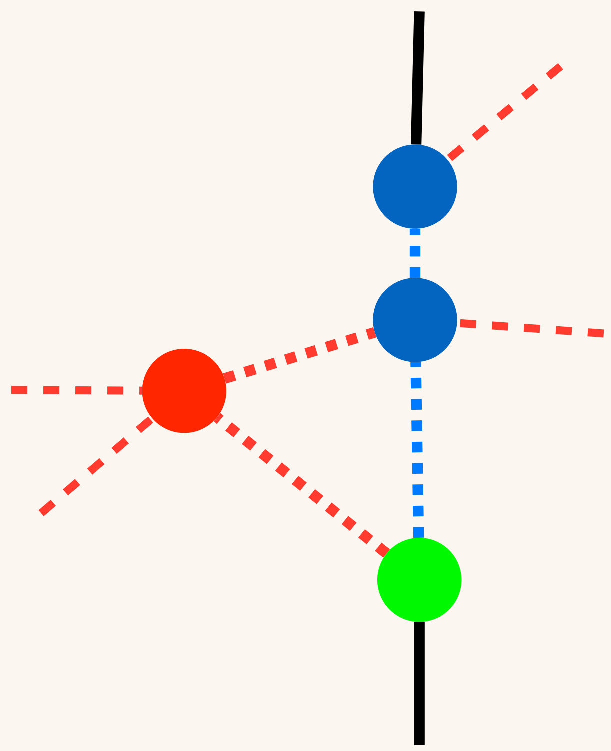
◉ Triad TRG



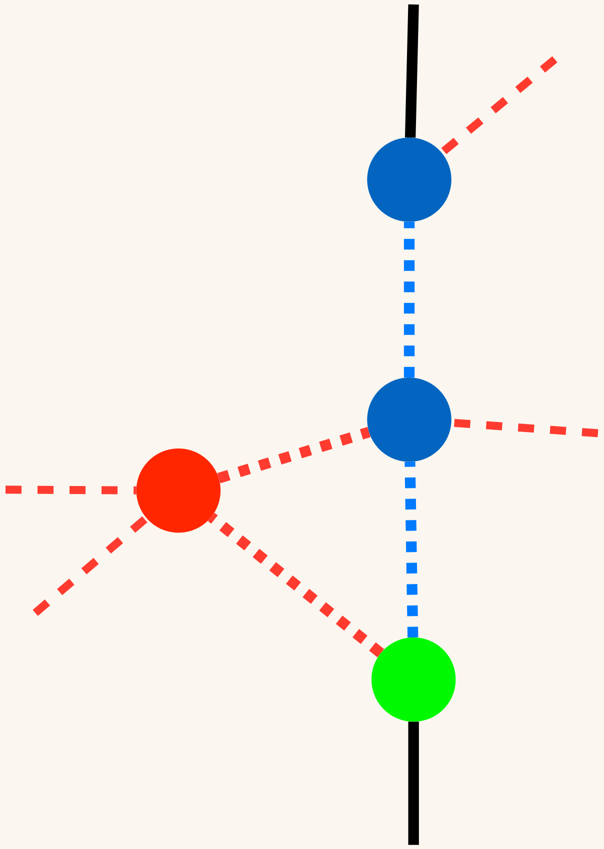
◉ Triad TRG



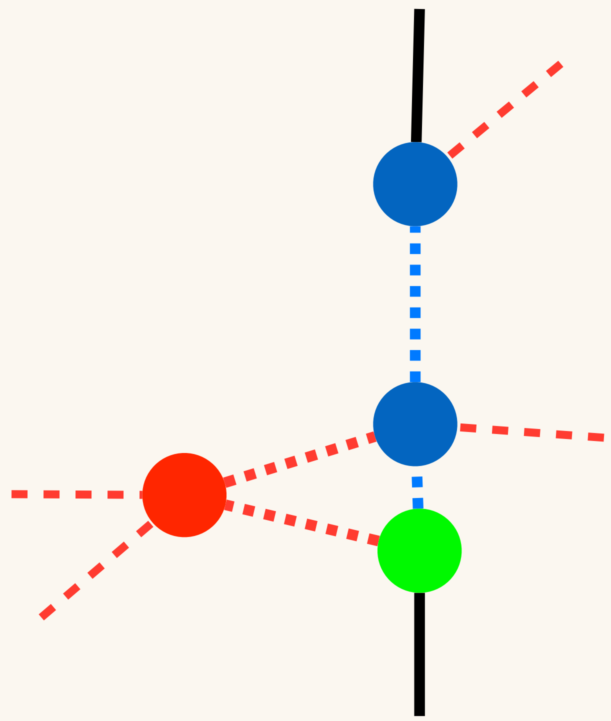
◉ Triad TRG



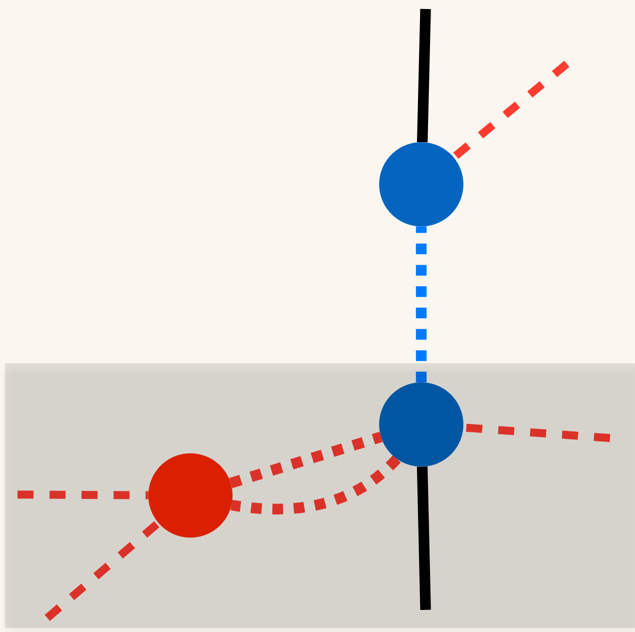
◉ Triad TRG



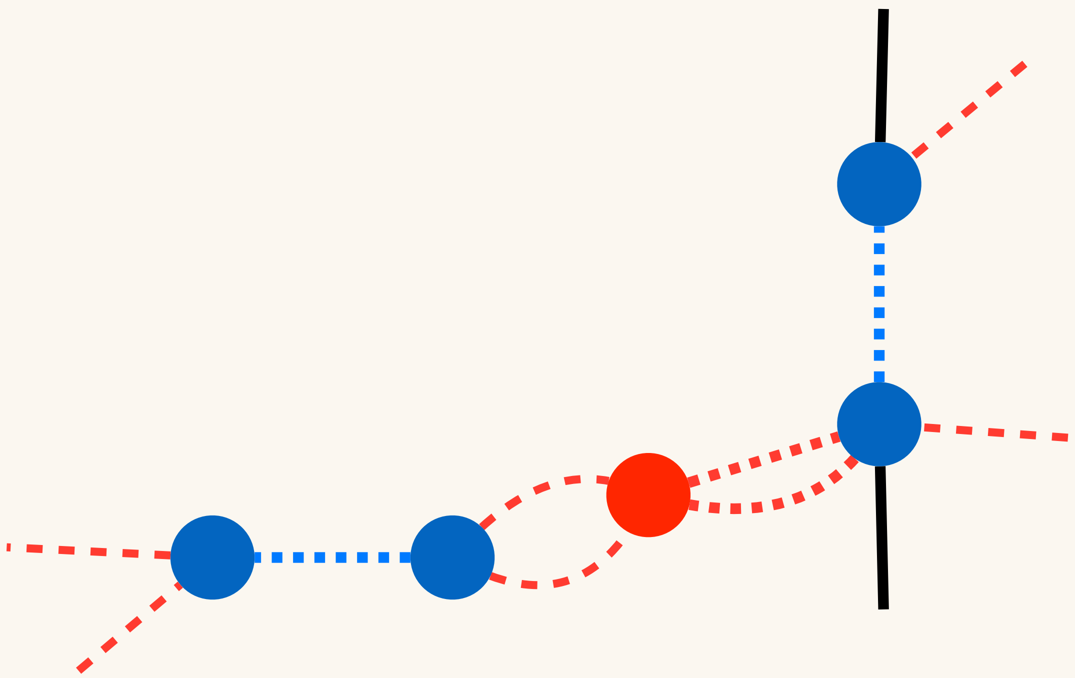
◉ Triad TRG



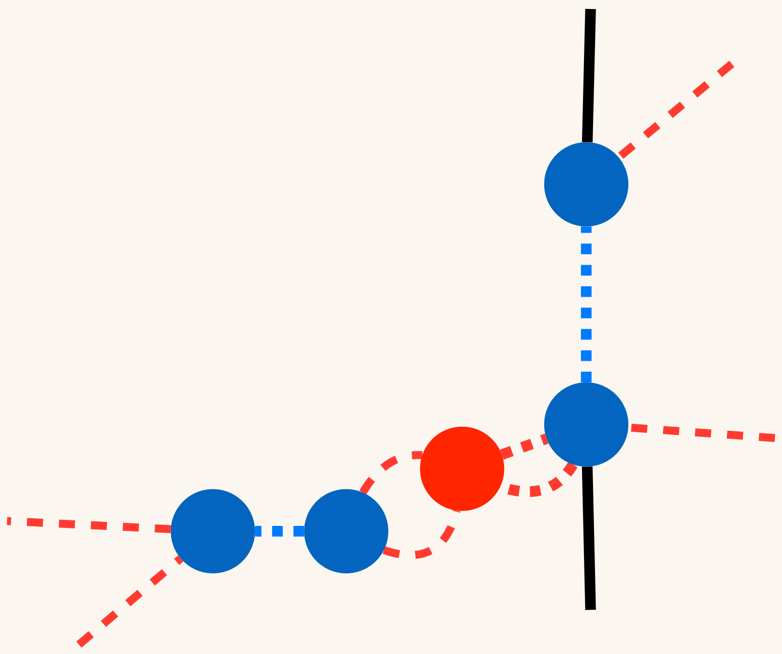
◉ Triad TRG



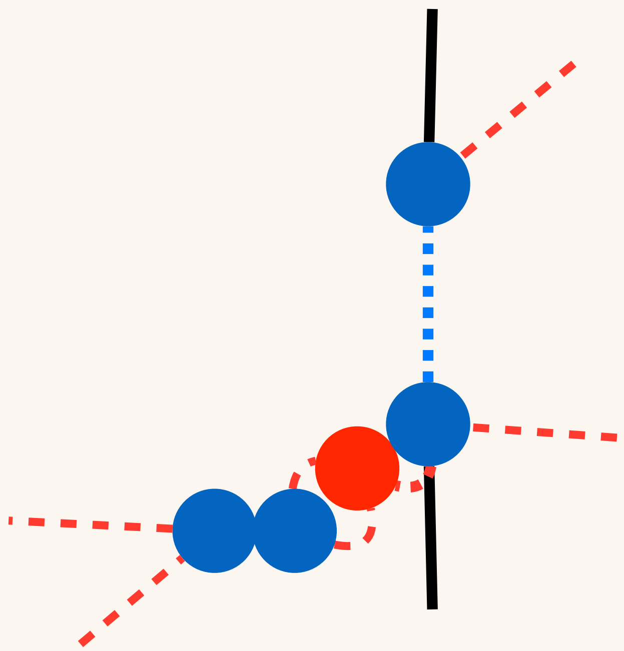
◉ Triad TRG



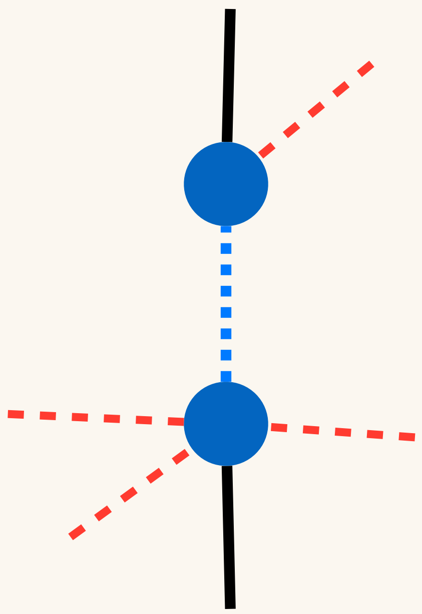
◉ Triad TRG



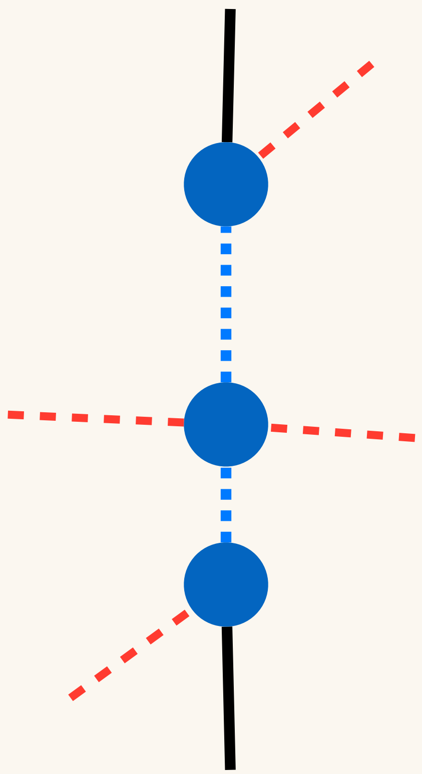
◉ Triad TRG



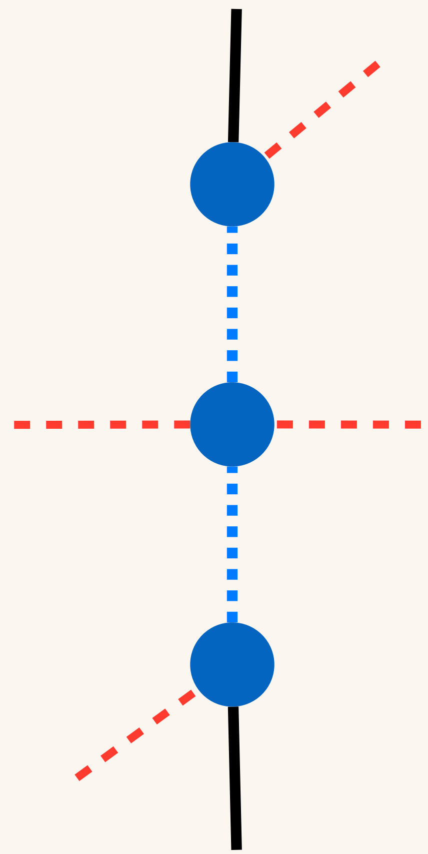
◉ Triad TRG



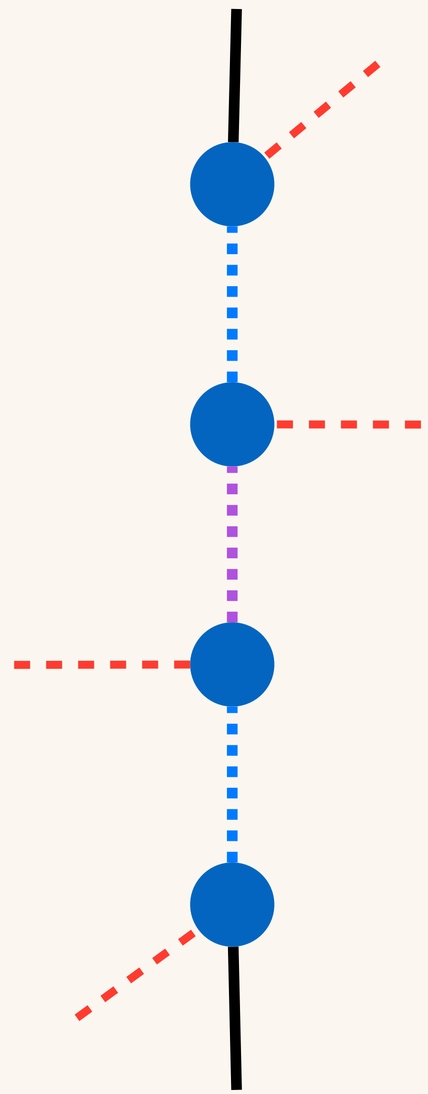
◉ Triad TRG



◉ Triad TRG



◉ Triad TRG

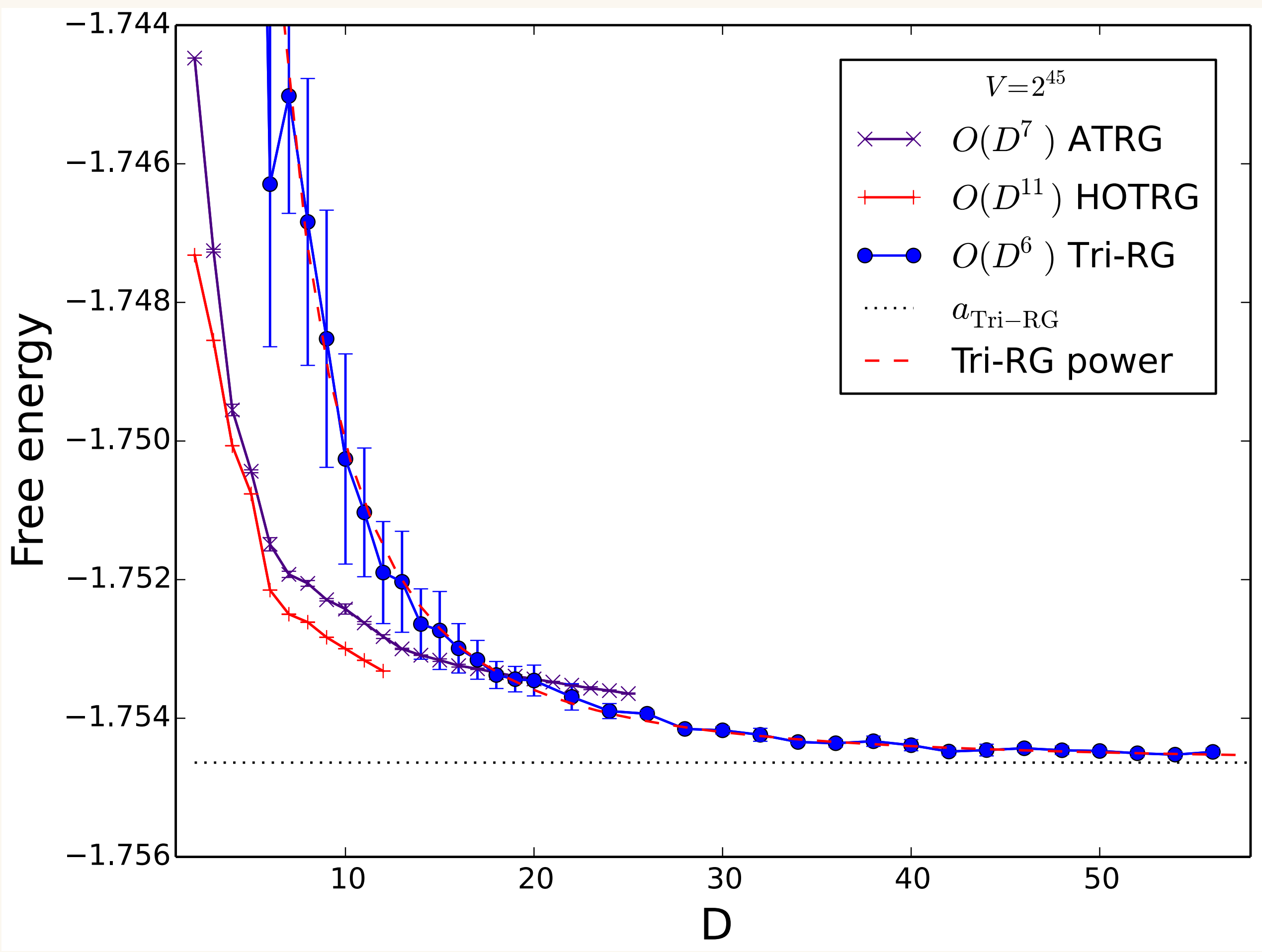


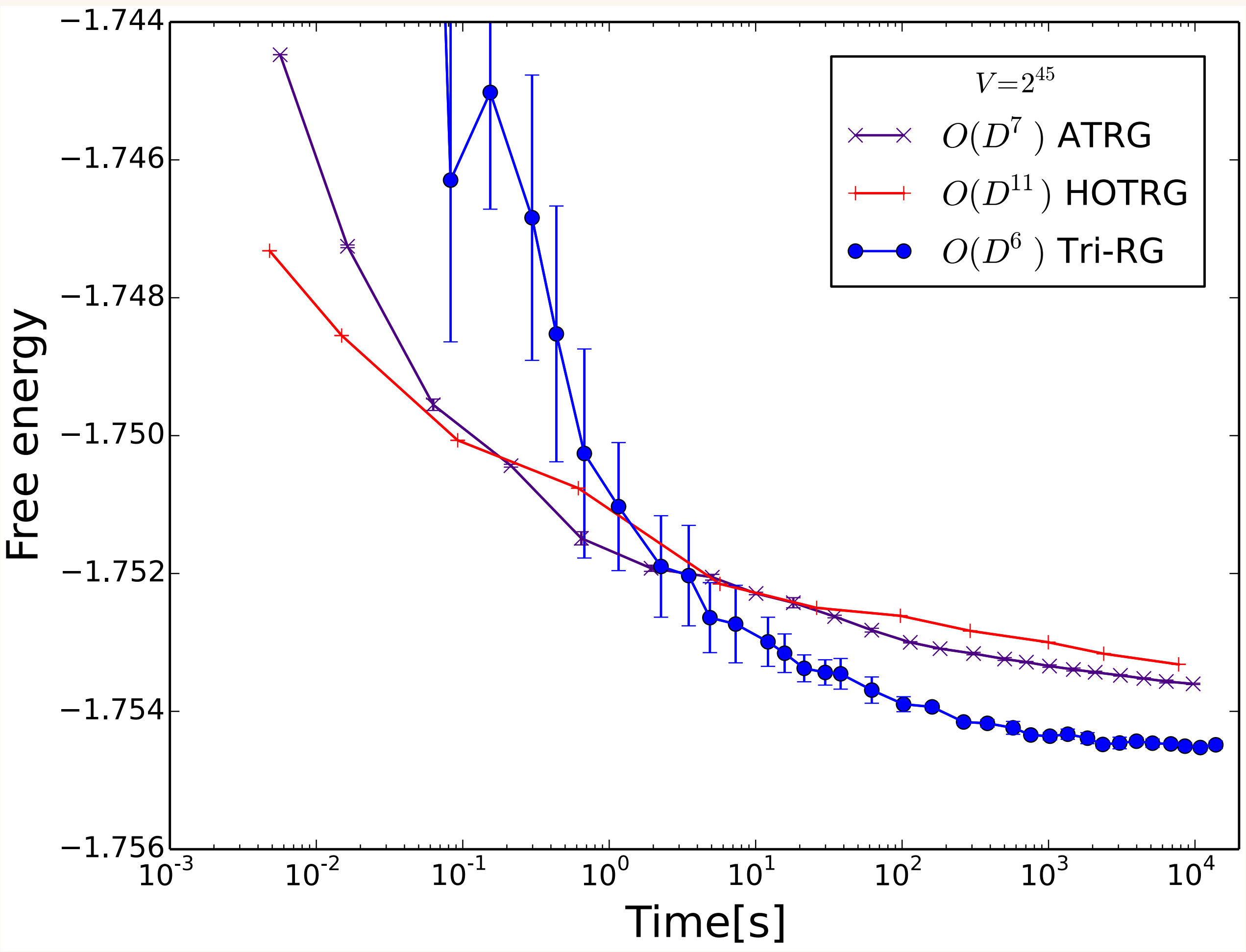
◉ Triad RG

◇ Triad rep. reduces the cost [D. Kadoh and K.N. arXiv:1912.02414]

$$O(D^{4\mathrm{dim}-1}) \to O(D^{\mathrm{dim}+3})$$

◇ 3-dim Ising



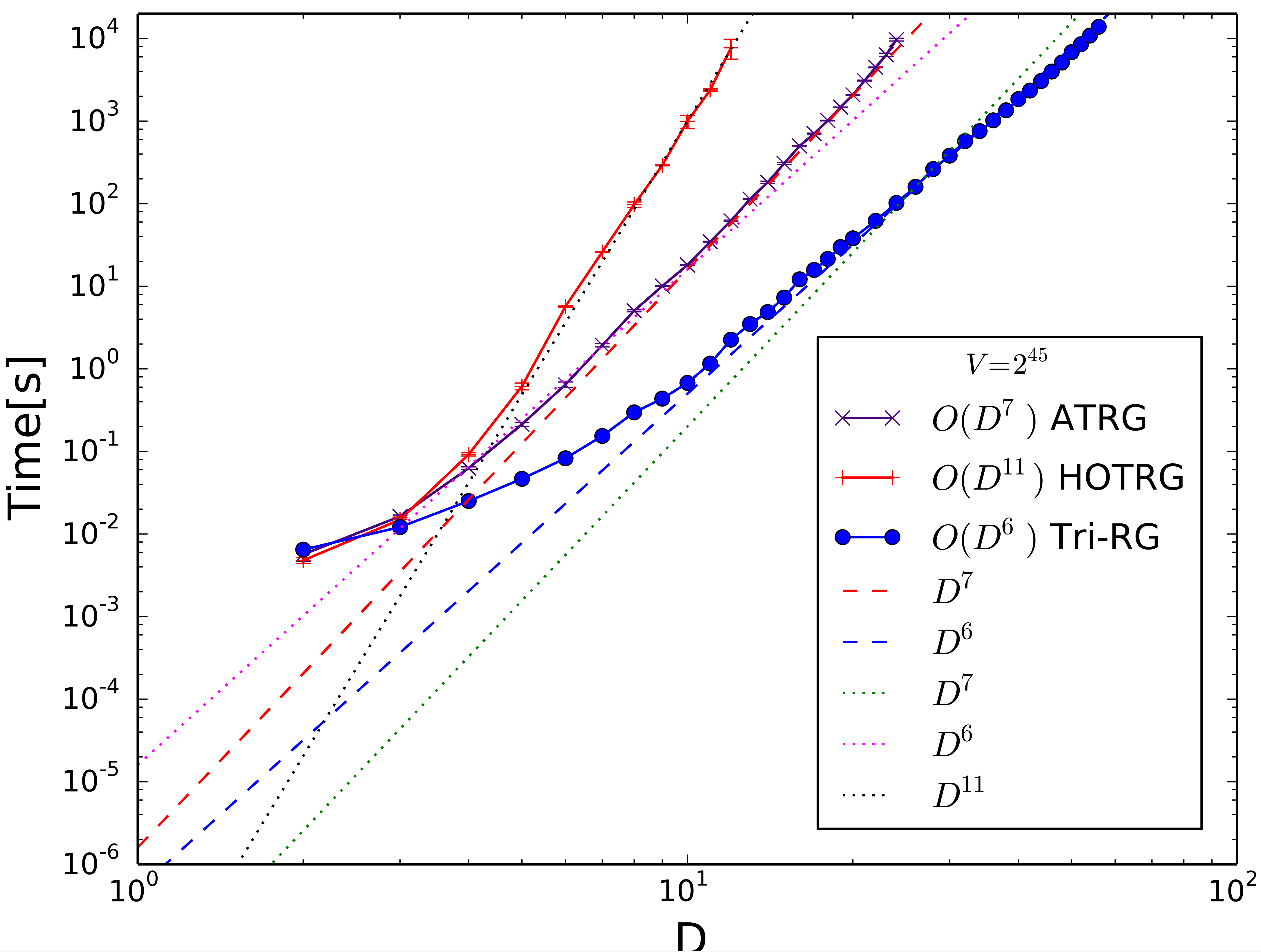


→ 計算量のスケール仕方が削減できている。

追加の分解における打ち切りで同じDでの精度は落ちる。

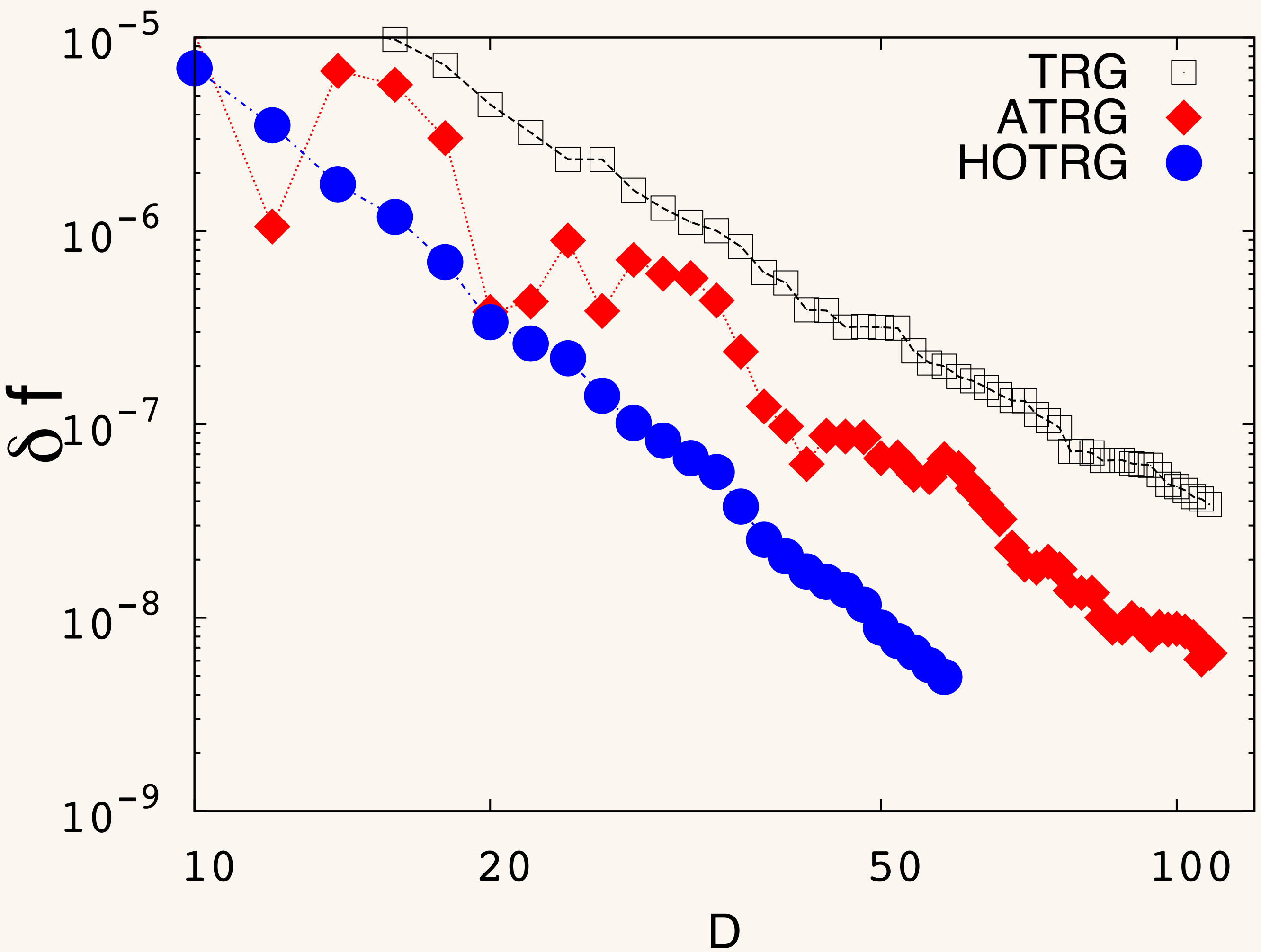
Triad RG

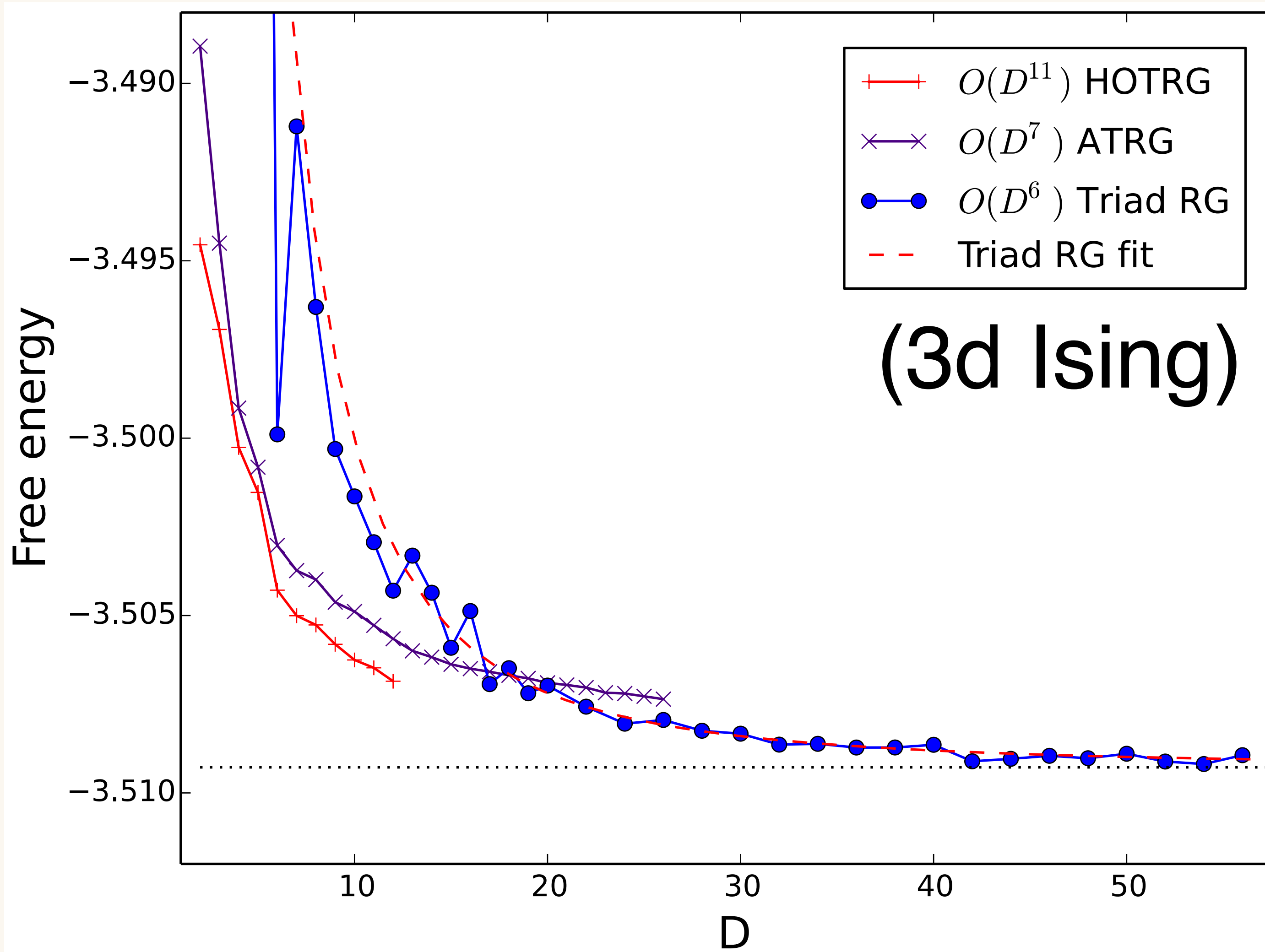
[D. Kadoh and K.N. arXiv:1912.02414]



◉ Free energy density of 3d-Ising model

[D. Adachi, T.Okubo, S. Todo. arXiv:1906.02007]





[D. Kadoh, K.N. arXiv:1912.02414]

→ 追加の分解は追加の系統誤差を与える

◉ Motivation: 系統誤差の起源

◇ HOTRG [Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

系統誤差: 射影テンソル (Isometry)

計算量: $O(D^{4d-1})$

d :空間次元

D :打ち切り添字サイズ

◇ Anisotropic TRG(ATRG) [D. Adachi, T.Okubo, S. Todo. arXiv:1906.02007]

系統誤差: (射影テンソル), 追加の分解, 乱拓SVD (R-SVD)

計算量: $O(D^{2d+1})$

◇ TriadTRG (TTRG) [D. Kadoh, K.N. arXiv:1912.02414]

系統誤差: 射影テンソル, 追加の分解, R-SVD

計算量: $O(D^{d+3})$

→ HOTRGにRandomized-SVDを使うとどうなるのか？

→ 追加の分解からくる系統誤差を減らせないか？

◉ Motivation: 系統誤差の起源

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計算量: $O(D^{d+3})$

→ HOTRGにRandomized-SVDを使うとどうなるのか？

→ 追加の分解からくる系統誤差を減らせないか？

◉ HOTRG with R-SVD

	with R-SVD	w/o R-SVD
◇ HOTRG	?	$O(D^{4d-1})$
◇ ATRG	$O(D^{2d+1})$	$O(D^{3d})$
◇ TTRG	$O(D^{d+3})$	$O(D^{d+4})$

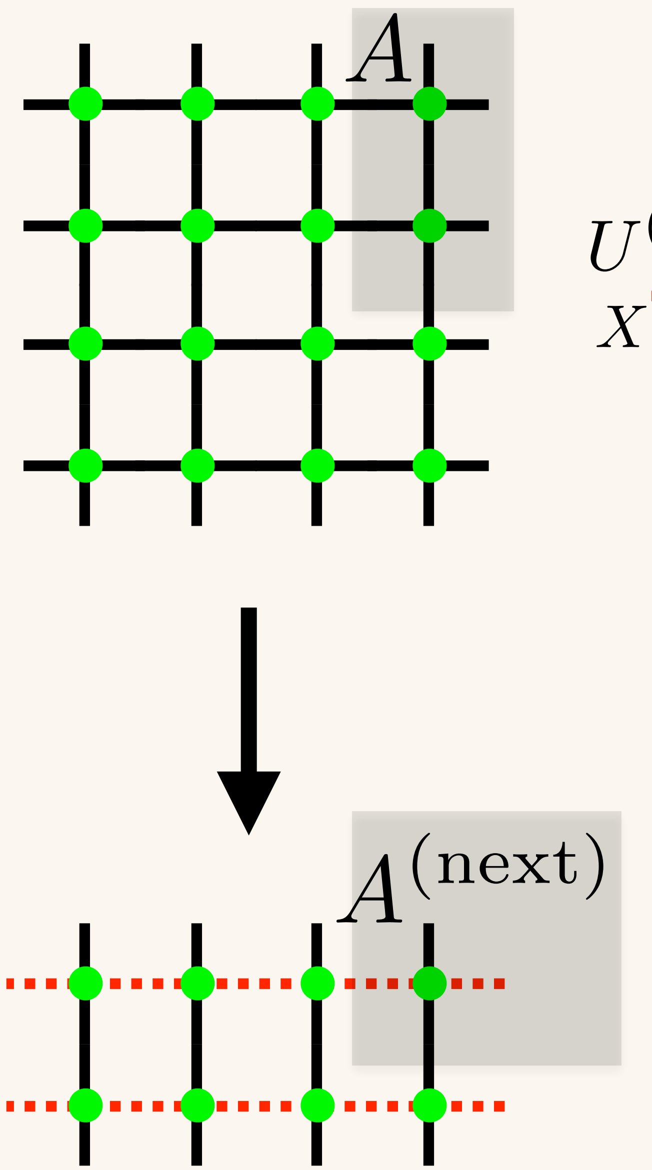
→ まずはHOTRGにR-SVDを適用してみる。

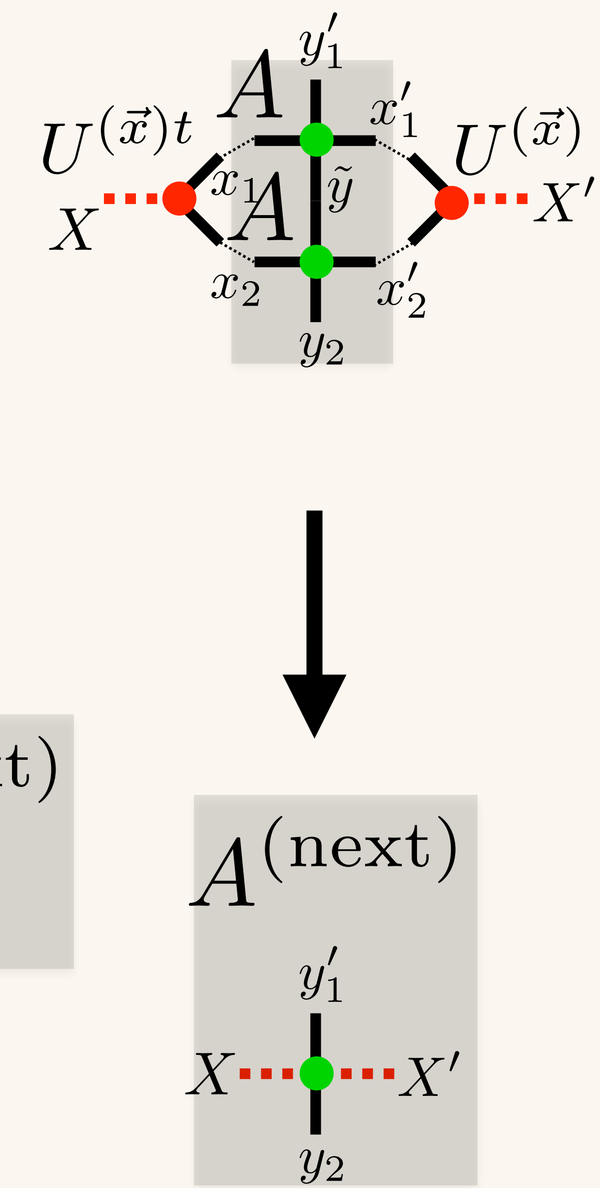
HOTRG with randomized SVD

◉ Higher-Order TRG (HOTRG)

[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

◇ 射影テンソルUを用いた近似的縮約





$$\Gamma^{(AA)} = AA \to A^{(\mathrm{next})}$$

→$U^{(\vec{x})}$は$\Gamma\Gamma^t$ のSVDから得る

$$[\Gamma\Gamma^t]_{[x_1 x_2][x_1^t x_2^t]} = \sum_{k=1}^{D^2} U^{(x)}_{[x_1 x_2]k} \lambda_k U^{(x)}_{[x_1^t x_2^t]k}$$

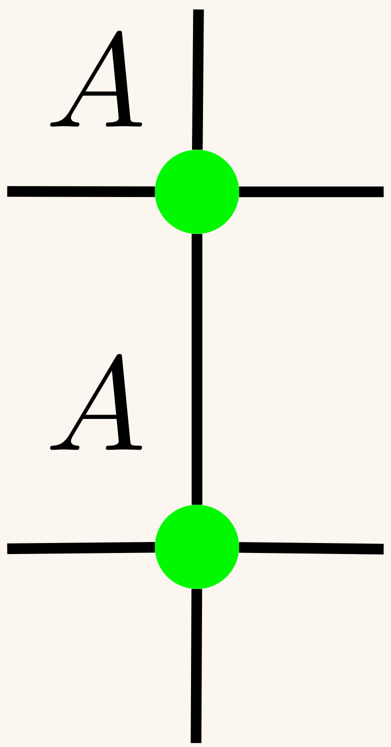
SVD打ち切り: $D^2 \to D$

射影テンソルの計算量:$O(D^6)$

$$U^t AAU = A^{(\mathrm{next})}$$

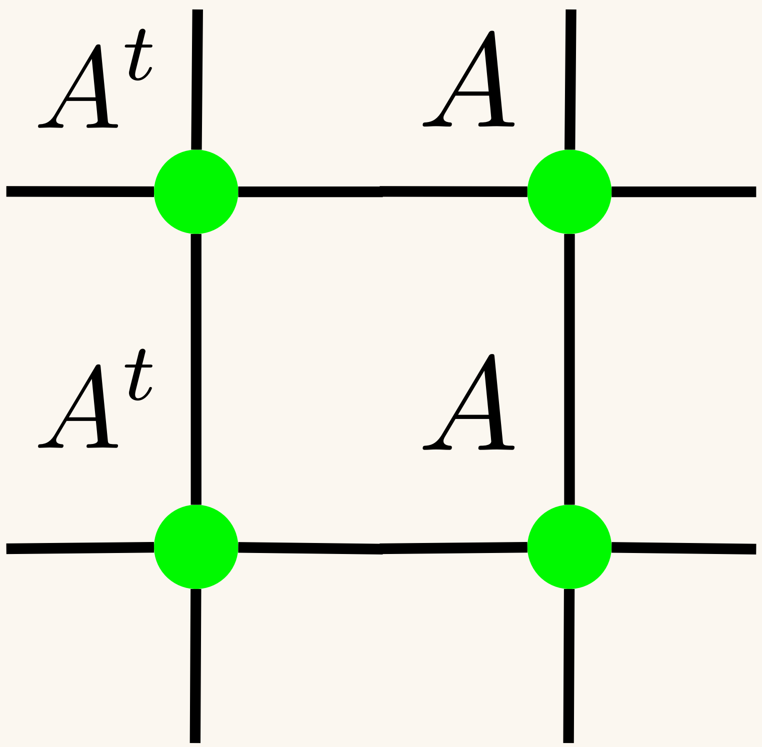
縮約の計算量: $O(D^7)$

HOTRG: Isometry step



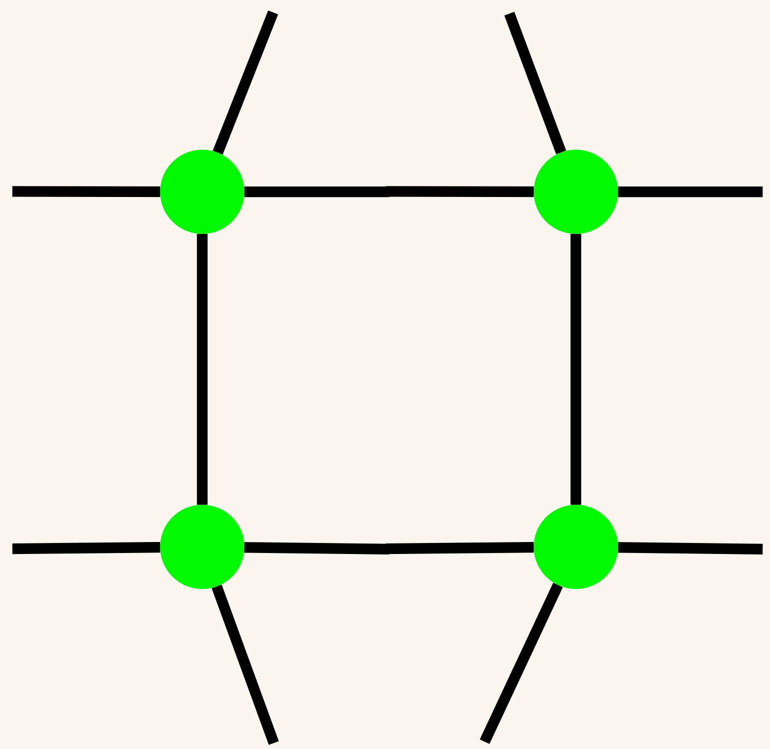
◇ Cost: $O(D^6) \rightarrow O(D^6) \rightarrow O(D^6)$

HOTRG: Isometry step



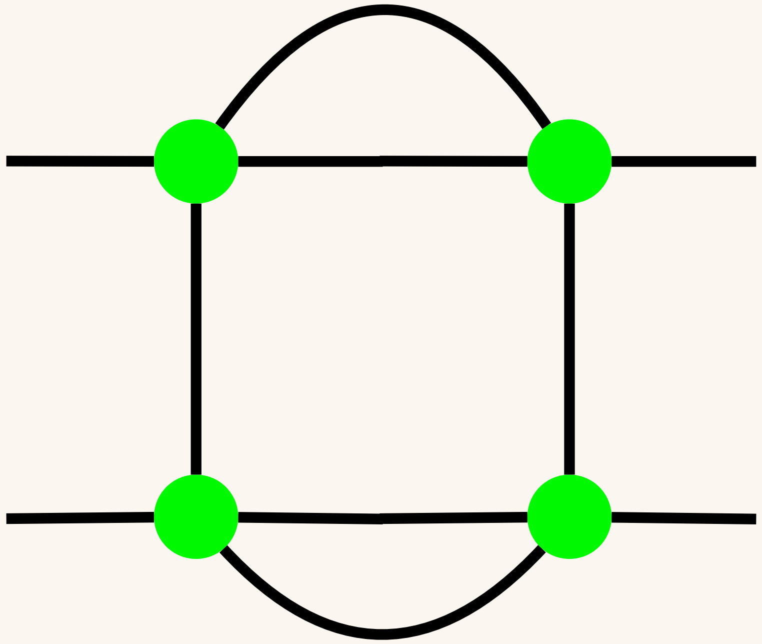
◇ Cost: $O(D^6) \rightarrow O(D^6) \rightarrow O(D^6)$

◉ HOTRG: Isometry step



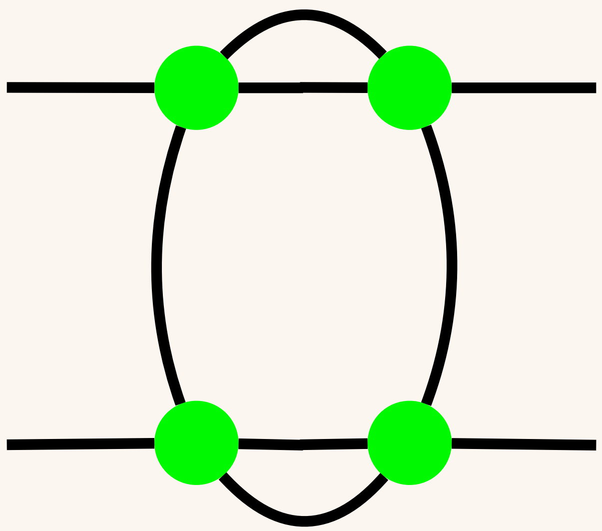
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



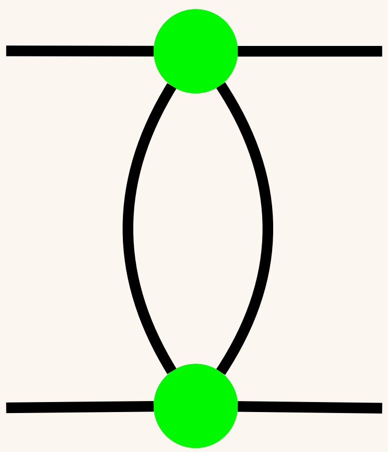
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



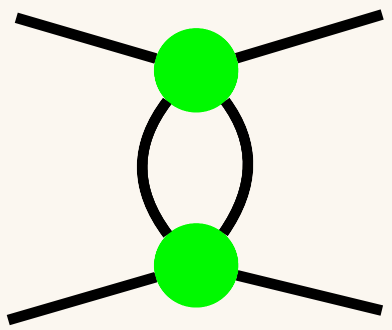
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



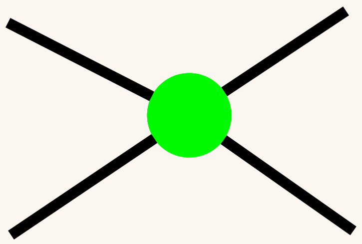
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



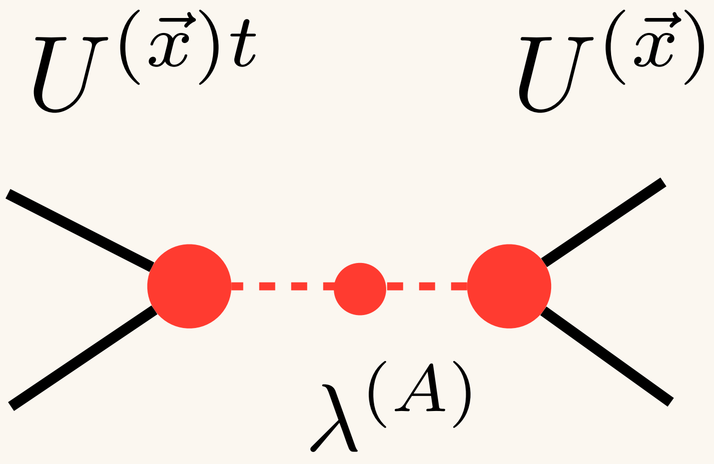
◇ Cost: $O(D^6) \to O(D^6) \to O(D^6)$

◉ HOTRG: Isometry step



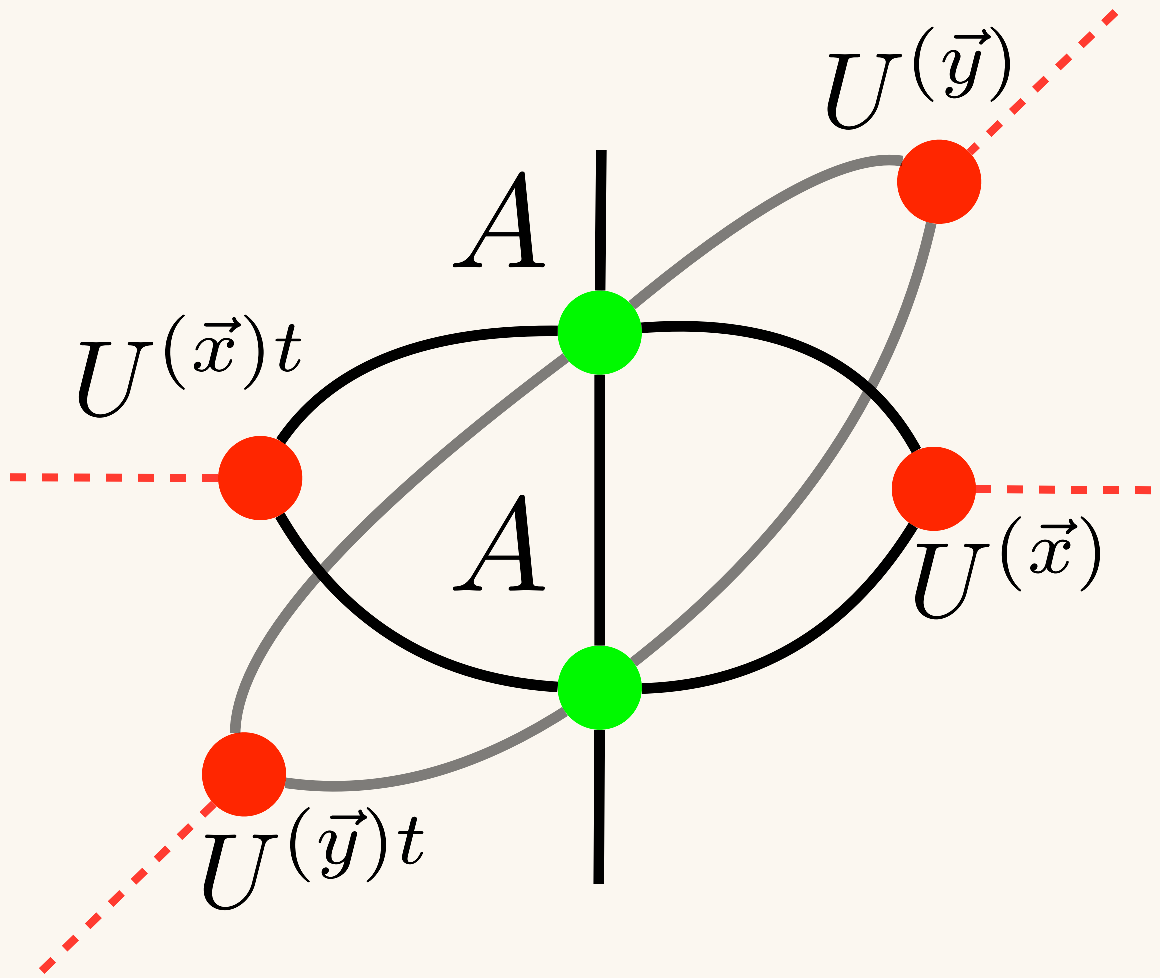
◇ Cost: $O(D^6) \rightarrow O(D^6) \rightarrow O(D^6)$

◉ HOTRG: Isometry step



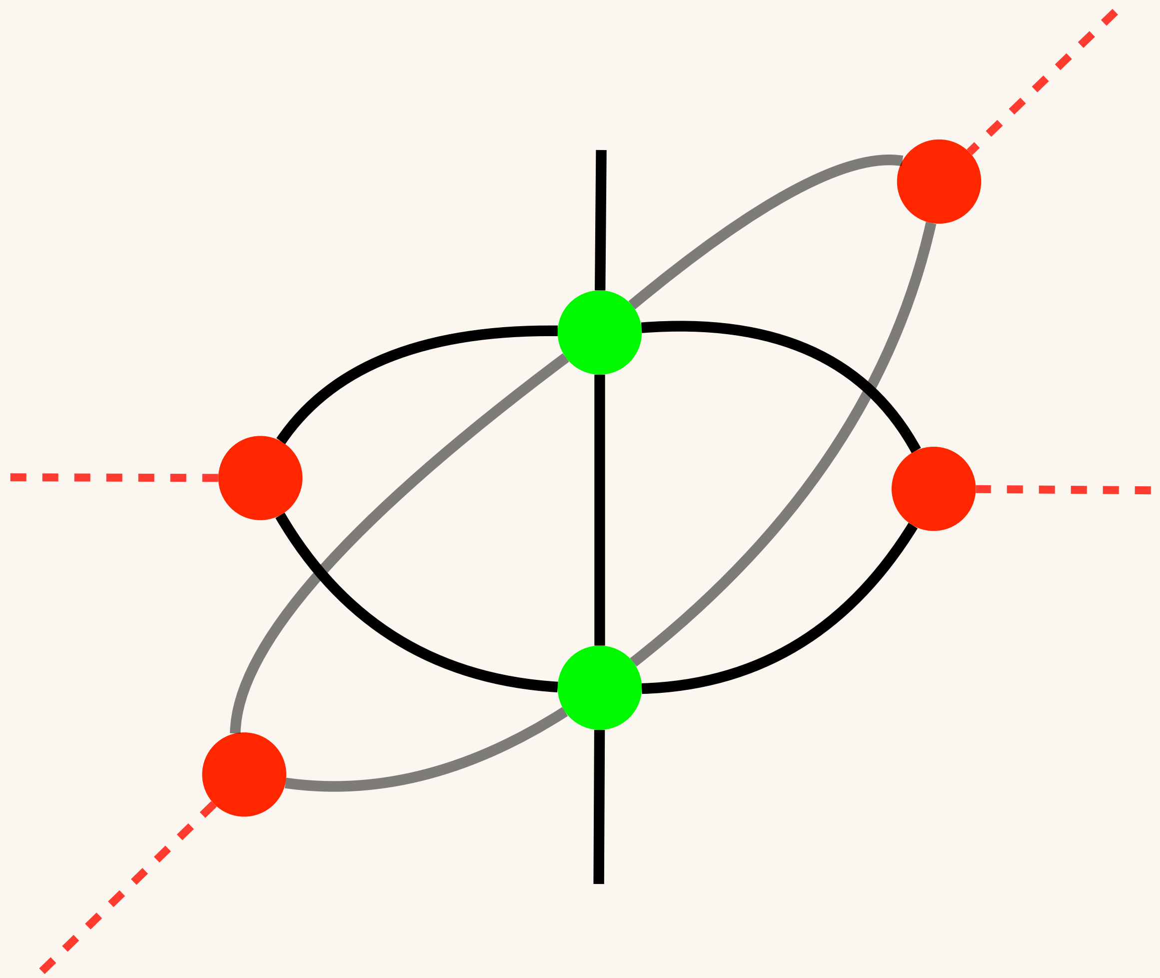
◇ Cost: $O(D^6) \rightarrow O(D^6) \rightarrow O(D^6)$

◉ HOTRG: Contraction step



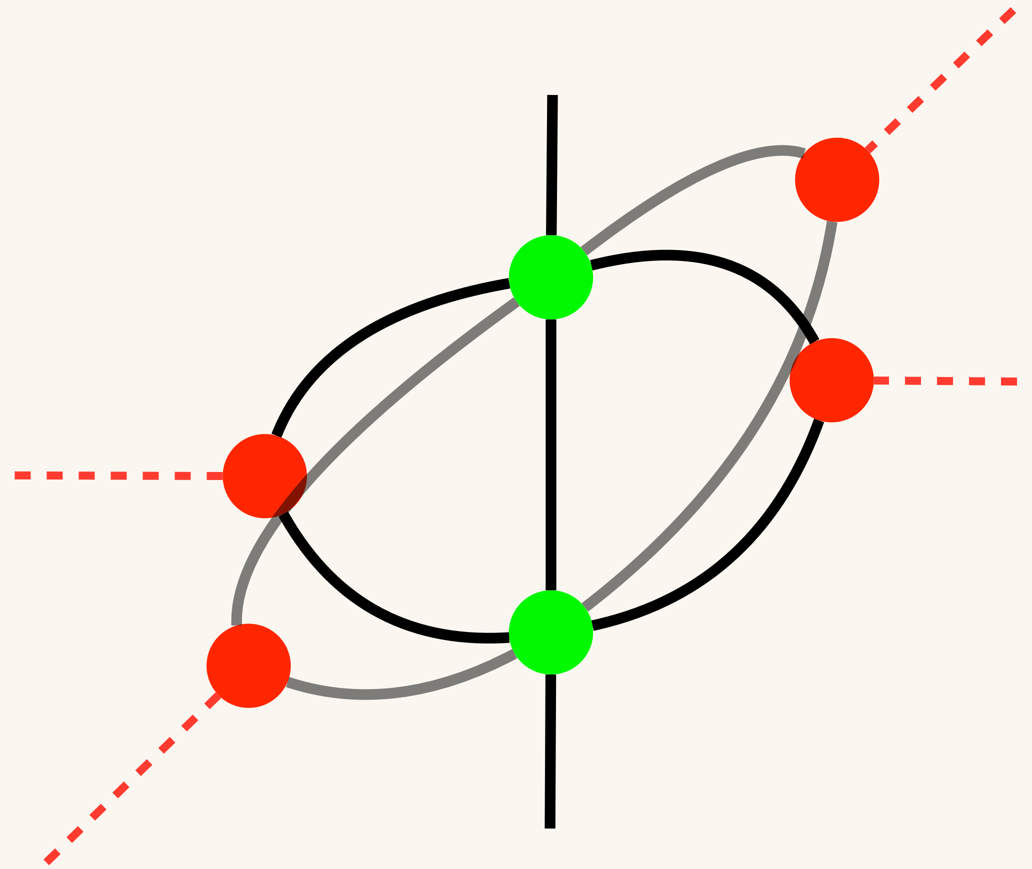
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



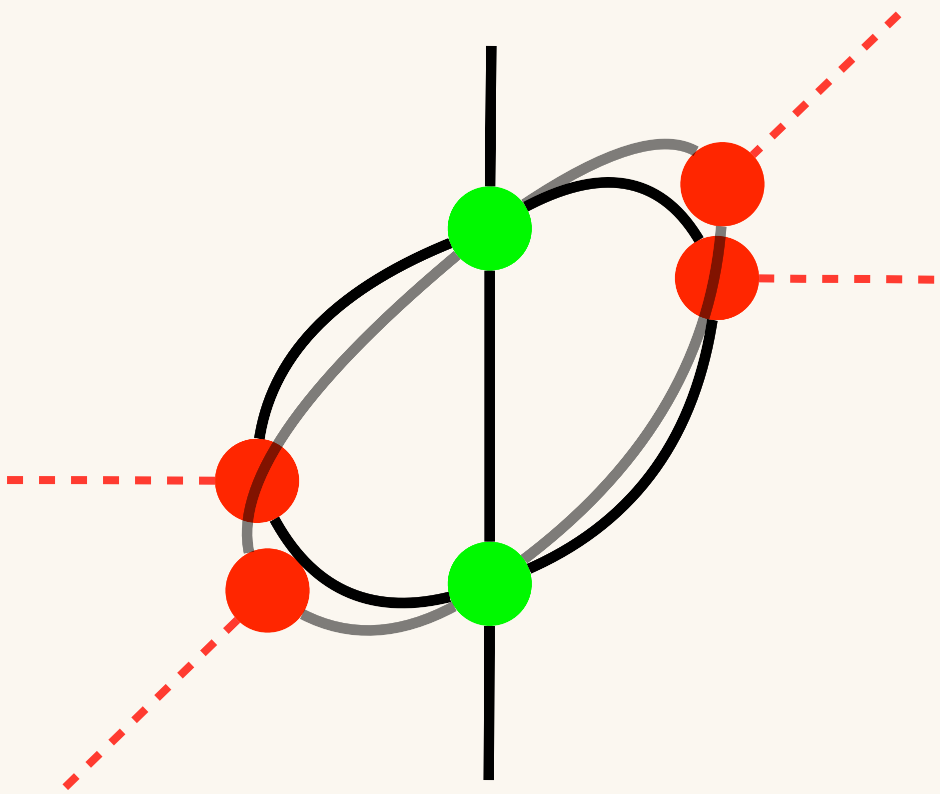
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



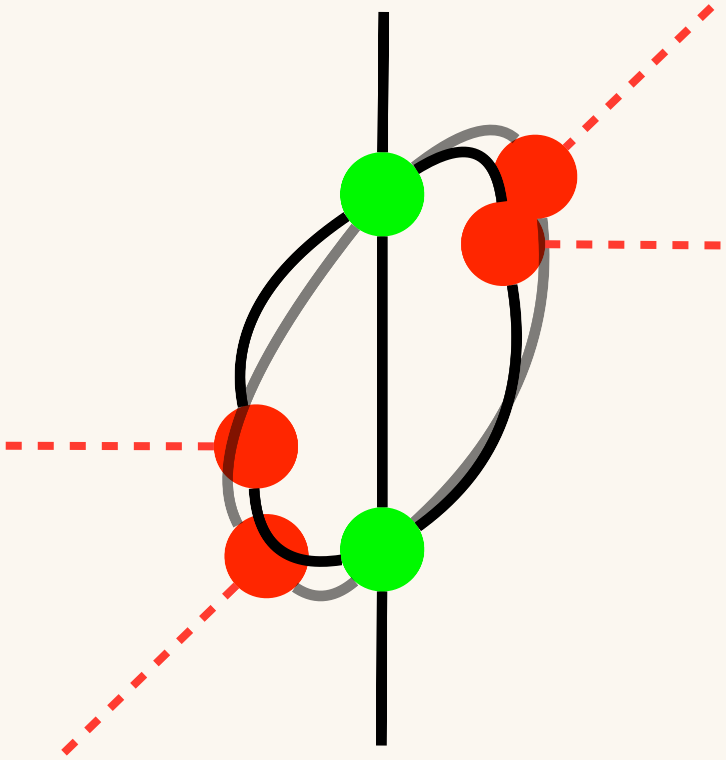
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



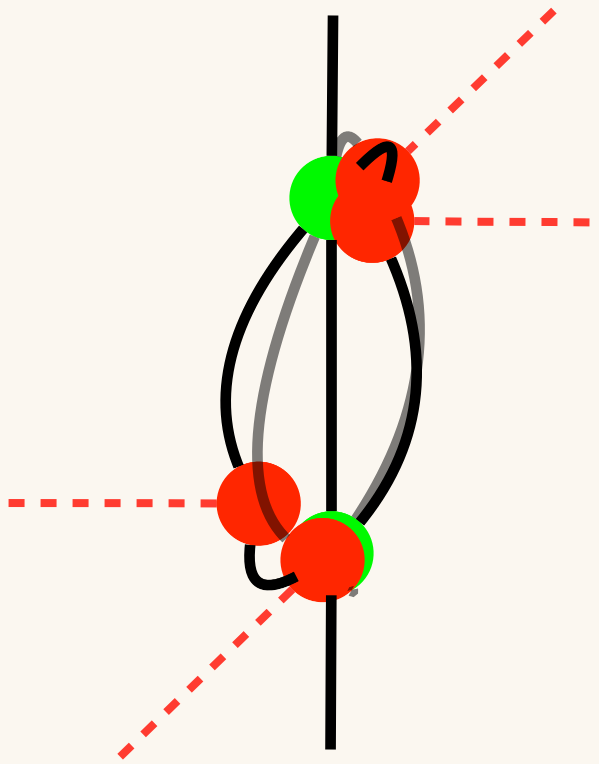
◇ Cost: $O(D^9) \rightarrow O(D^{11})$

◉ HOTRG: Contraction step



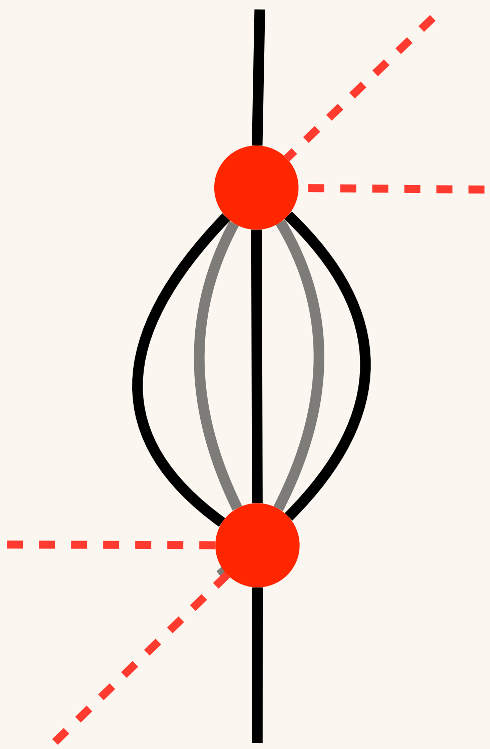
◇ Cost: $O(D^9) \to O(D^{11})$

◉ HOTRG: Contraction step



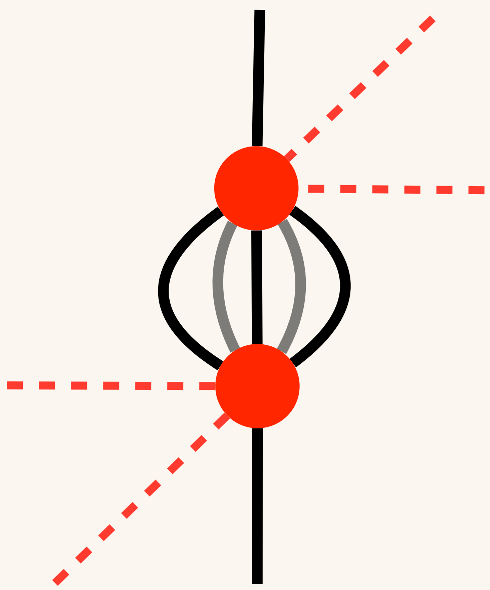
◇ Cost: $O(D^9) \rightarrow O(D^{11})$

◉ HOTRG: Contraction step



◇ Cost: $O(D^9) \to O(D^{11})$

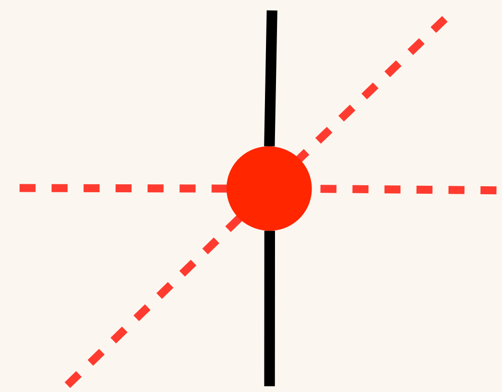
◉ HOTRG: Contraction step



◇ Cost: $O(D^9) \to O(D^{11})$

HOTRG: Contraction step

$A^{(\mathrm{next})}$



◇ Cost: $O(D^9) \to O(D^{11})$

◉ Higher-Order TRG (HOTRG)

[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

◇ なぜ今までHOTRGにR-SVDを適用してこなかったか?

◇ HOTRGの支配的な計算量は縮約ステップ

◇ R-SVDはSVD(分解ステップ)の近似と考えられている

↓

→ 分解の近似では縮約の近似を変えることはできない(?)

実際には…

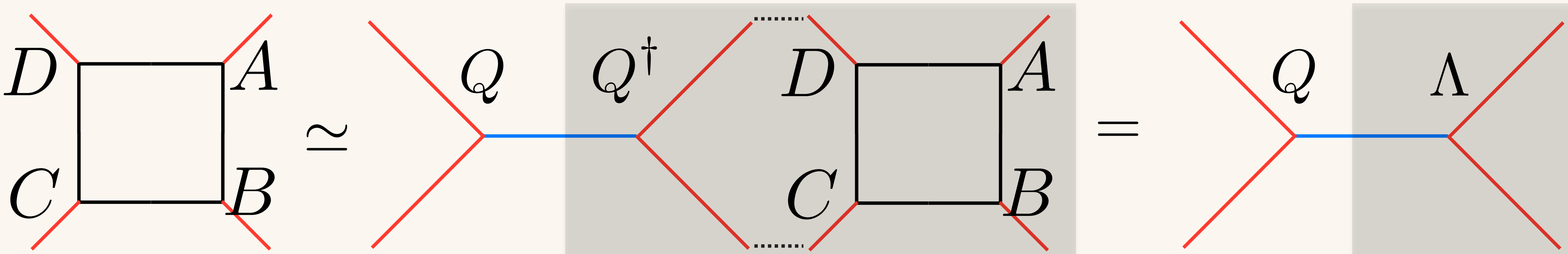
◇ R-SVDは縮約の近似としても利用できる

(この縮約近似手法自体はTriad TRGでも使われていた)

◉ 乱拓特異値分解(R-SVD)

[N. Halko, et al. arXiv:0909.4061]
[S. Morita, et al. arXiv:1712.01458]

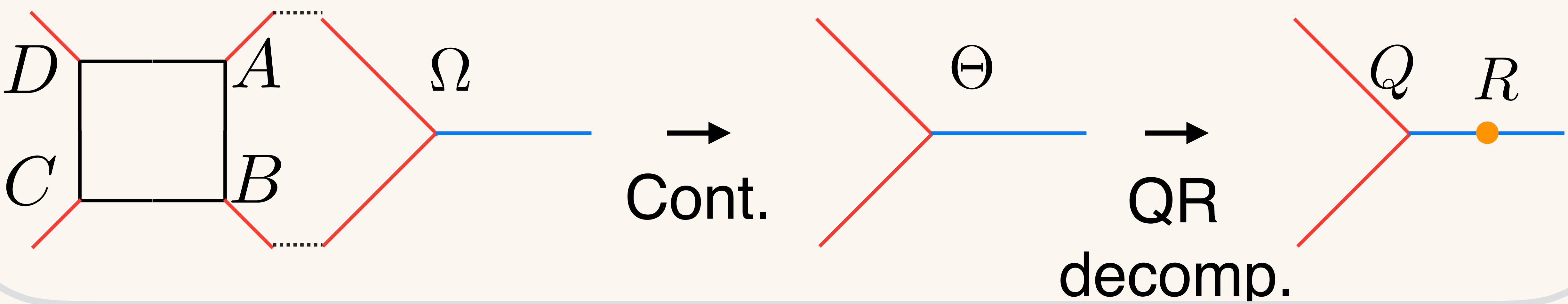
◇ 直交行列 Q による近似的な縮約法



◇ $\Lambda \equiv Q^\dagger ABCD$ の特異値分解なら添字の数が減って早い

◇ Q の準備に乱数とQR分解を使う

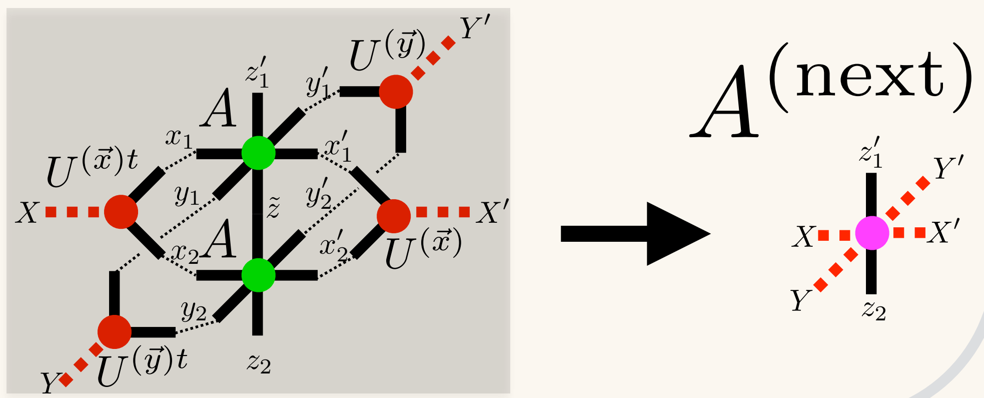
◇ 乱数テンソル Ω でサンプリングして近似している



● HOTRG [Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

◇ 射影テンソルUとの縮約

$$U^{(\vec{y})t}U^{(\vec{x})t}AAU^{(\vec{x})}U^{(\vec{y})} \to A^{(\mathrm{next})}$$



● HOTRG with R-SVD [K.N. arXiv:2307.14191] [D. Kadoh, K.N. arXiv:1912.02414]

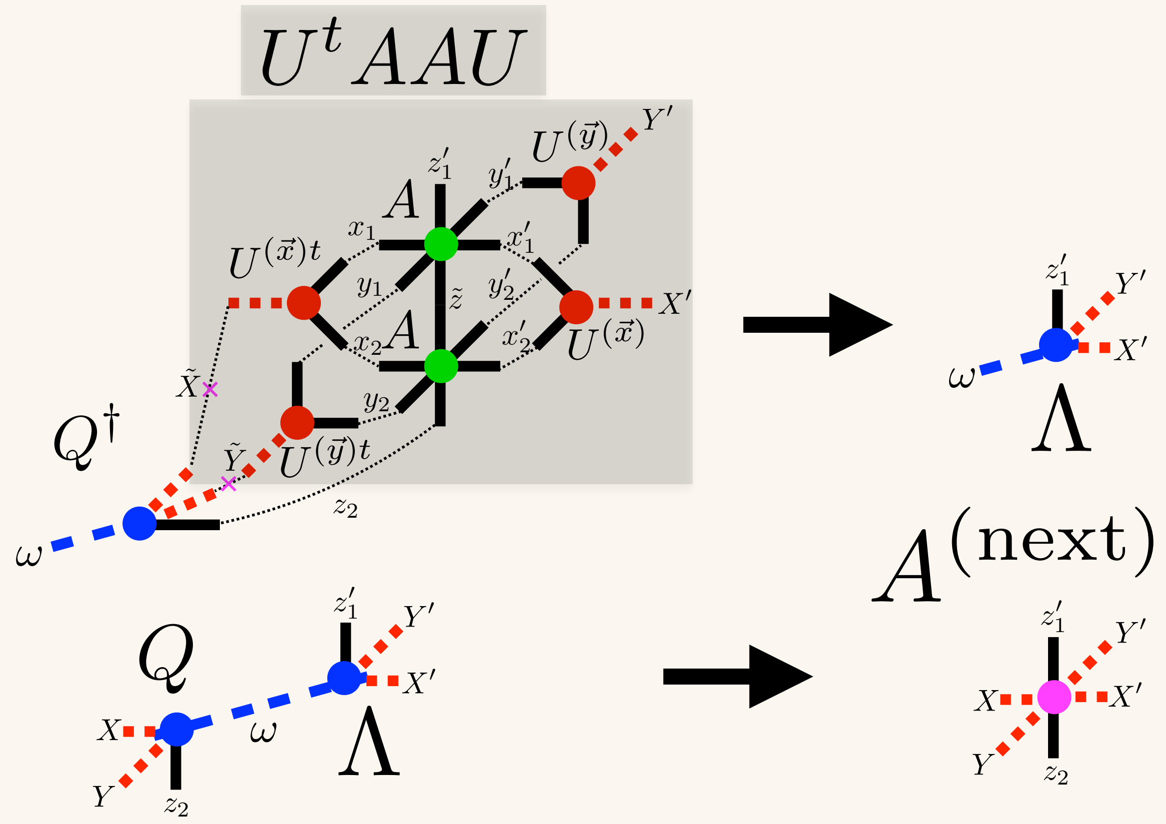
◇ 射影テンソルU、Q との縮約

$$QQ^{\dagger}U^{(\vec{y})t}U^{(\vec{x})t}AAU^{(\vec{x})}U^{(\vec{y})} \simeq A^{(\mathrm{next})}$$

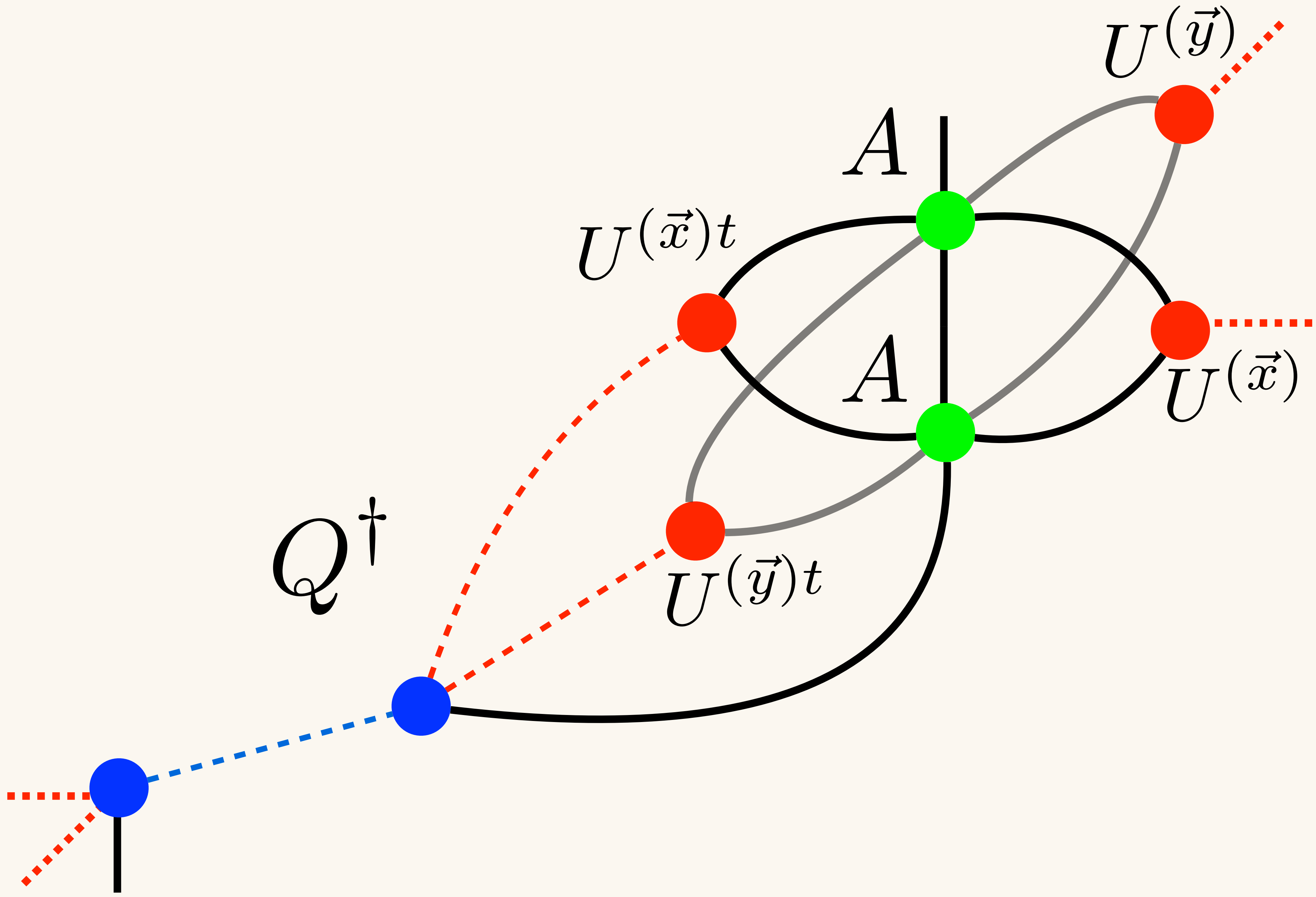
◇ 計算量削減

$$O(D^{4d-1}) \to O(D^{3d})$$

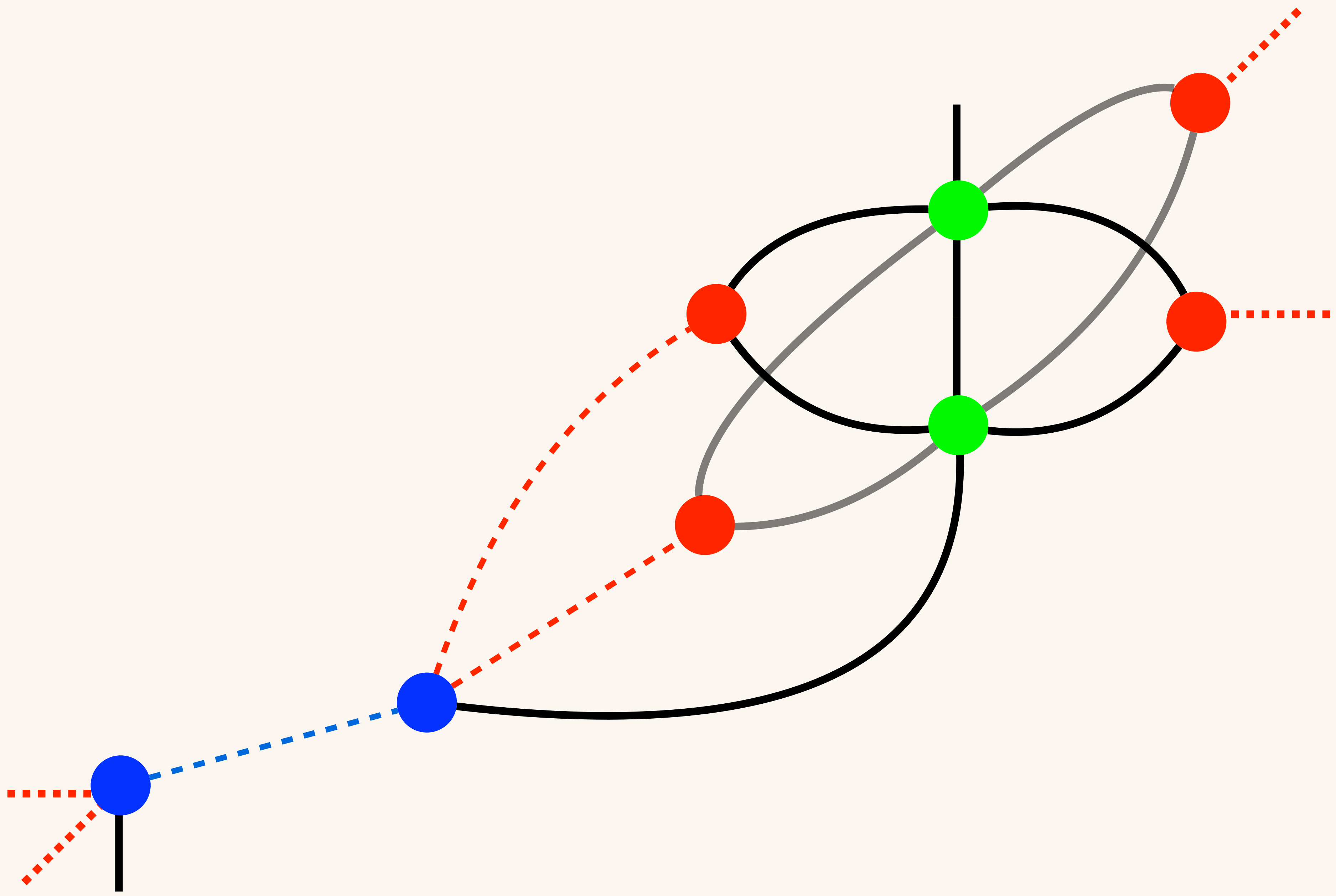
→ もっと減らせないか？



R-HOTRG: Contraction step

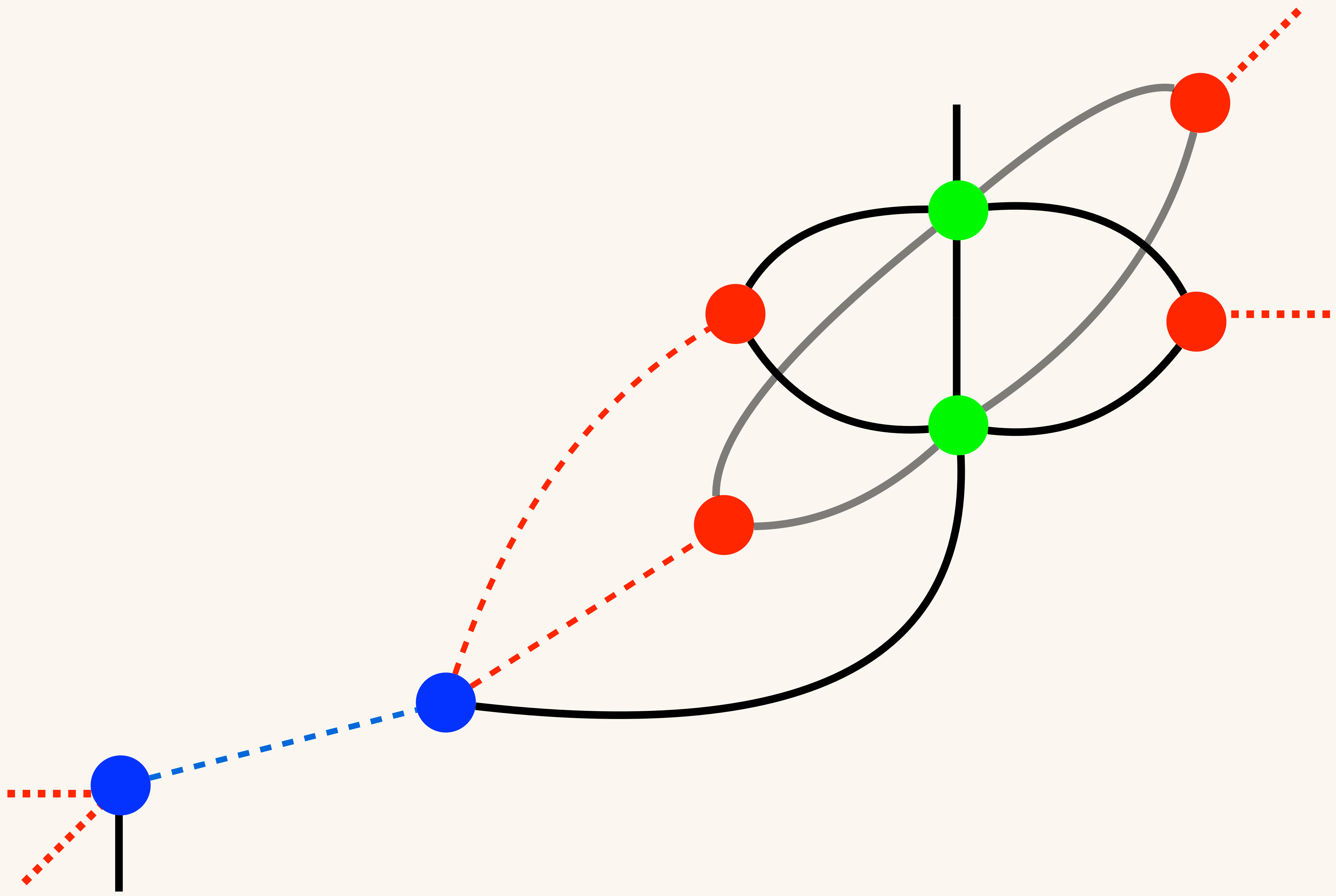


◉ R-HOTRG: Contraction step



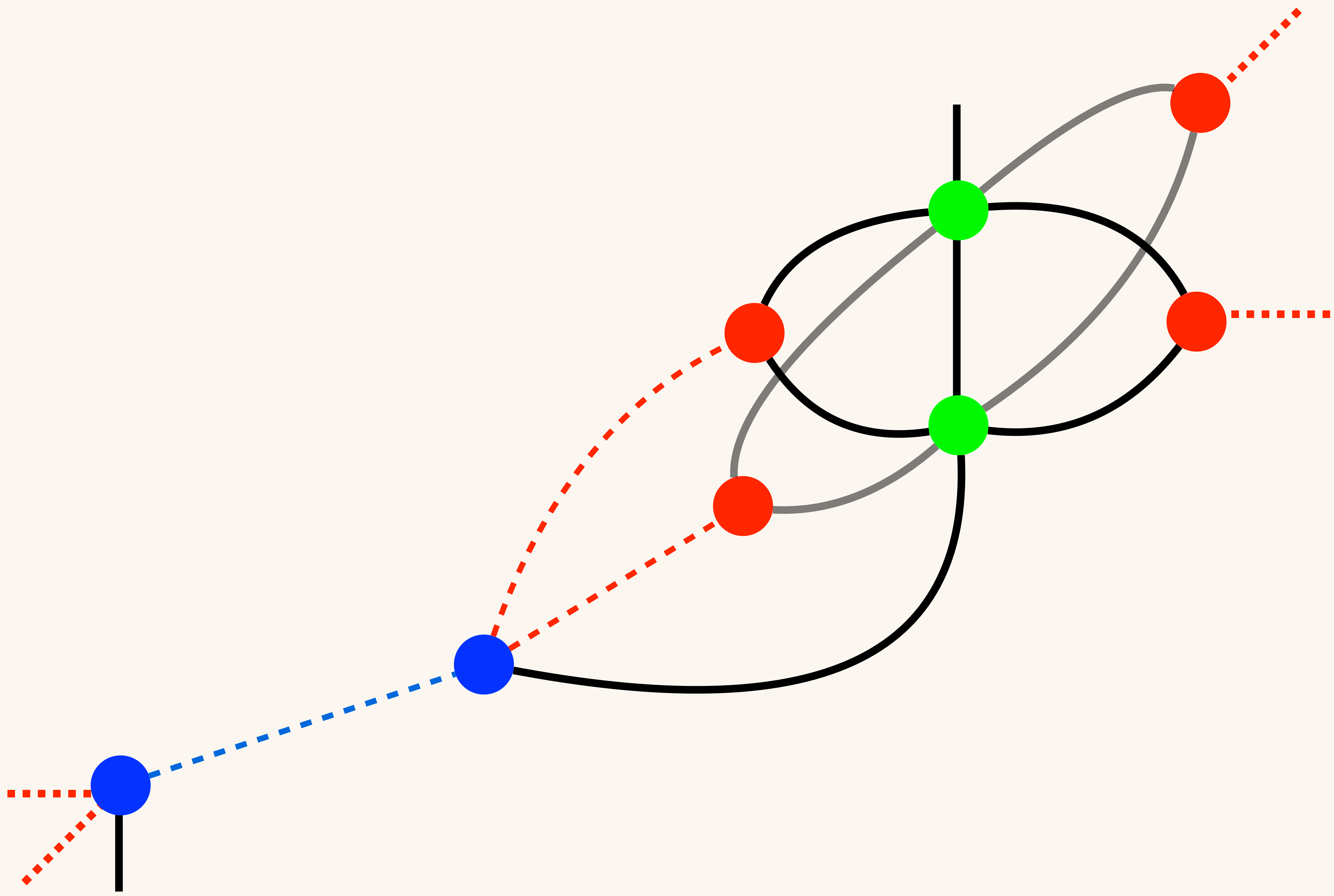
◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



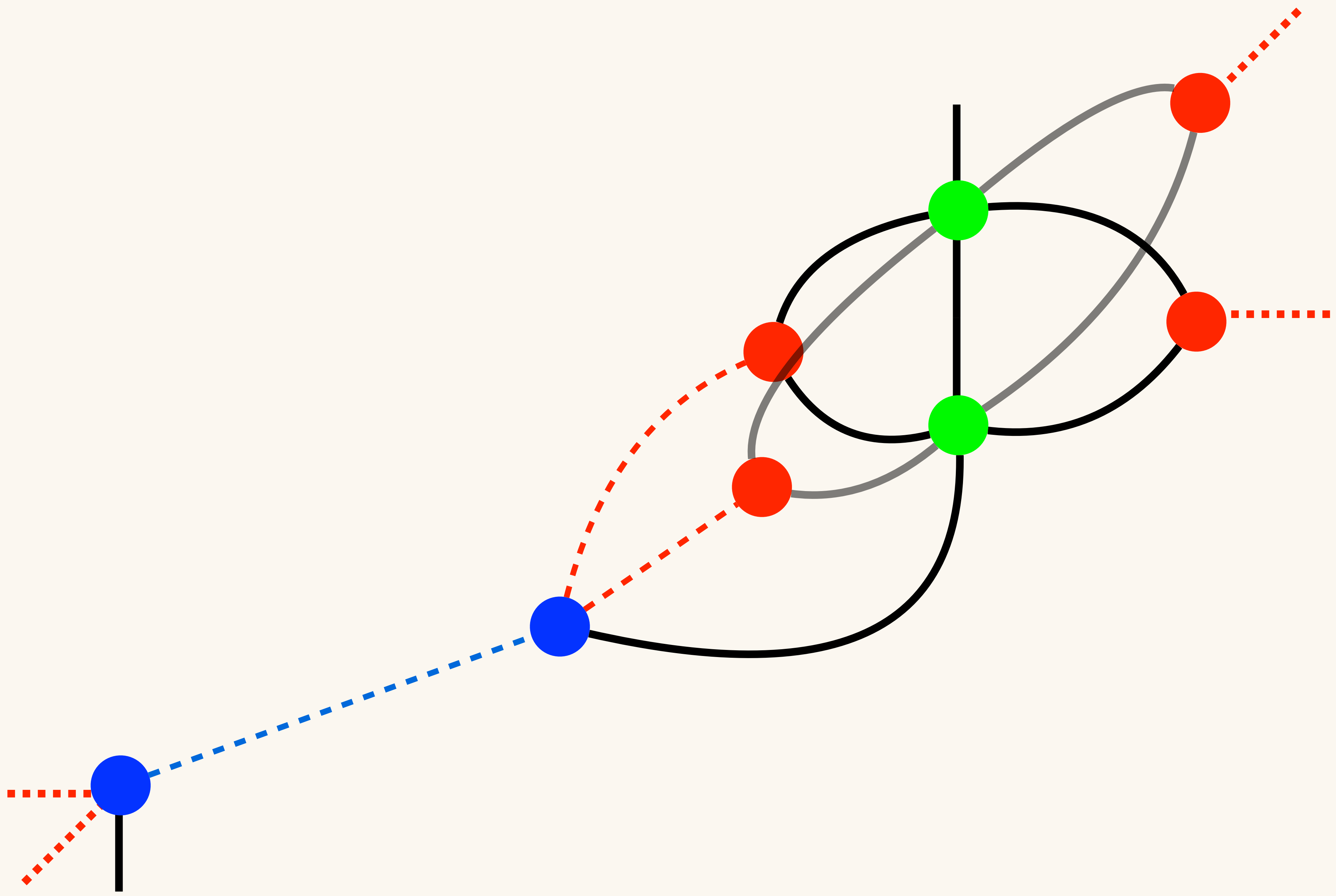
◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



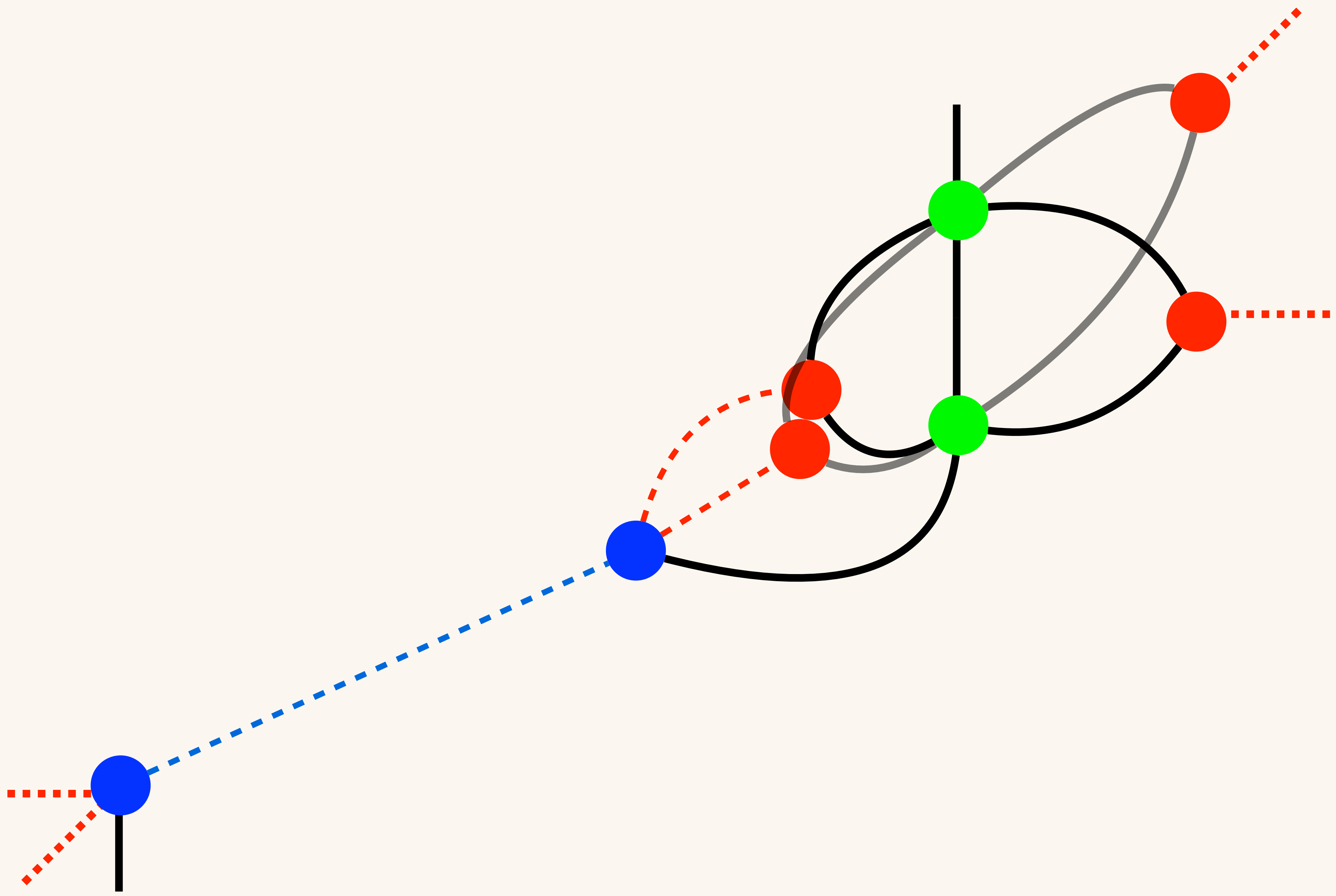
◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



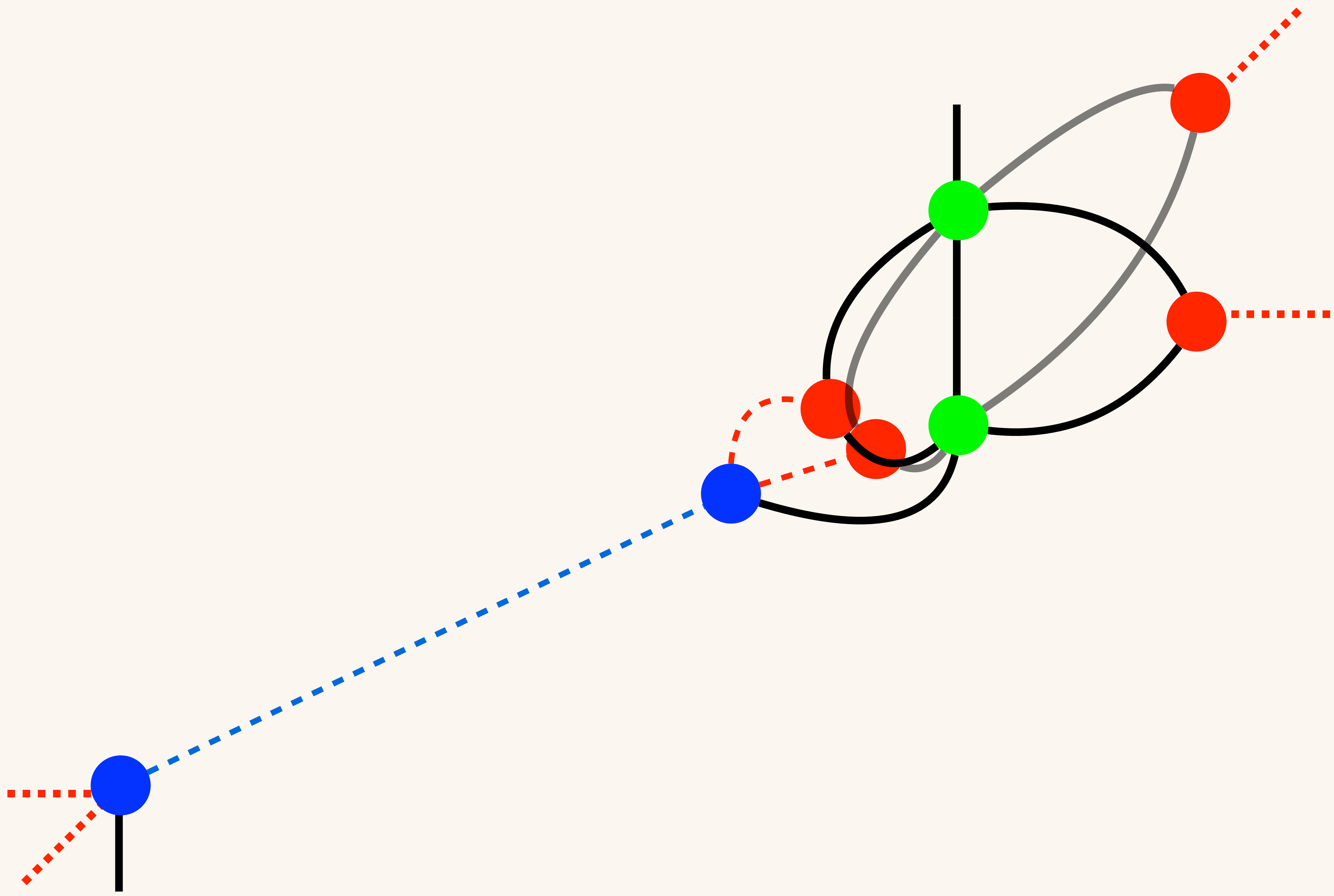
◇ Cost: $O(D^9) \rightarrow O(D^9)$

◉ R-HOTRG: Contraction step



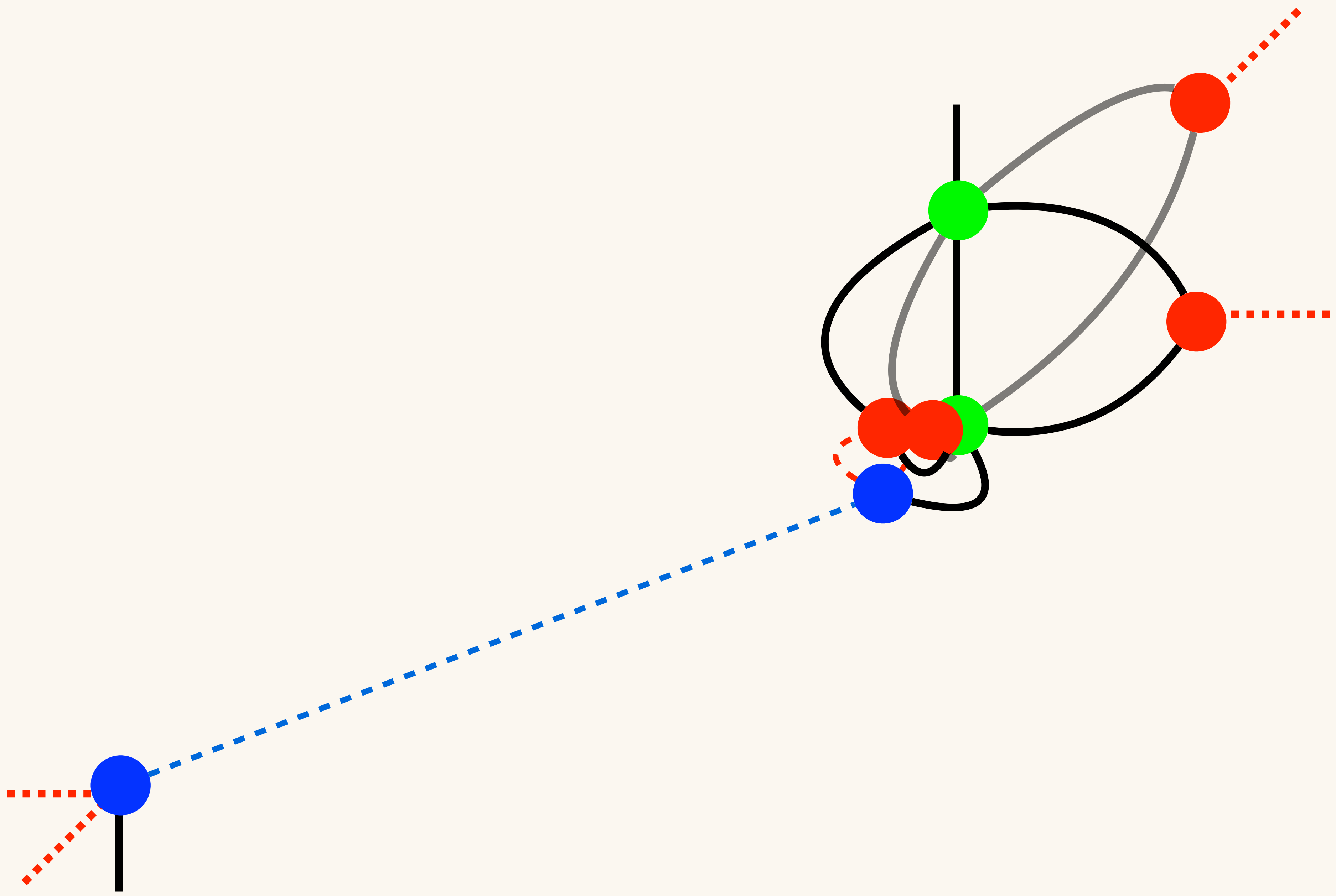
◇ Cost: $O(D^9) \rightarrow O(D^9)$

◉ R-HOTRG: Contraction step



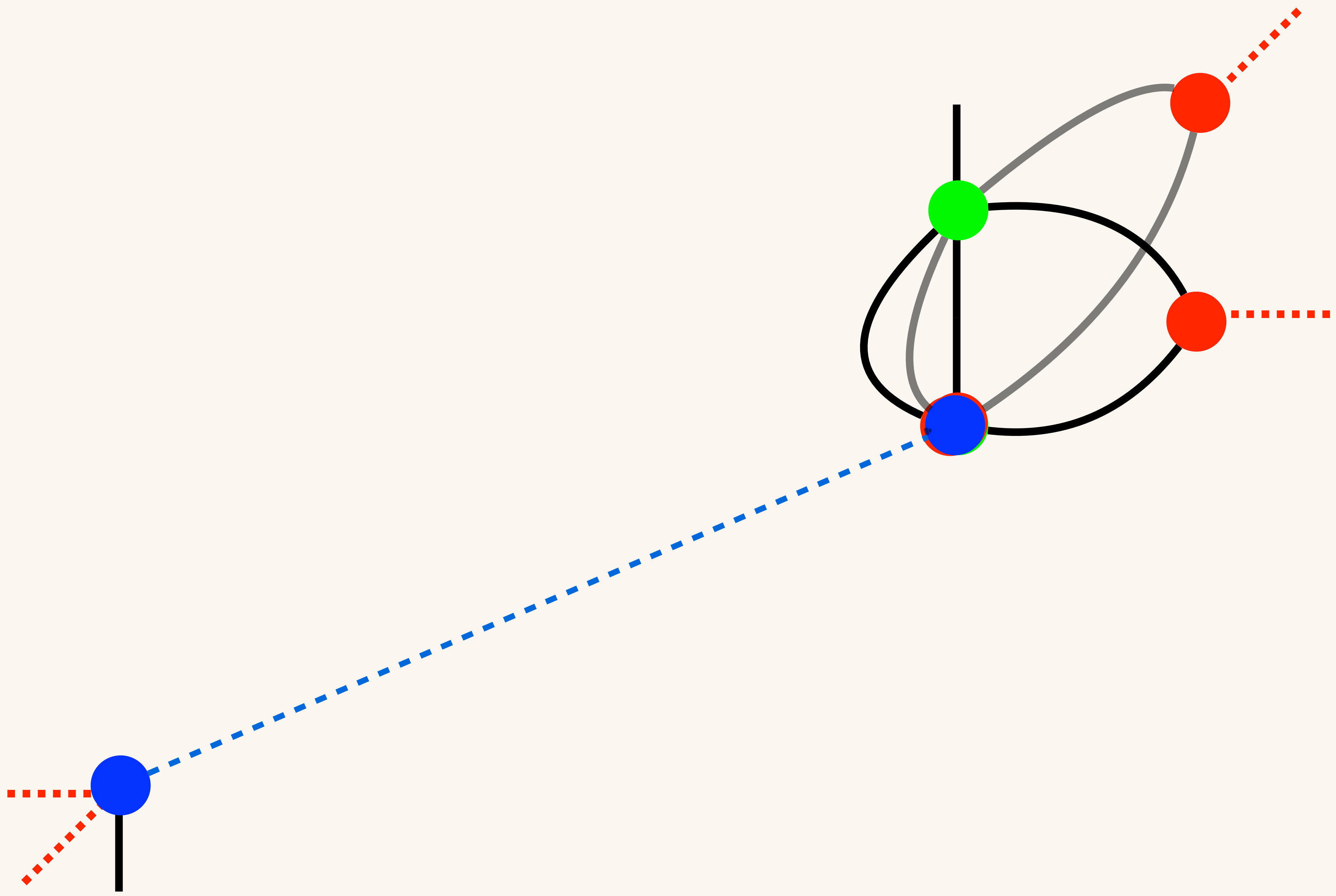
◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



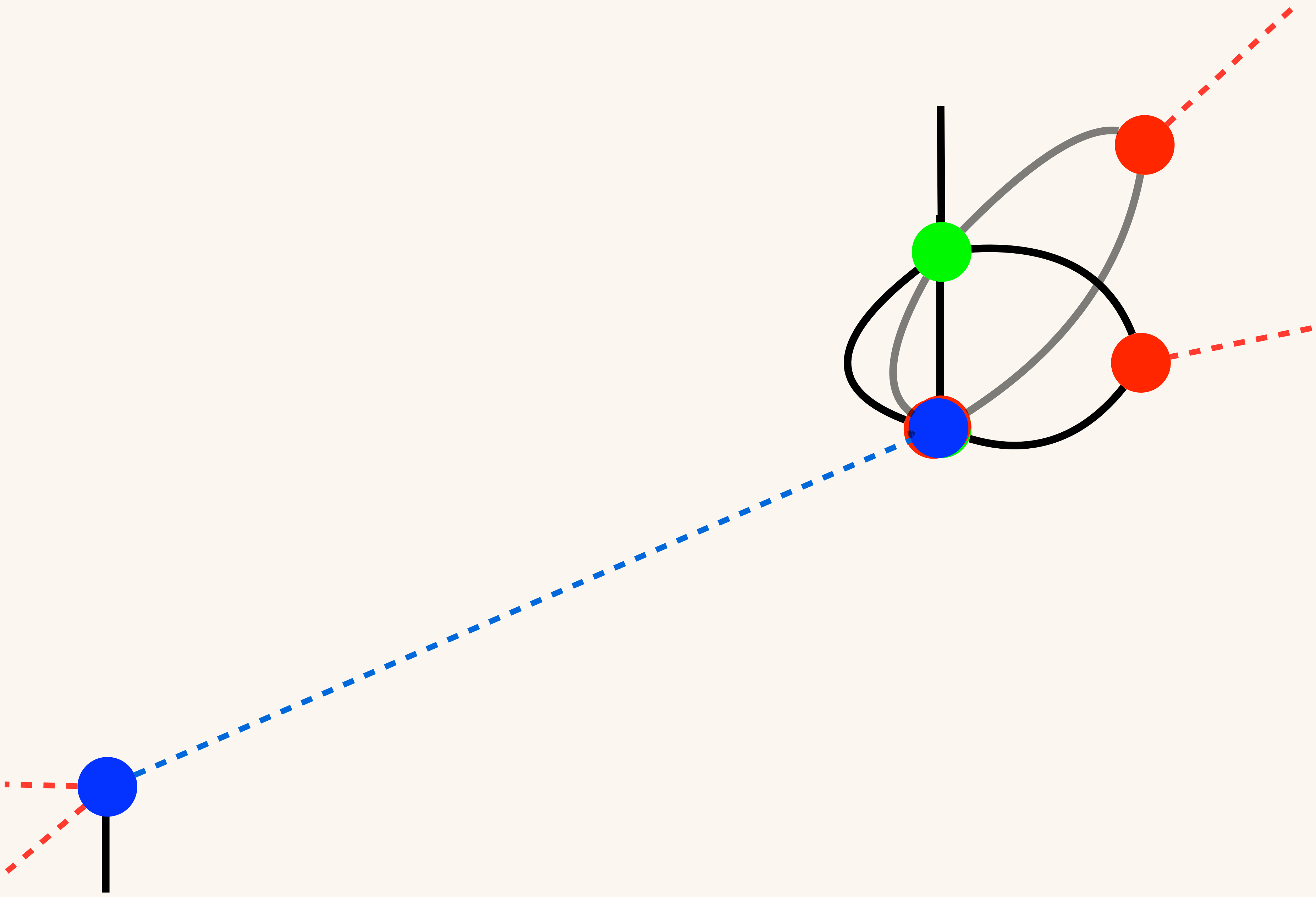
◇ Cost: $O(D^9) \rightarrow O(D^9)$

◉ R-HOTRG: Contraction step



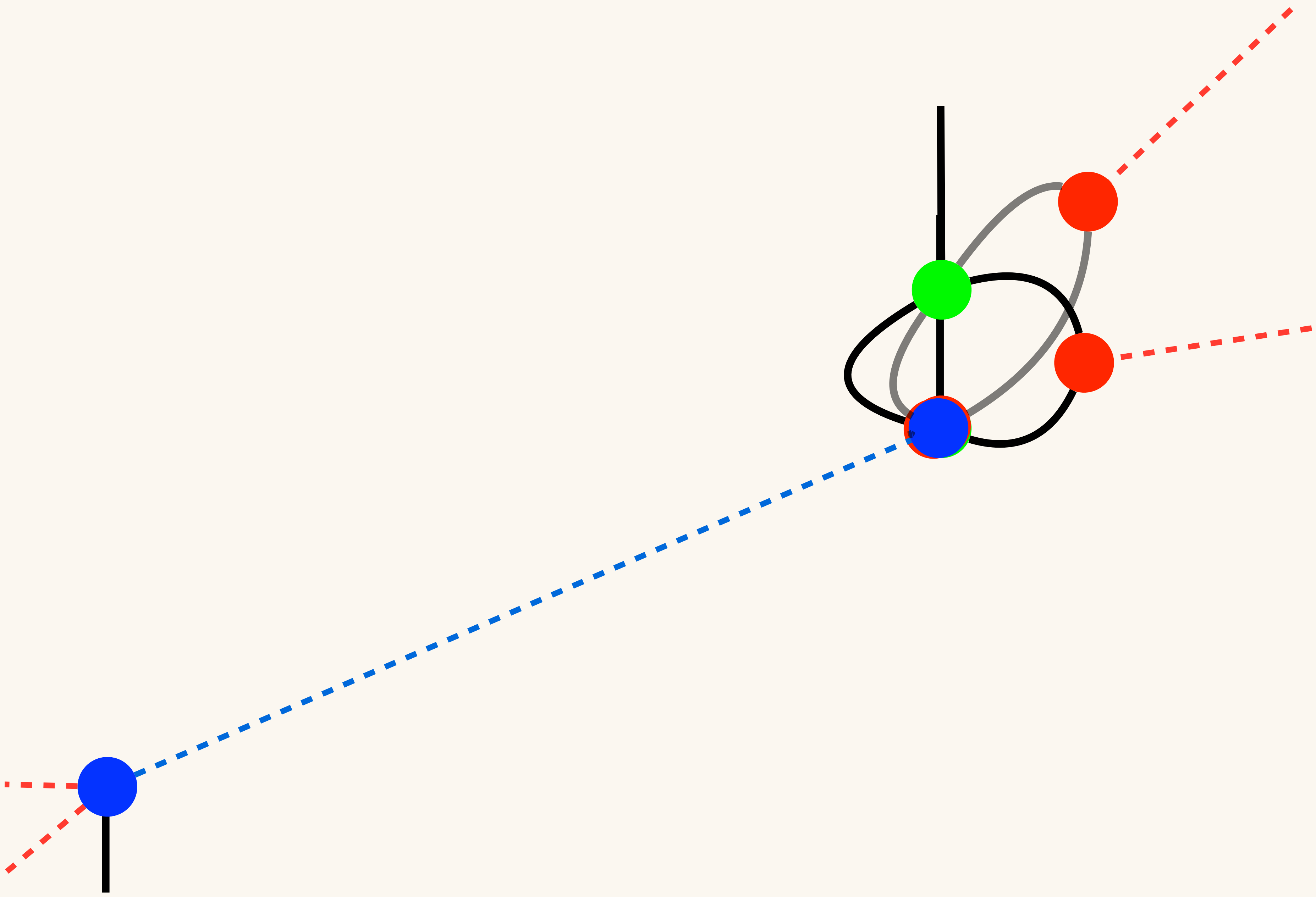
◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



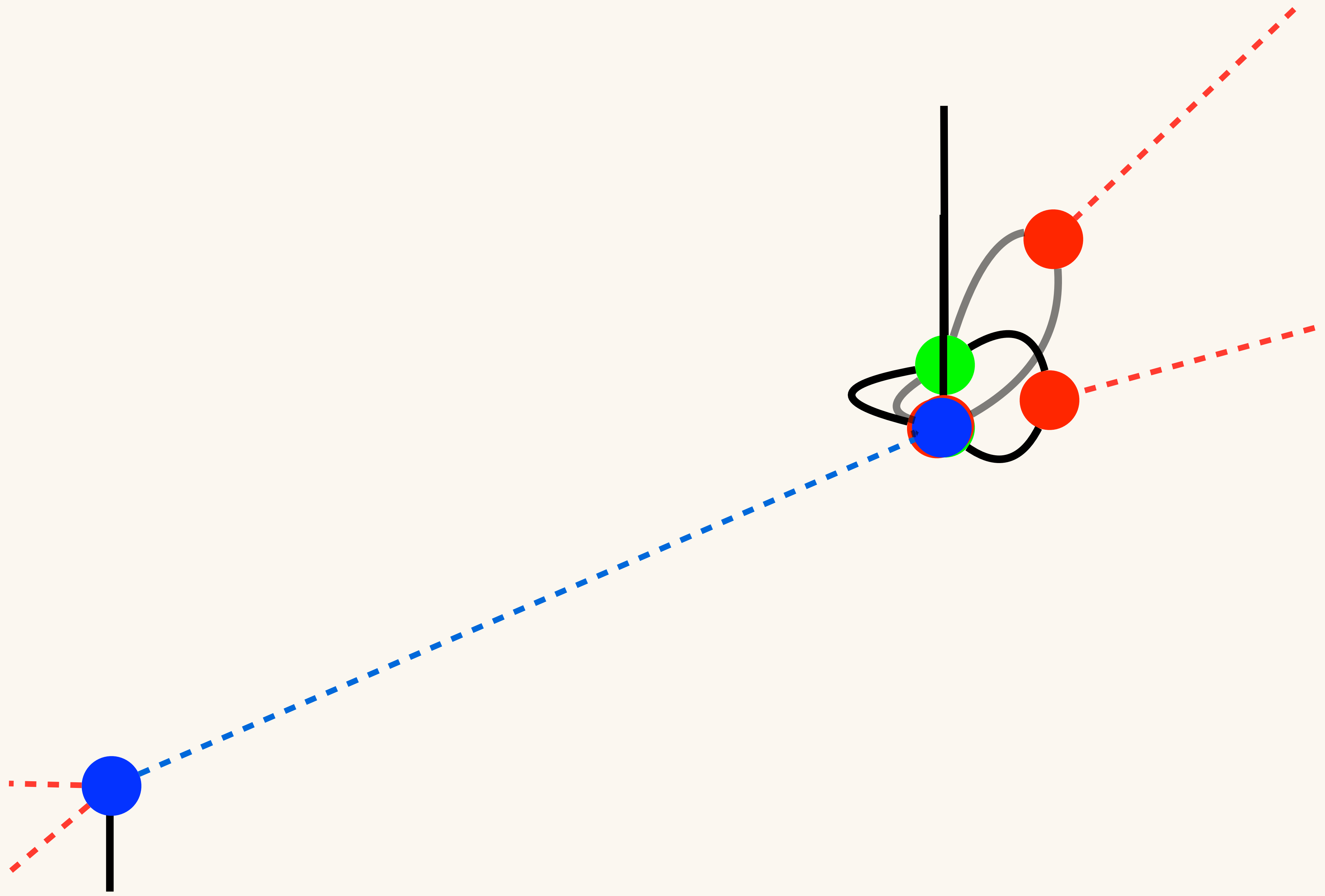
◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



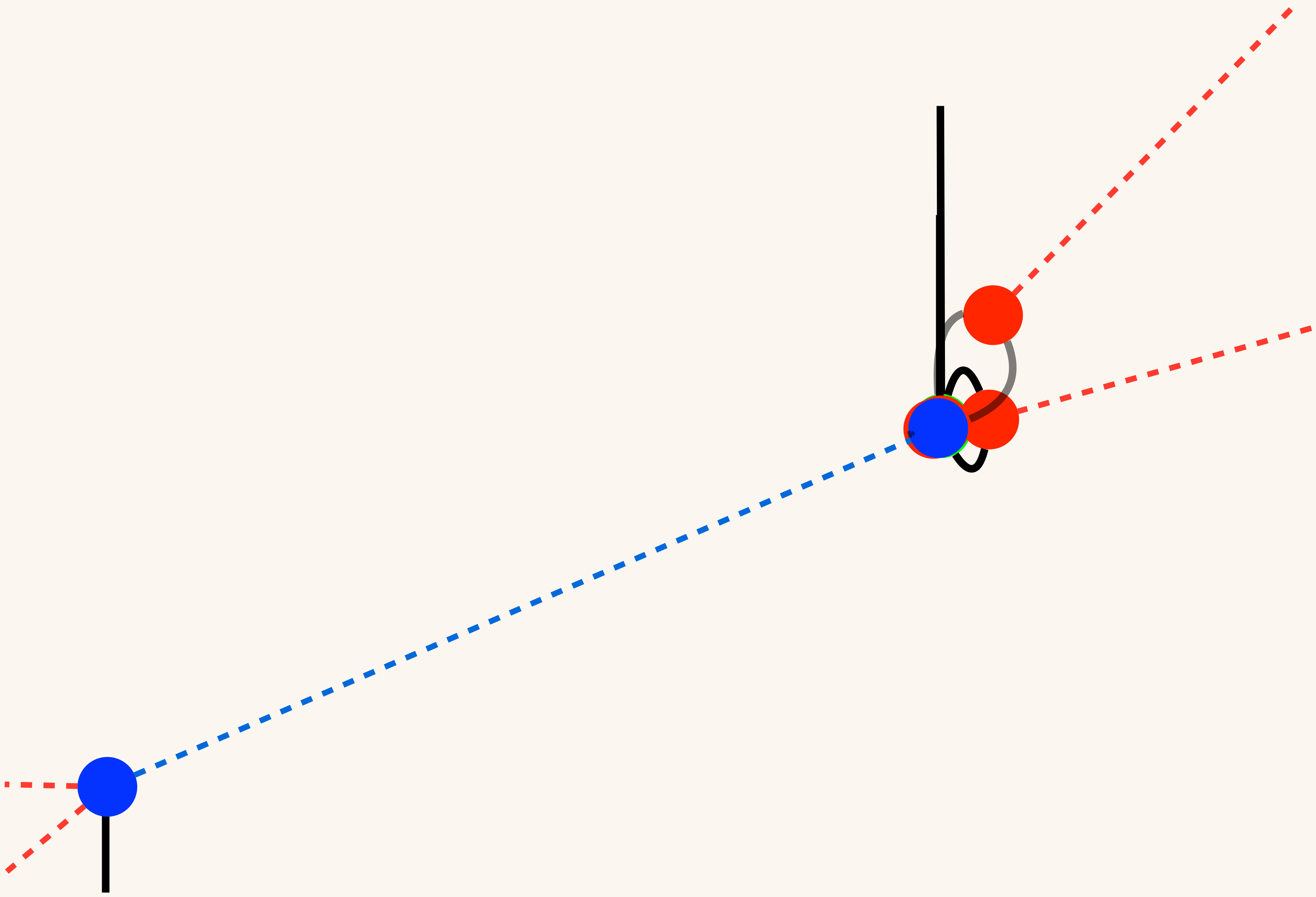
◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



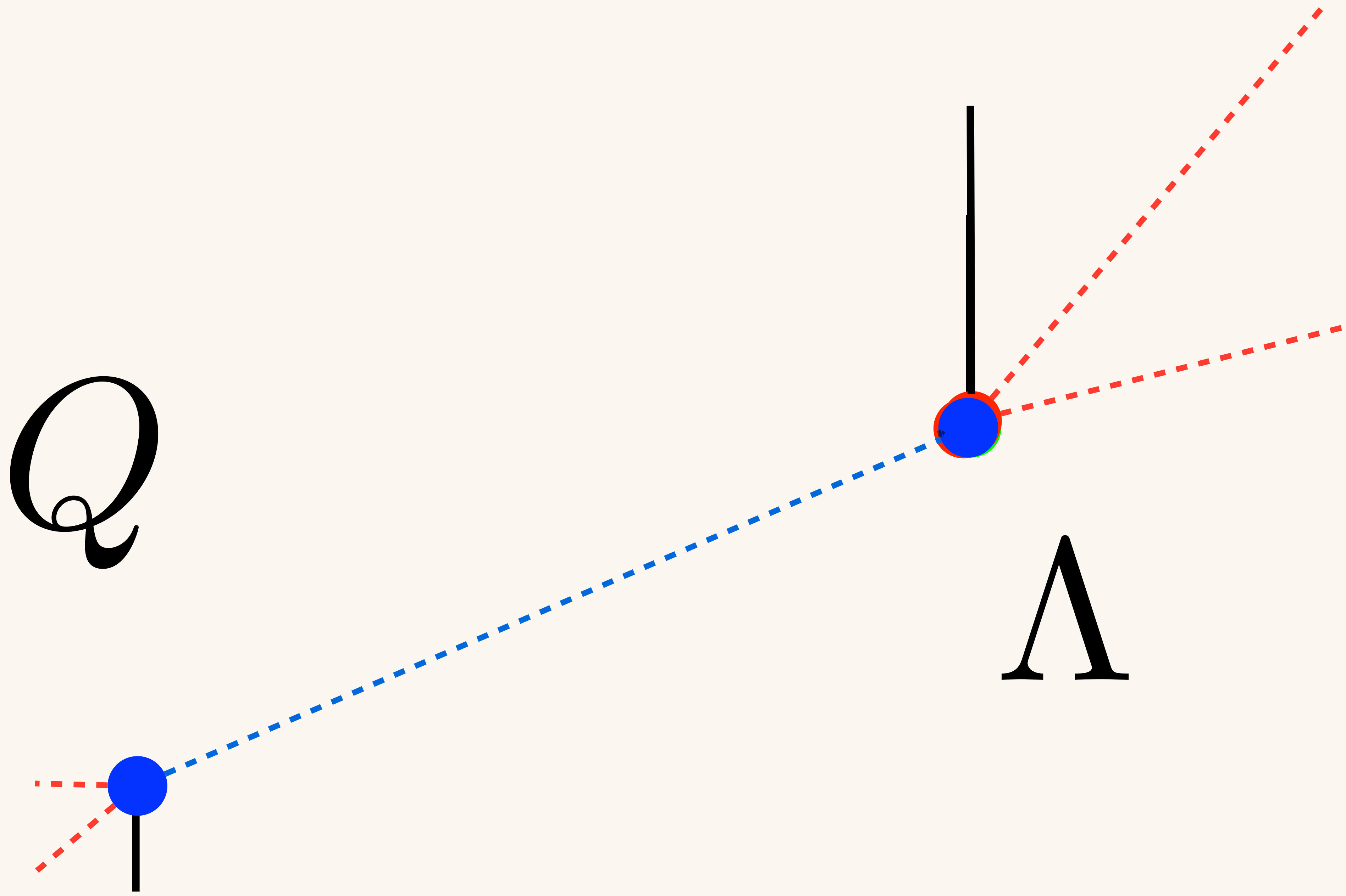
◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



◇ Cost: $O(D^9) \to O(D^9)$

◉ R-HOTRG: Contraction step



◇ Cost: $O(D^9) \to O(D^9)$

計算量と系統誤差の削減

◉ Minimally-decomposed TRG(MDTRG)

→ 分解で計算量削減を誤差なしで

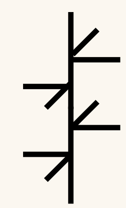
近似
SVD(Isometry)

精度改善
広い近似範囲

計算量削減
追加分解

打ち切りSVD

近似範囲



→ 全ての分解や縮約の近似範囲がHOTRGと一致。

全ての分解や縮約の近似を外からIsometryを演算する形に。

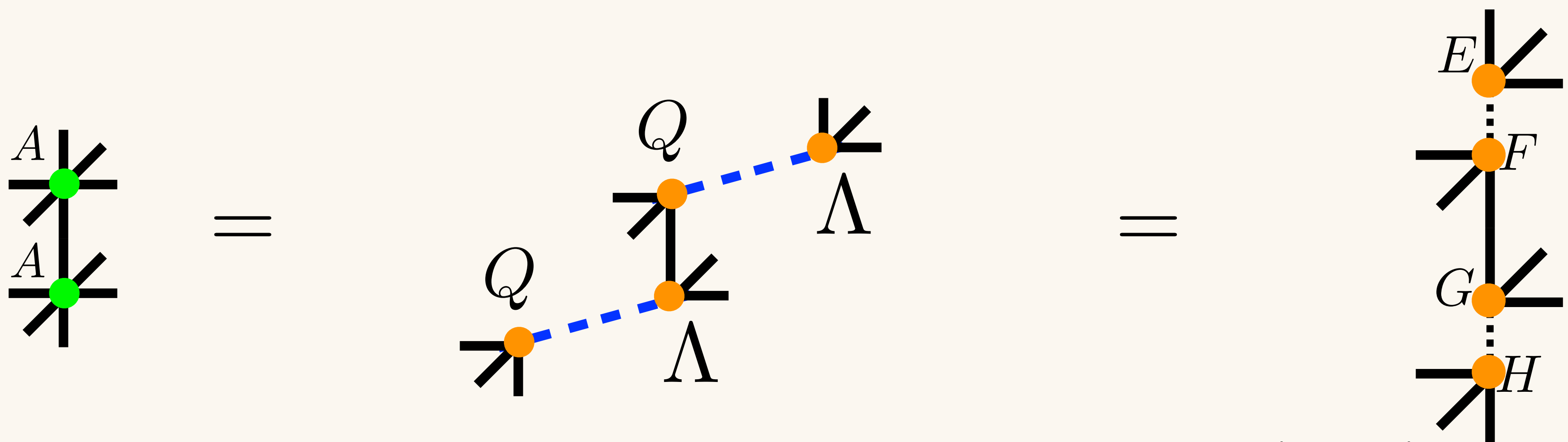
↓

HOTRGの精度のままで計算量だけ落としたい。

◉ Minimally-decomposed TRG(MDTRG)

[K.N. arXiv:2307.14191]

→ 実は既にd+1本の添字のテンソル表現をQ と Λでしてる

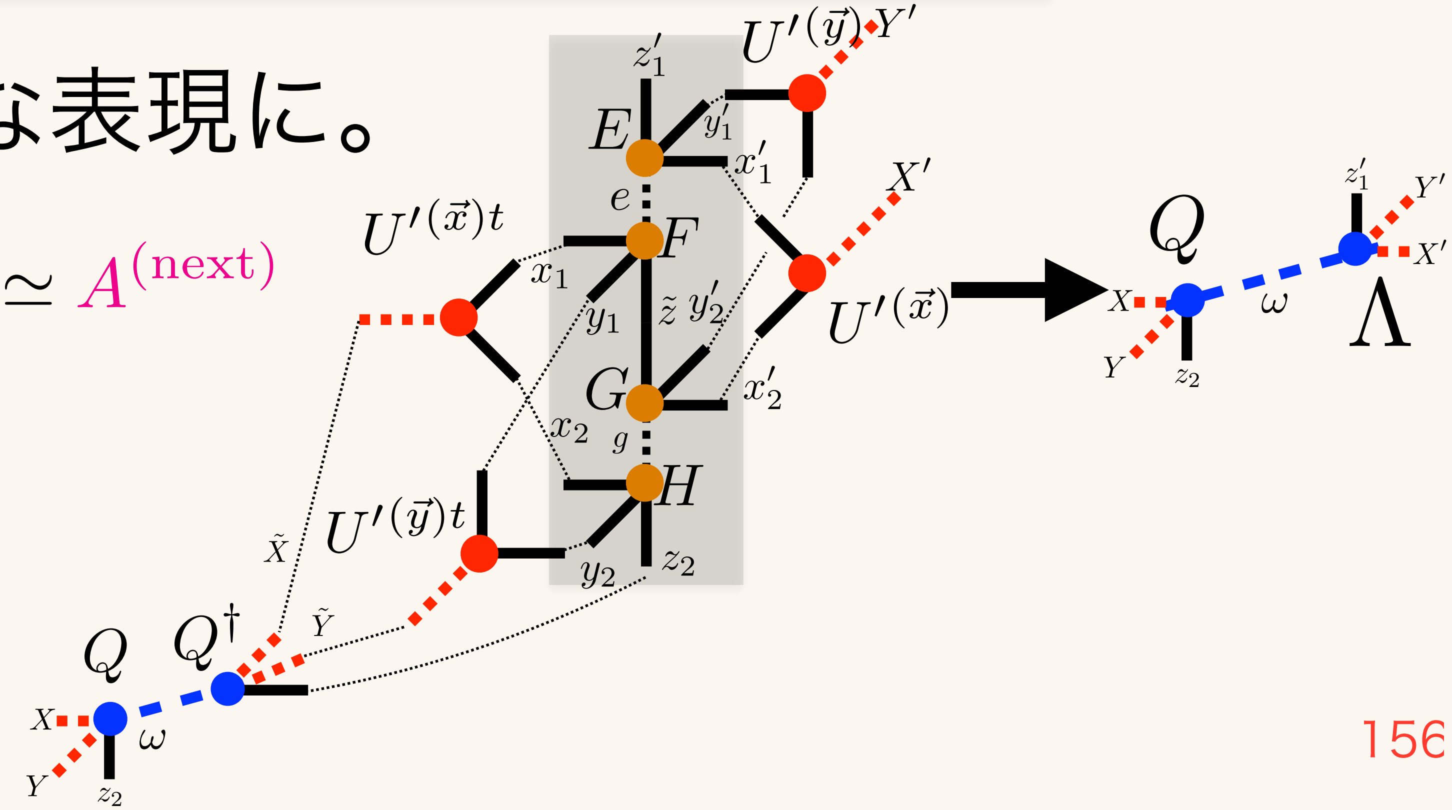


$$EFGH = Q\Lambda Q\Lambda$$

A:2d本　　E,F,G,H:d+1本　　Q, Λ:d+1本

◇ AでなくEFGHを基本的な表現に。

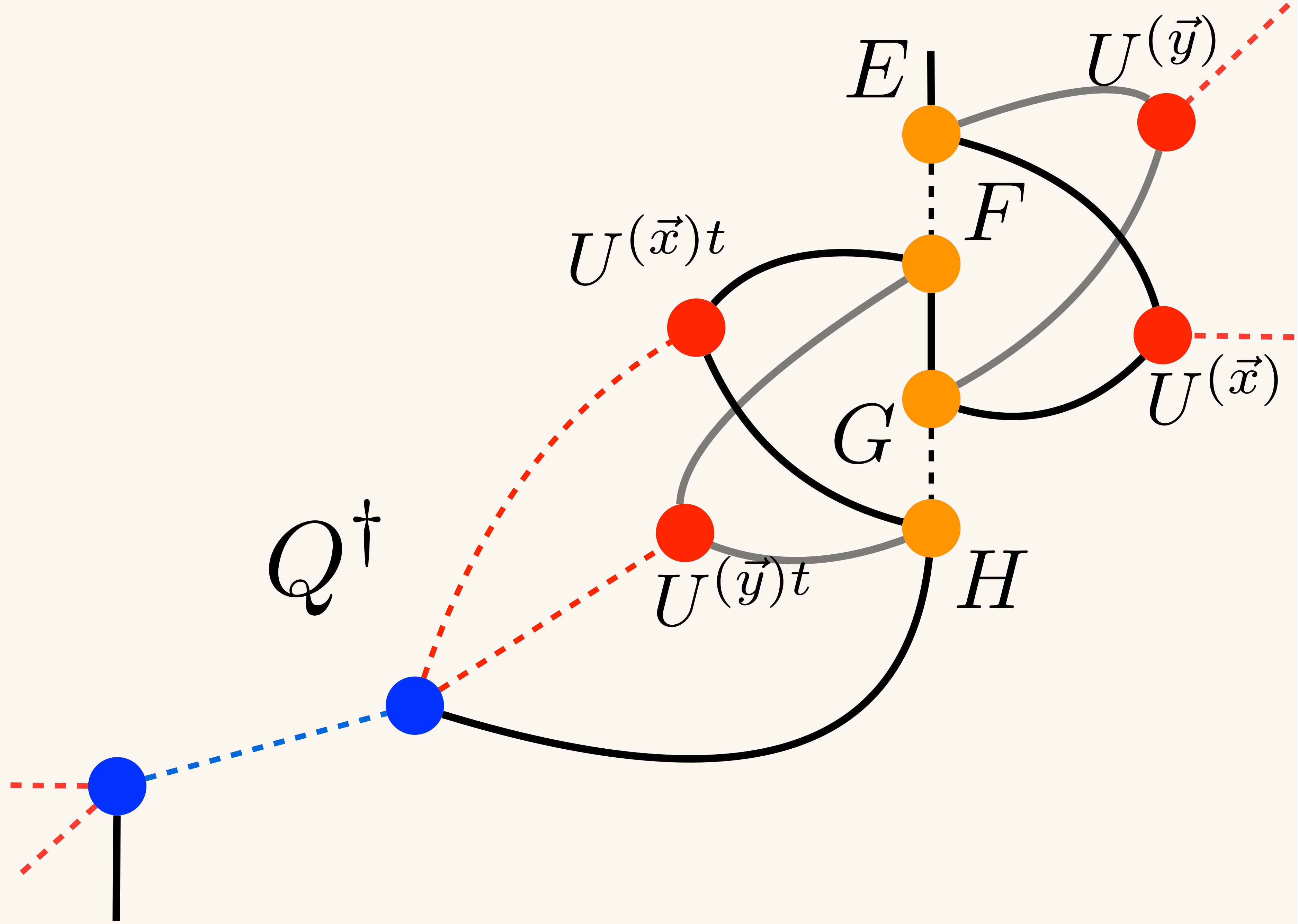
$$QQ^{\dagger}U'^{(\vec{y})t}U'^{(\vec{x})t}EFGHU'^{(\vec{x})}U'^{(\vec{y})} = Q\Lambda \simeq A^{(\mathrm{next})}$$



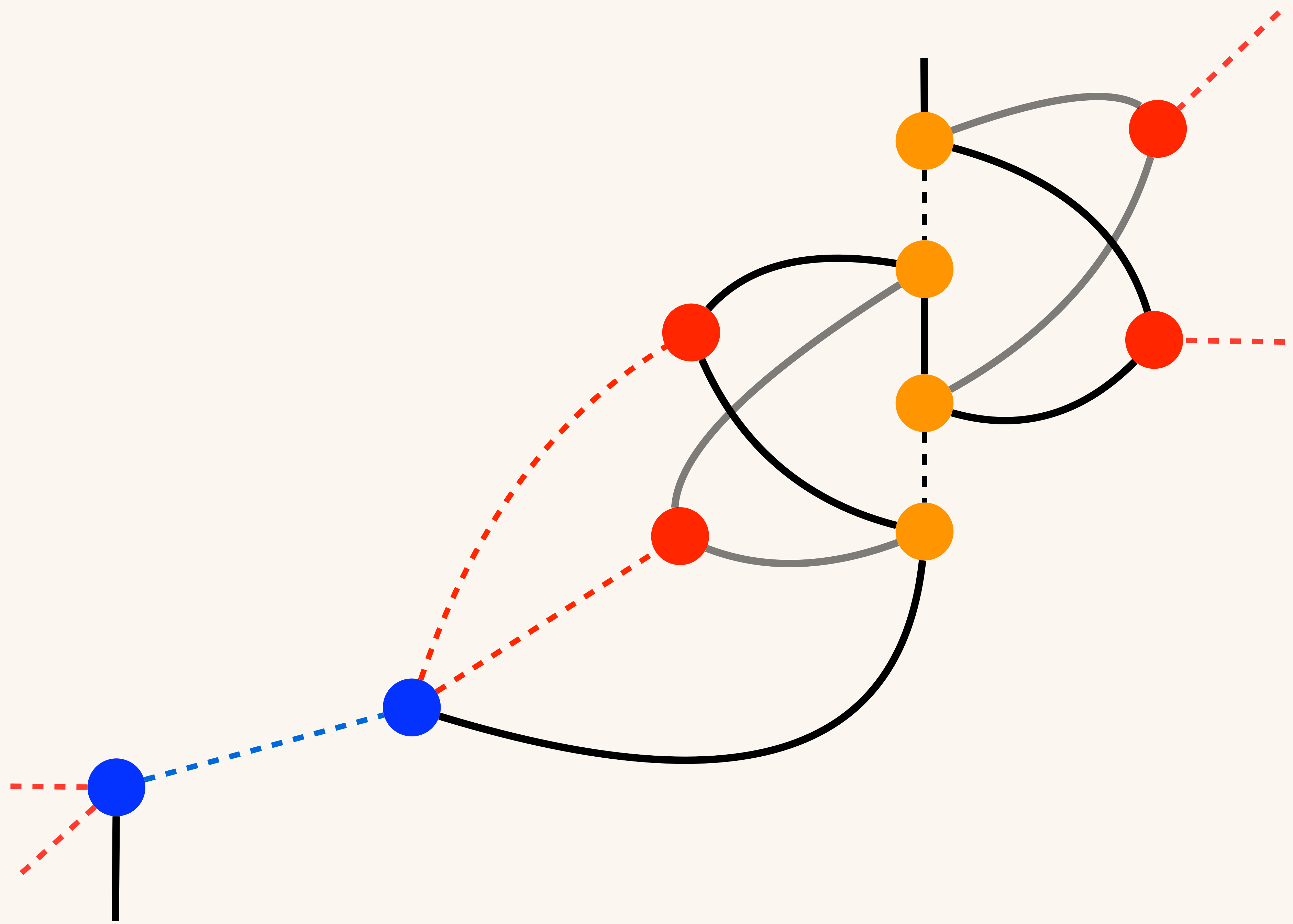
◇ 計算量削減

$$O(D^{3d}) \to O(D^{2d+1})$$

◉ MDTRG: Contraction step

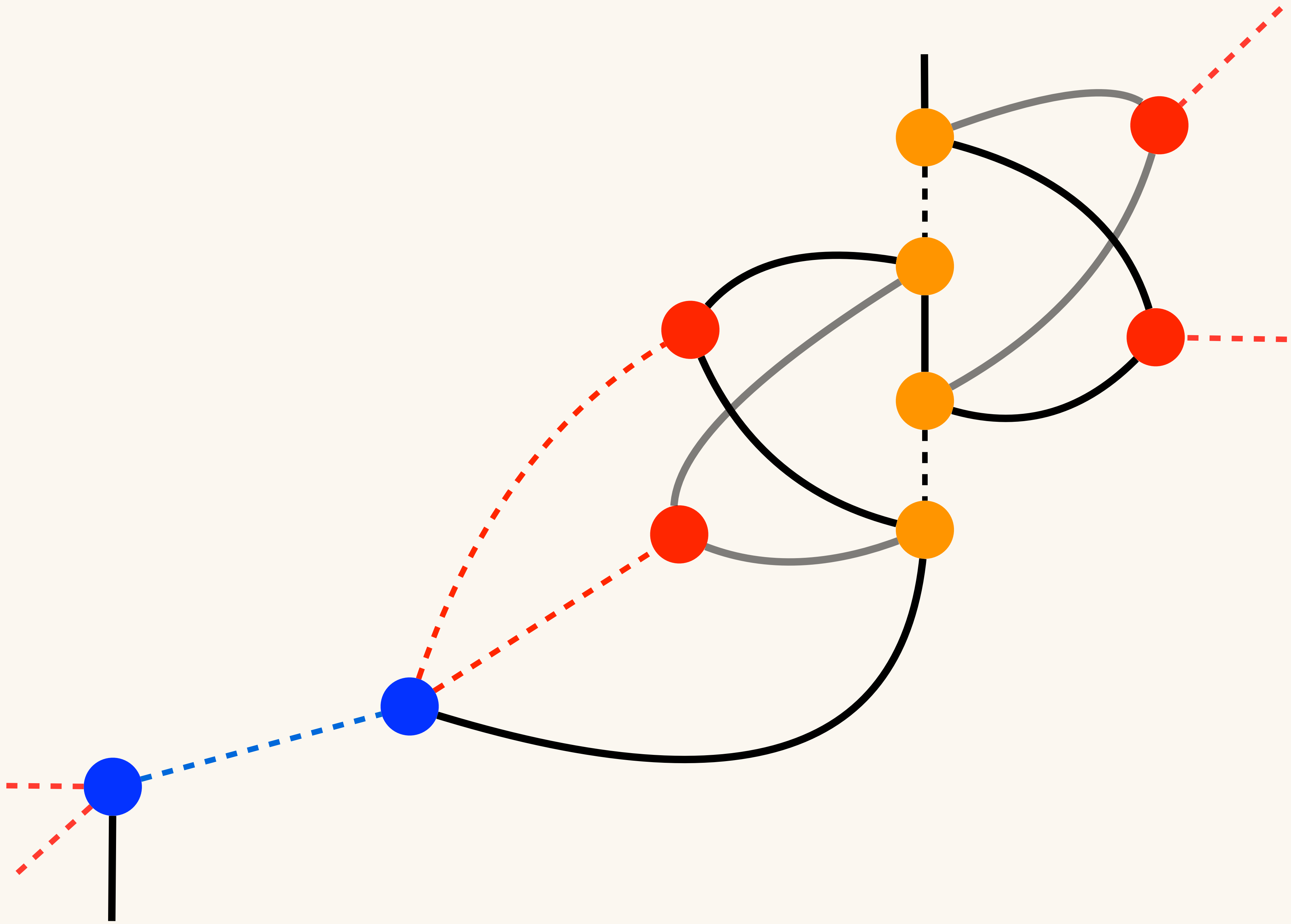


◉ MDTRG: Contraction step



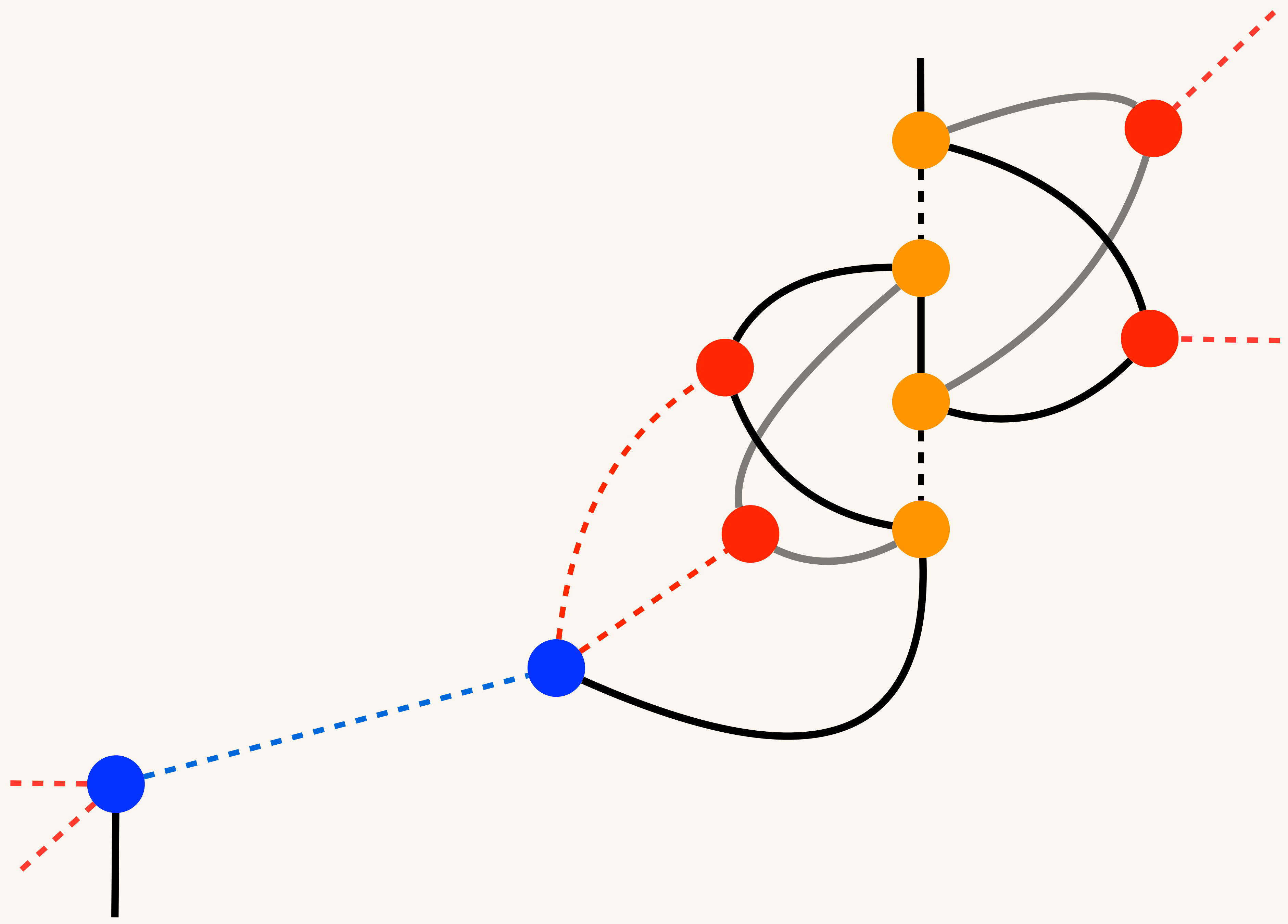
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



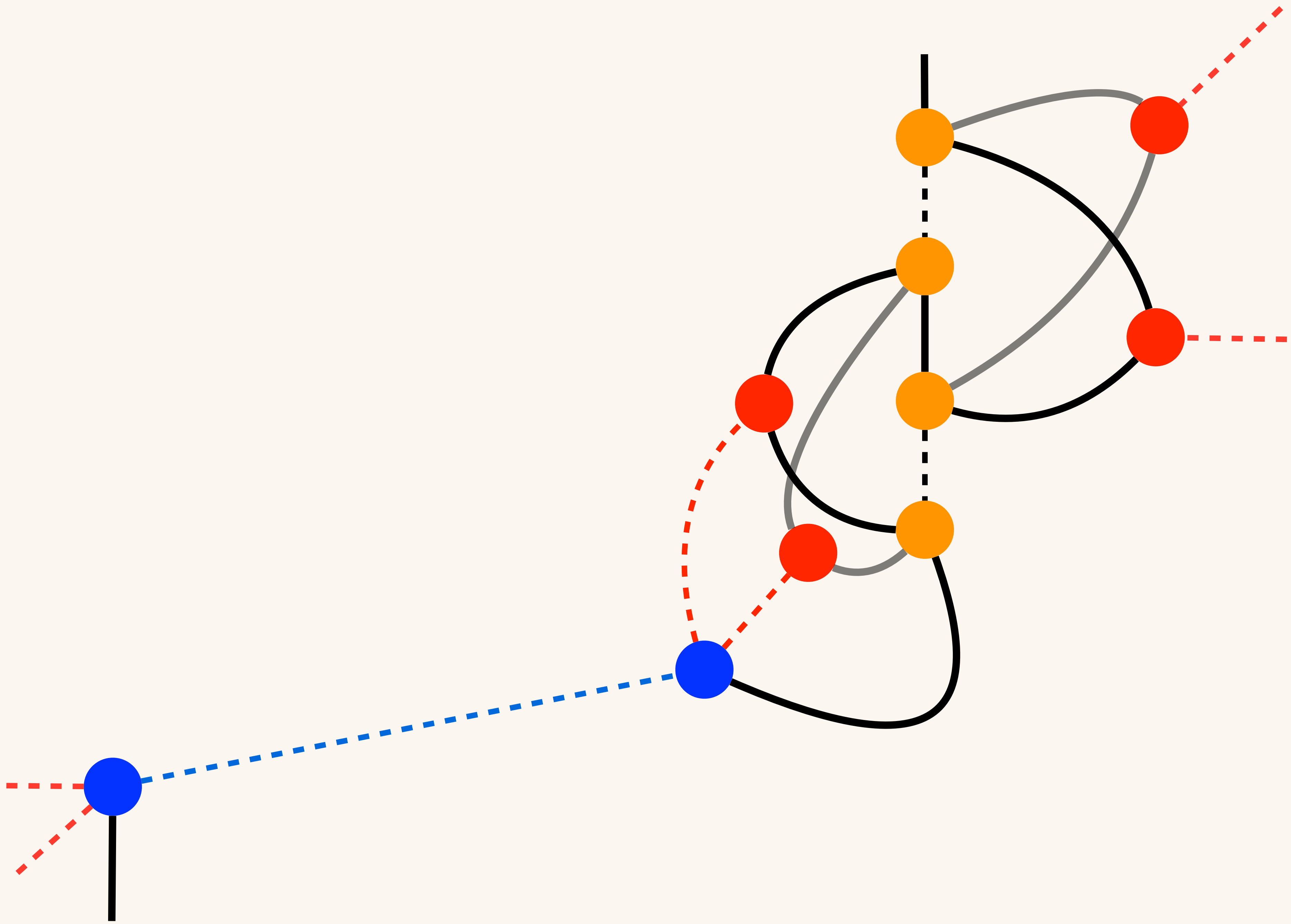
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



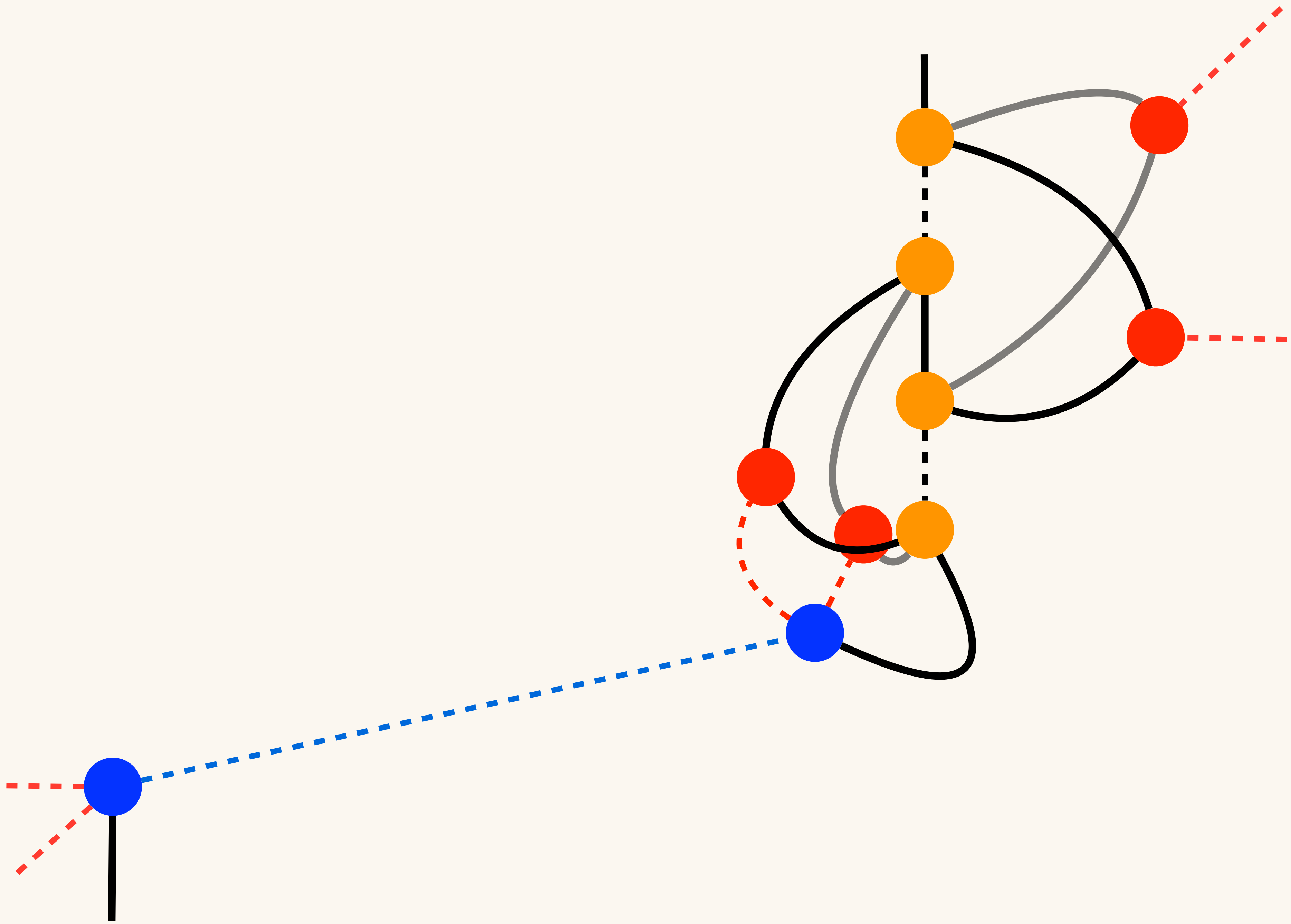
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



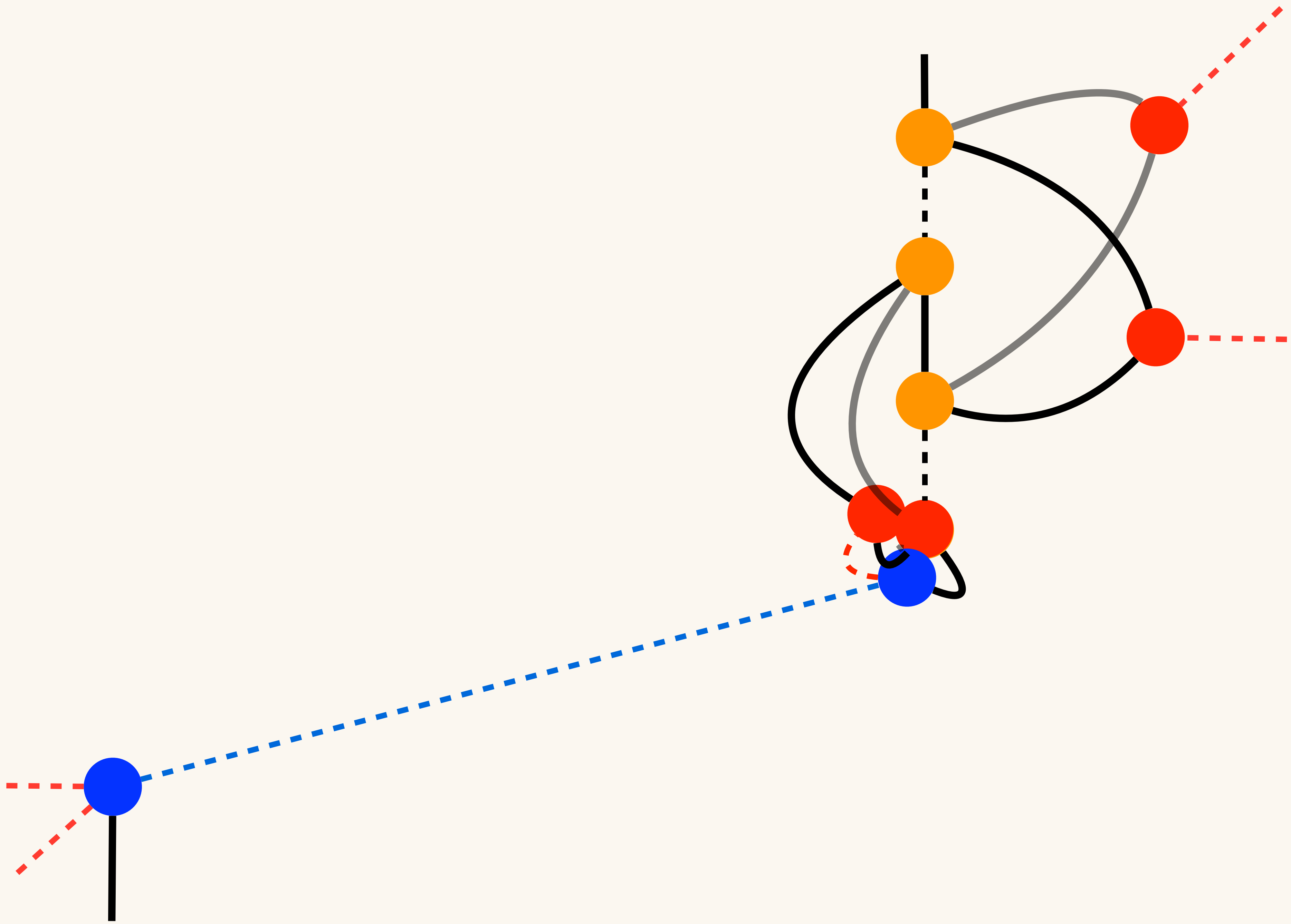
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



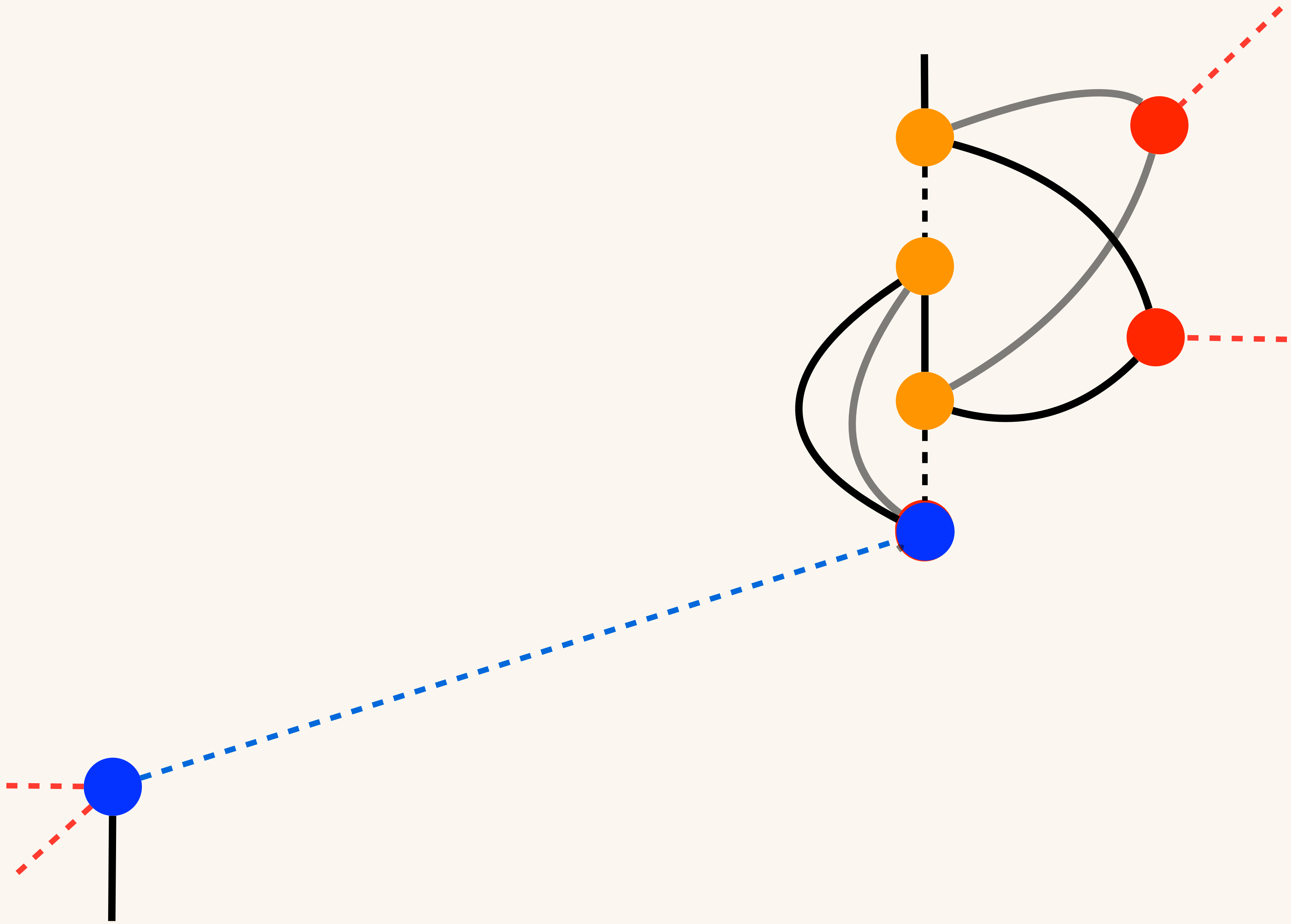
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



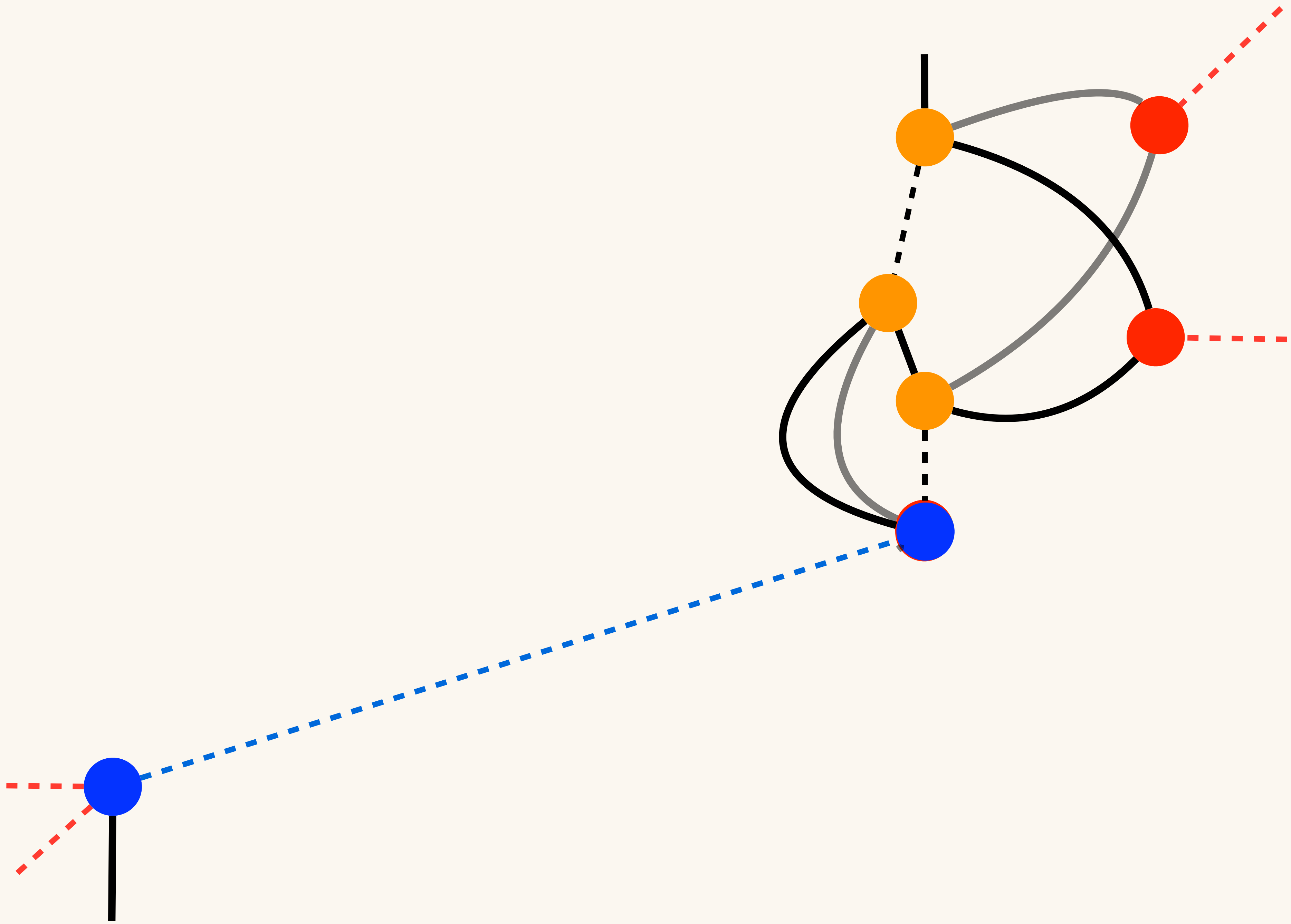
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



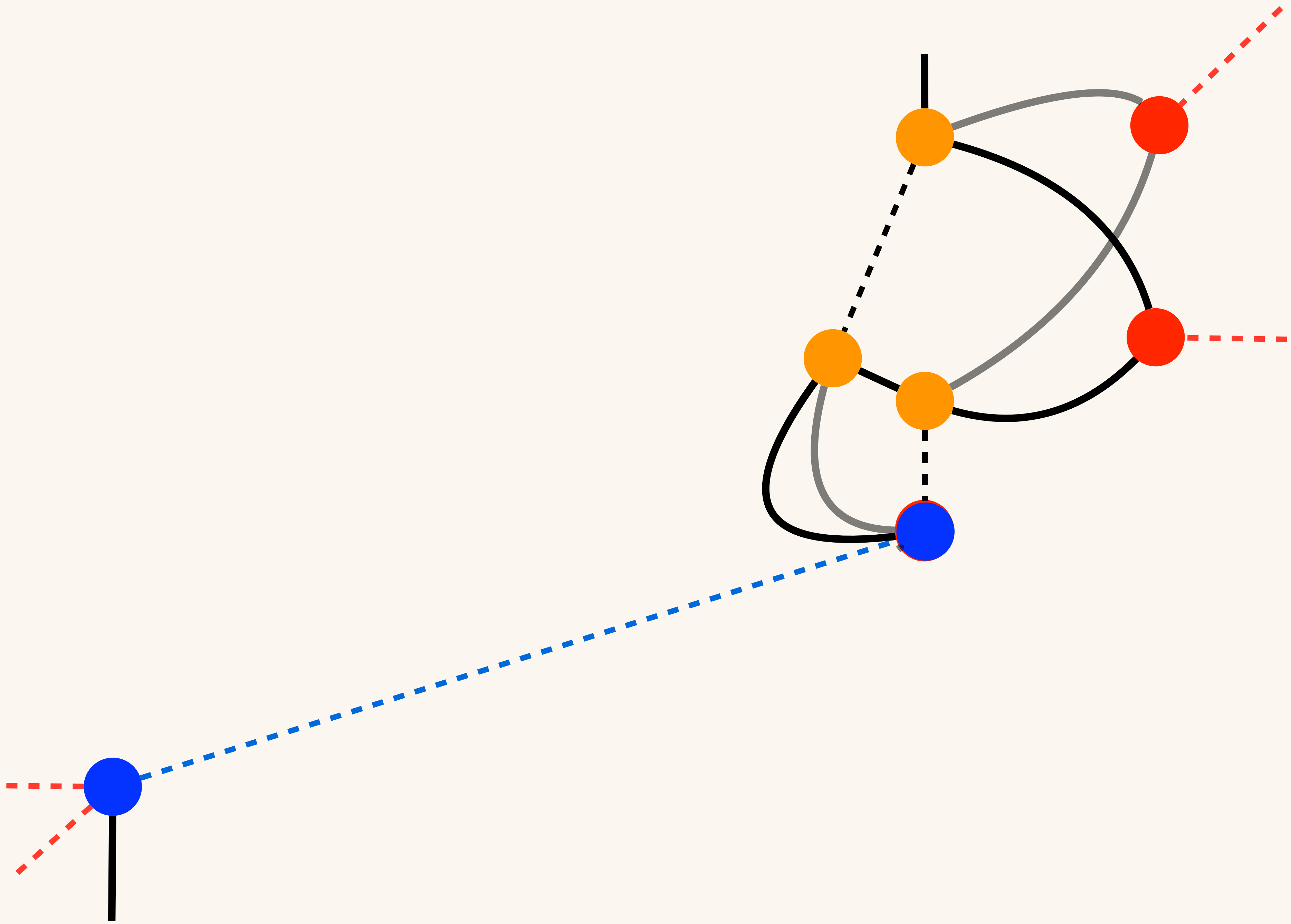
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



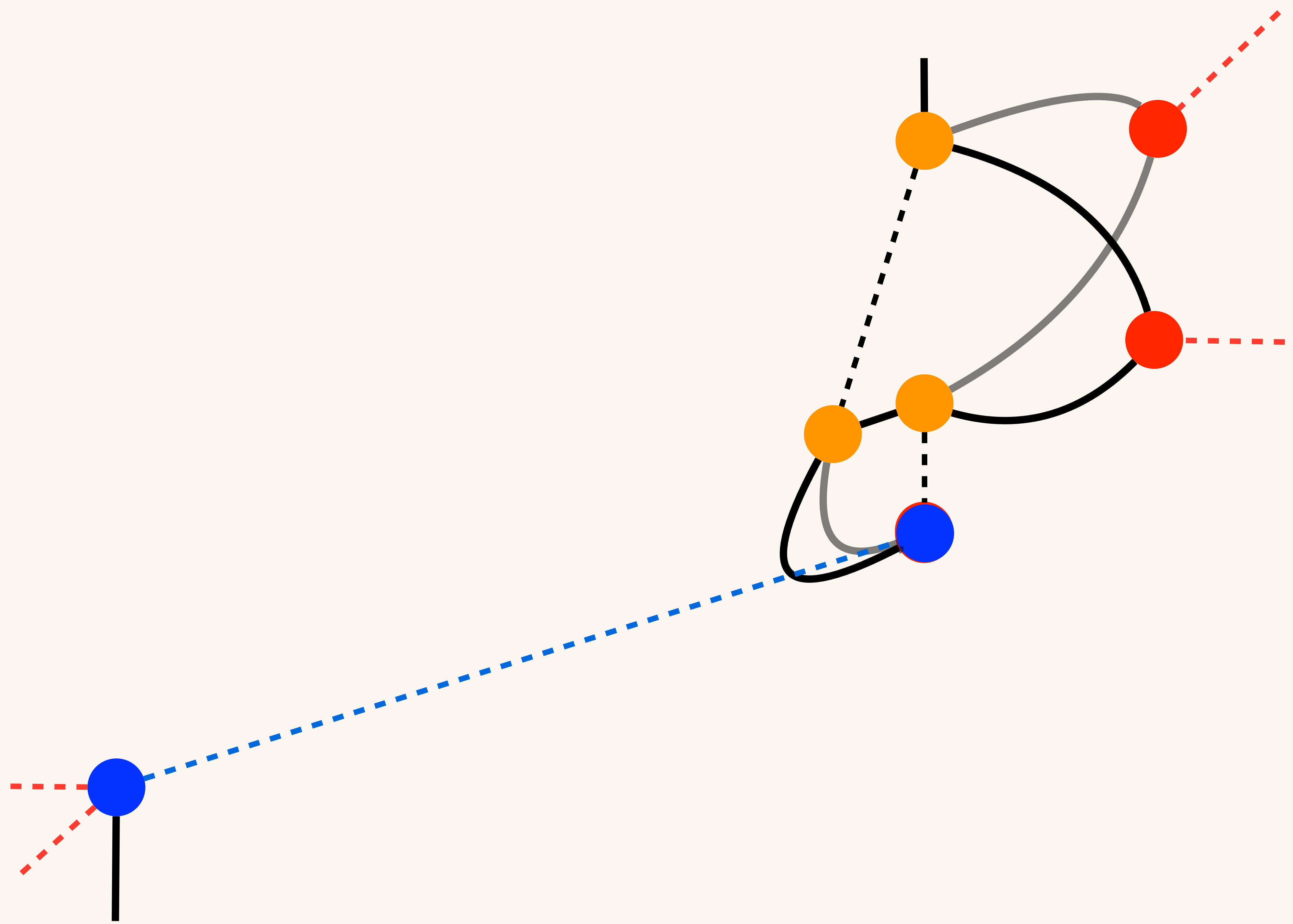
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

MDTRG: Contraction step



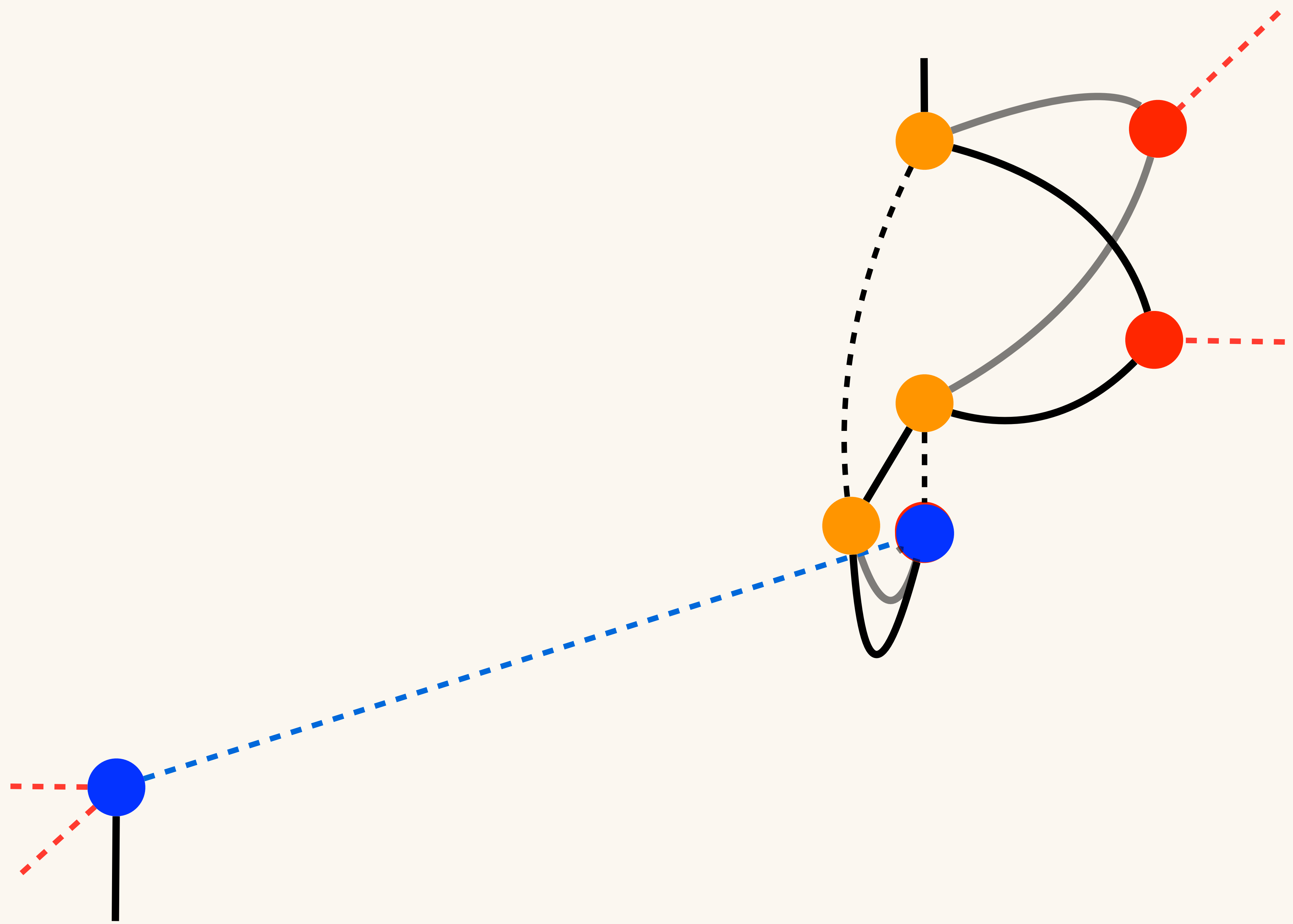
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



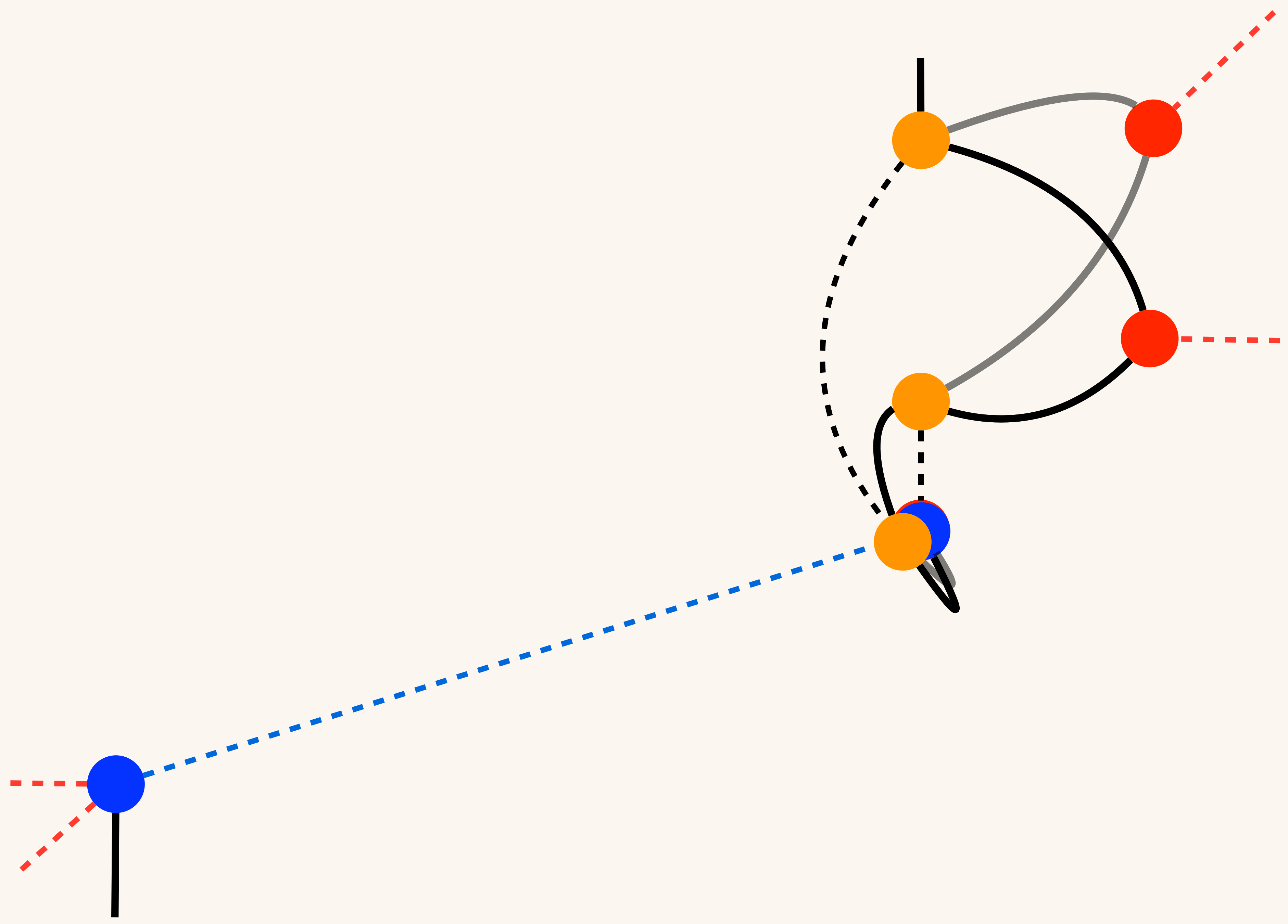
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

MDTRG: Contraction step



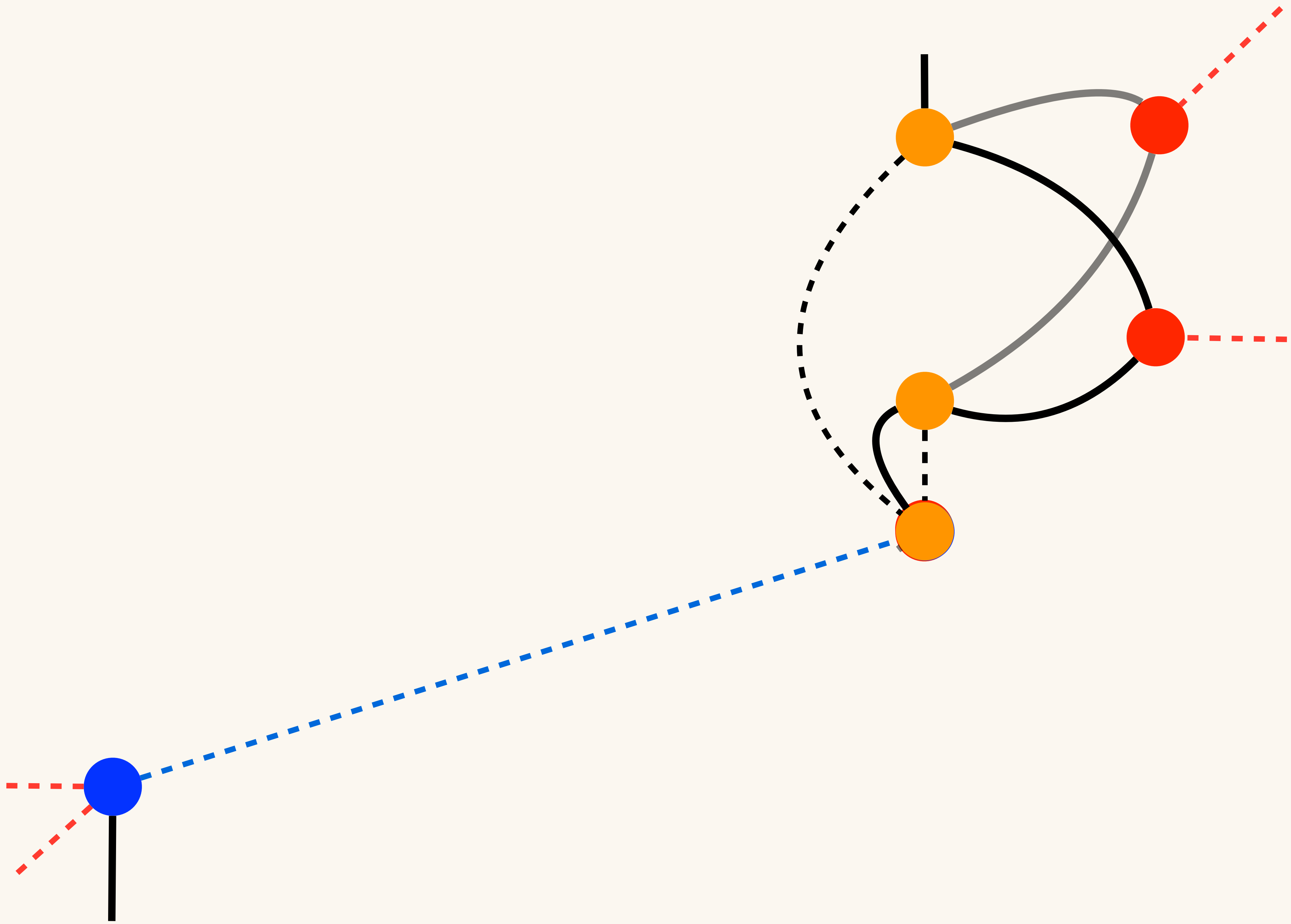
$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$

MDTRG: Contraction step



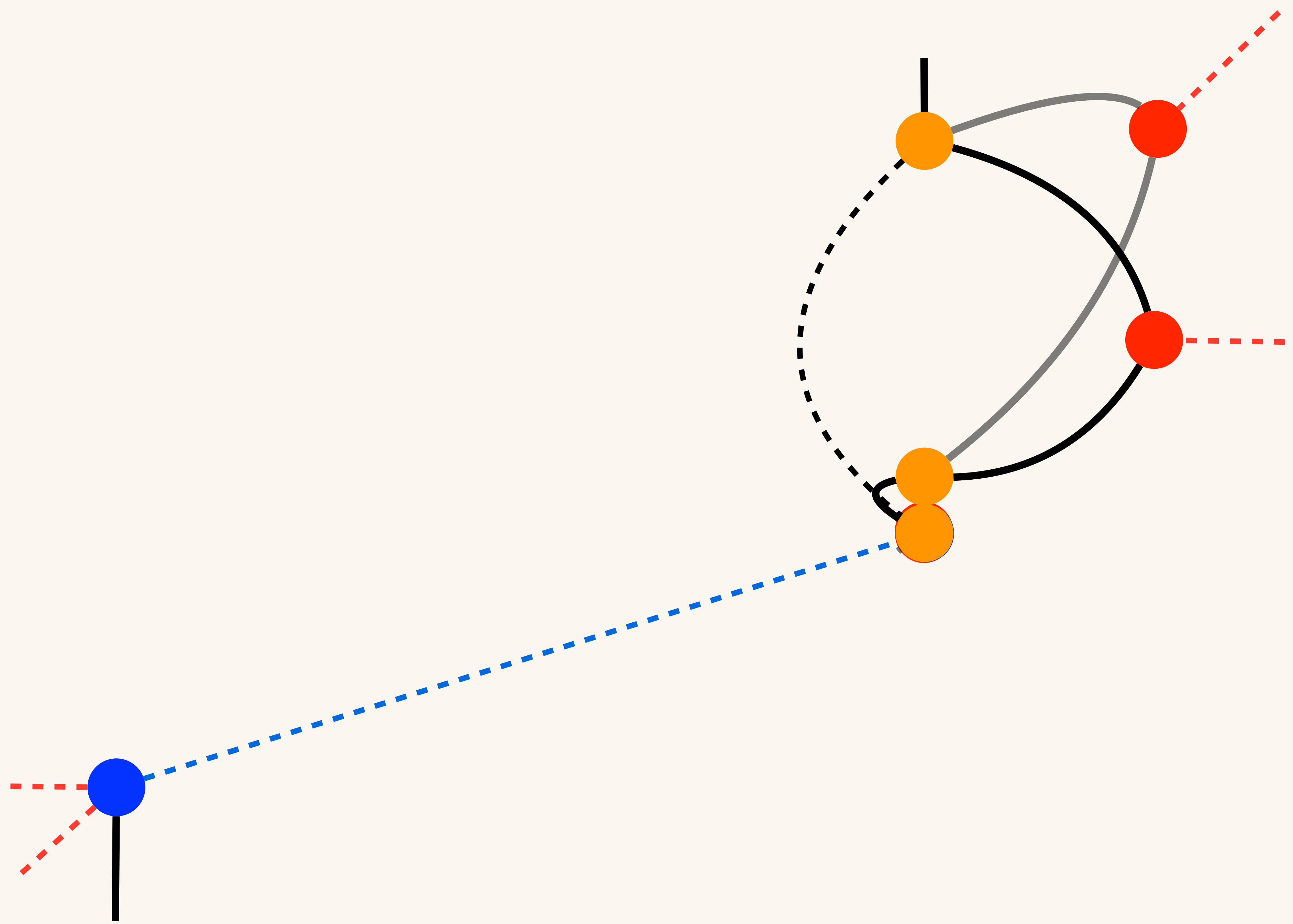
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

MDTRG: Contraction step



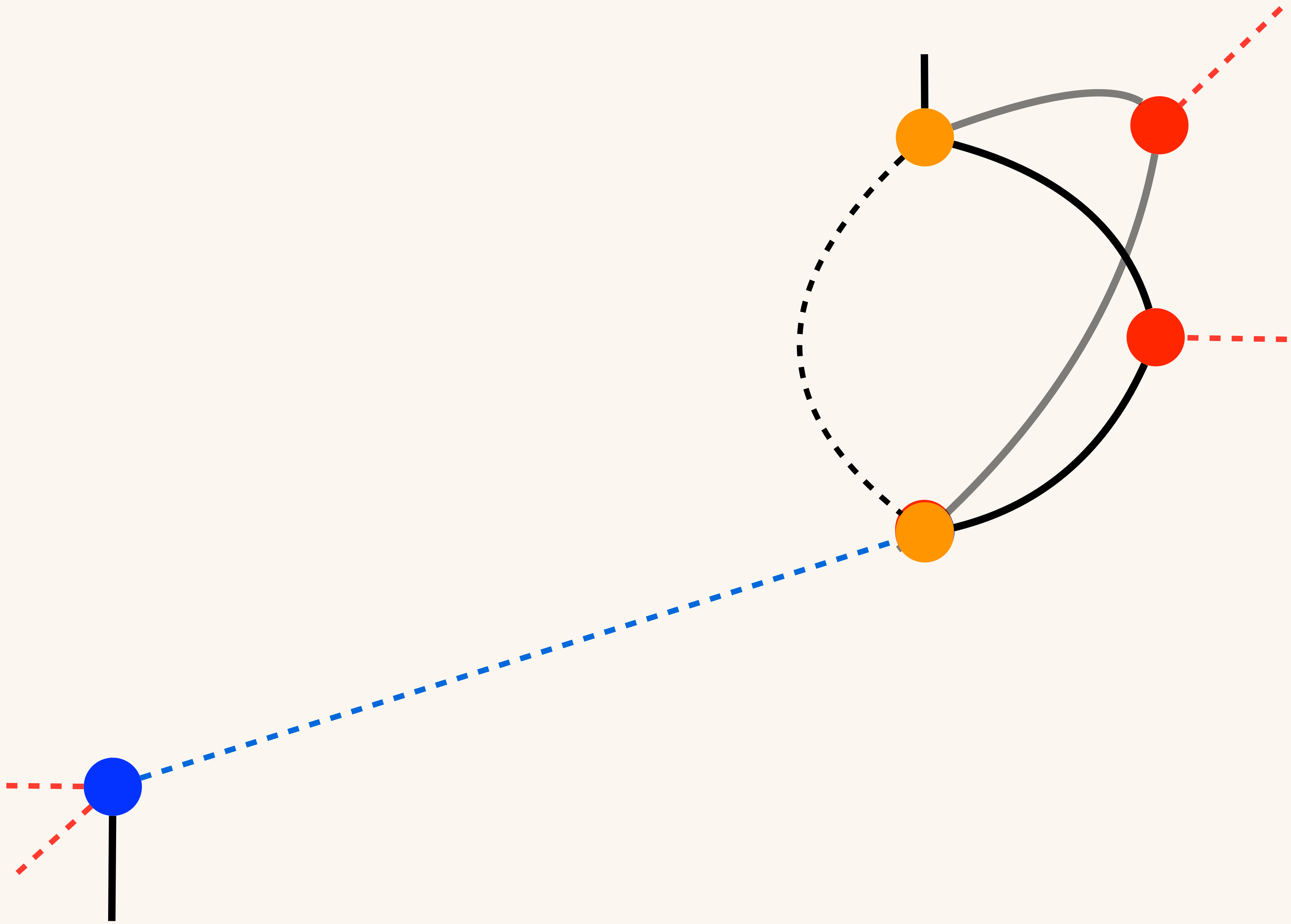
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



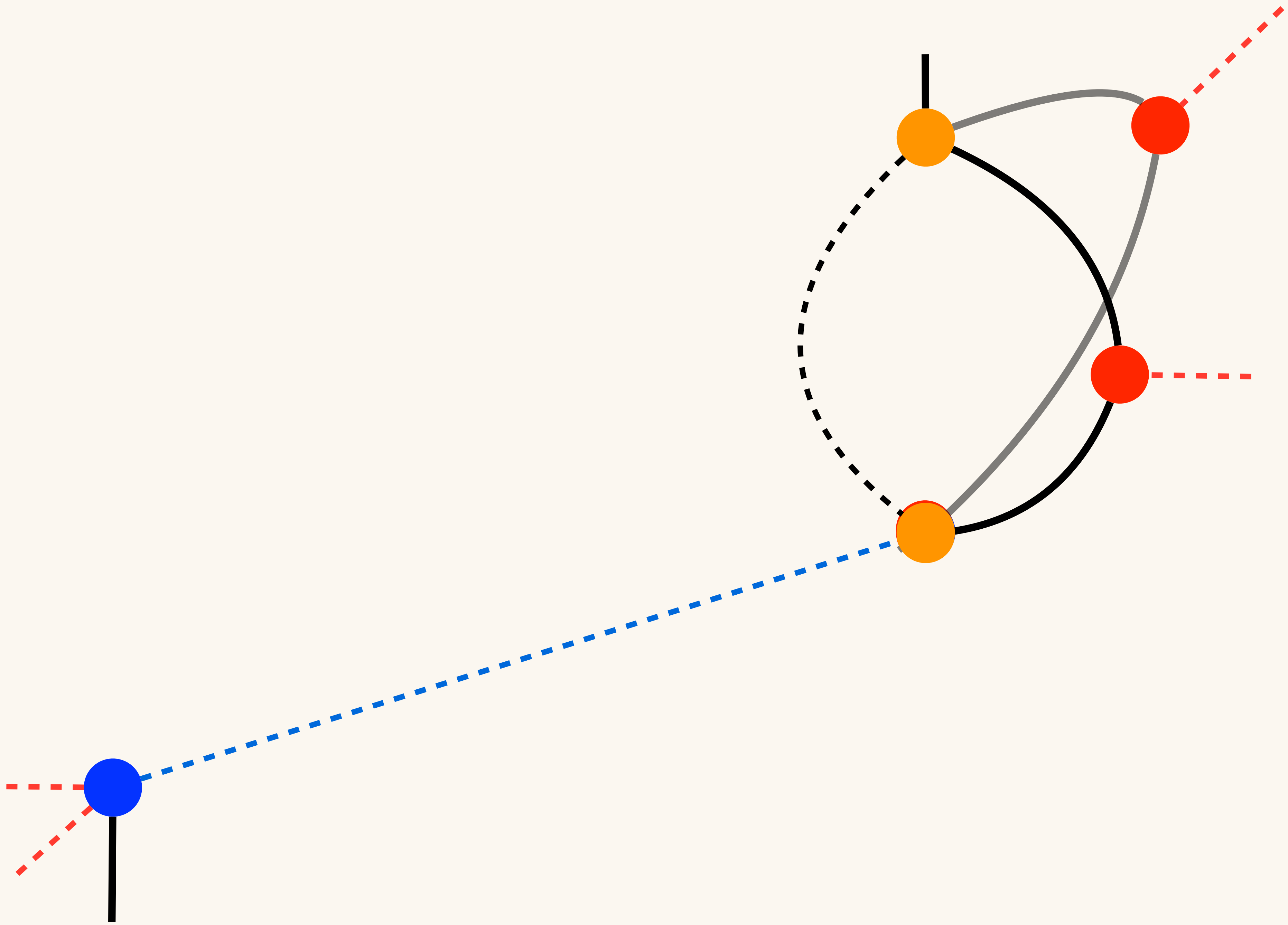
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



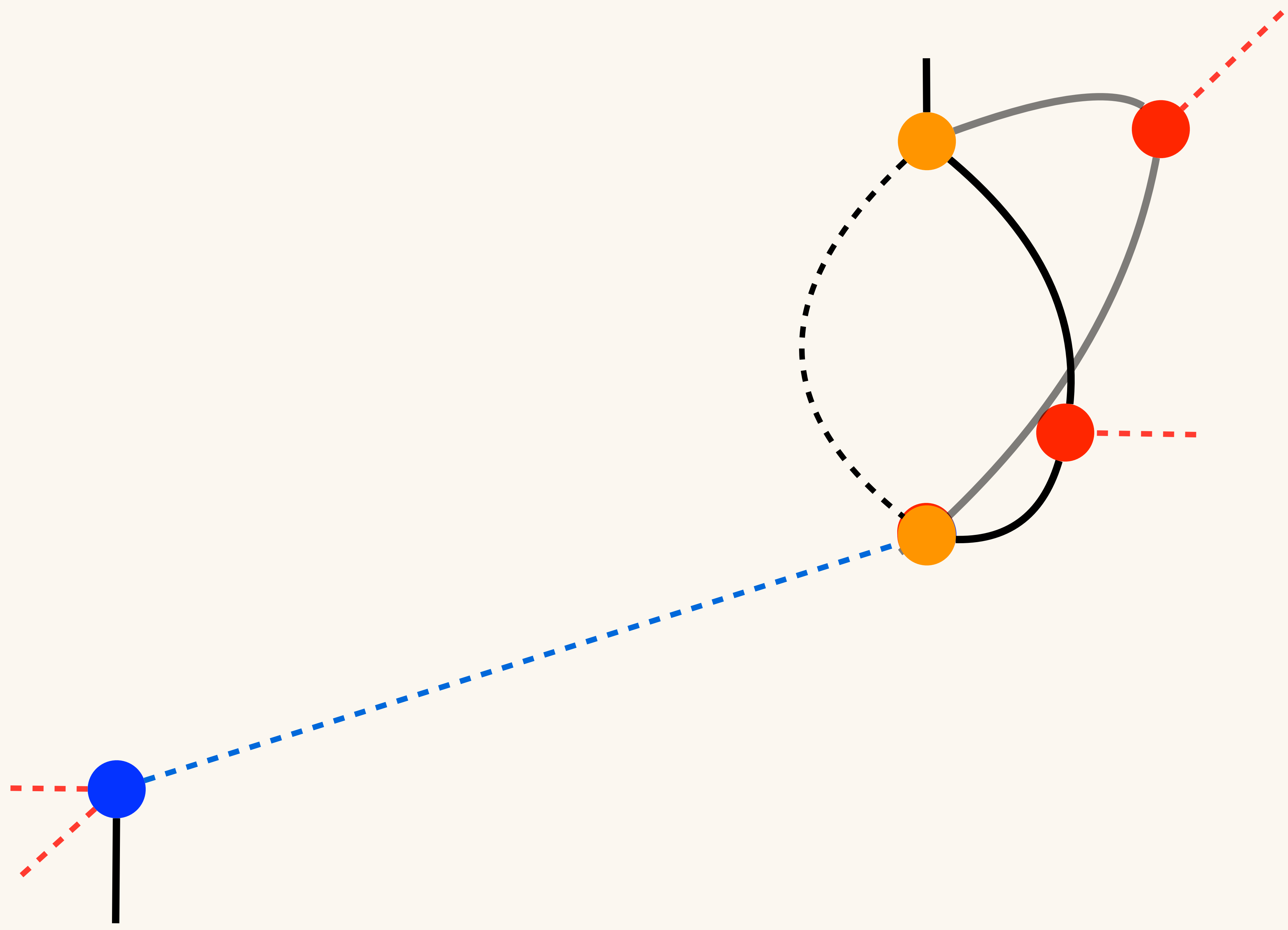
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



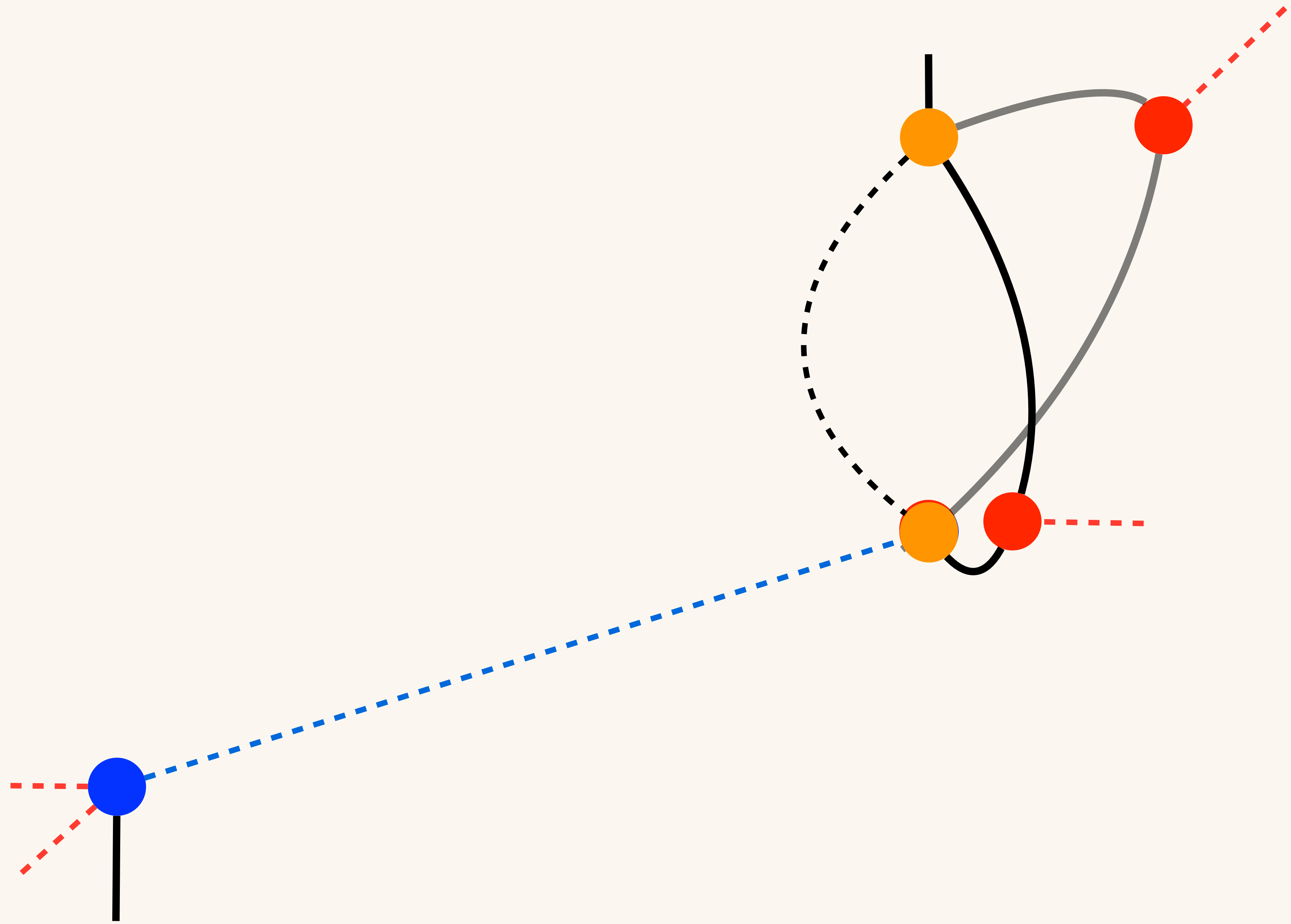
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



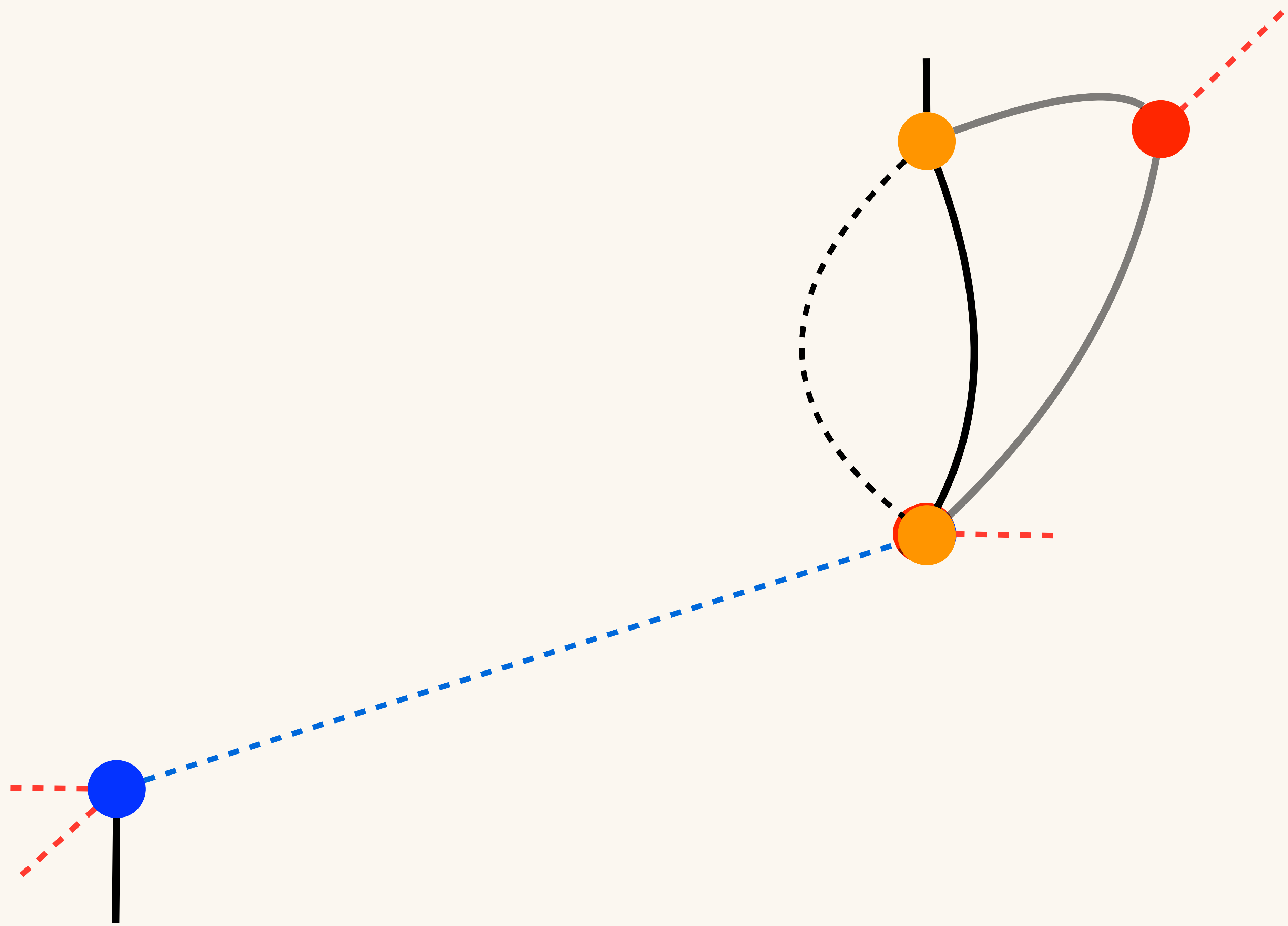
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

MDTRG: Contraction step



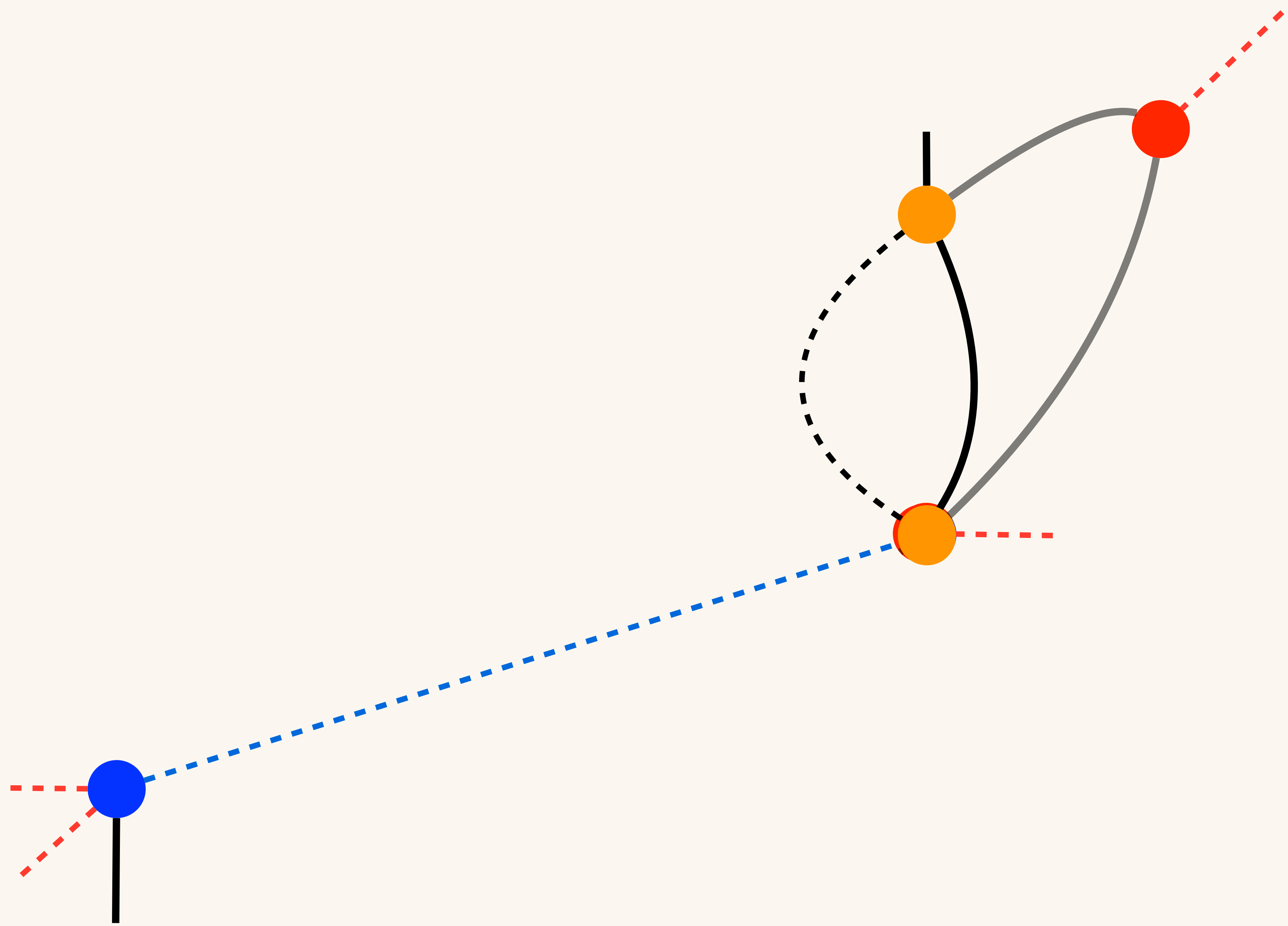
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



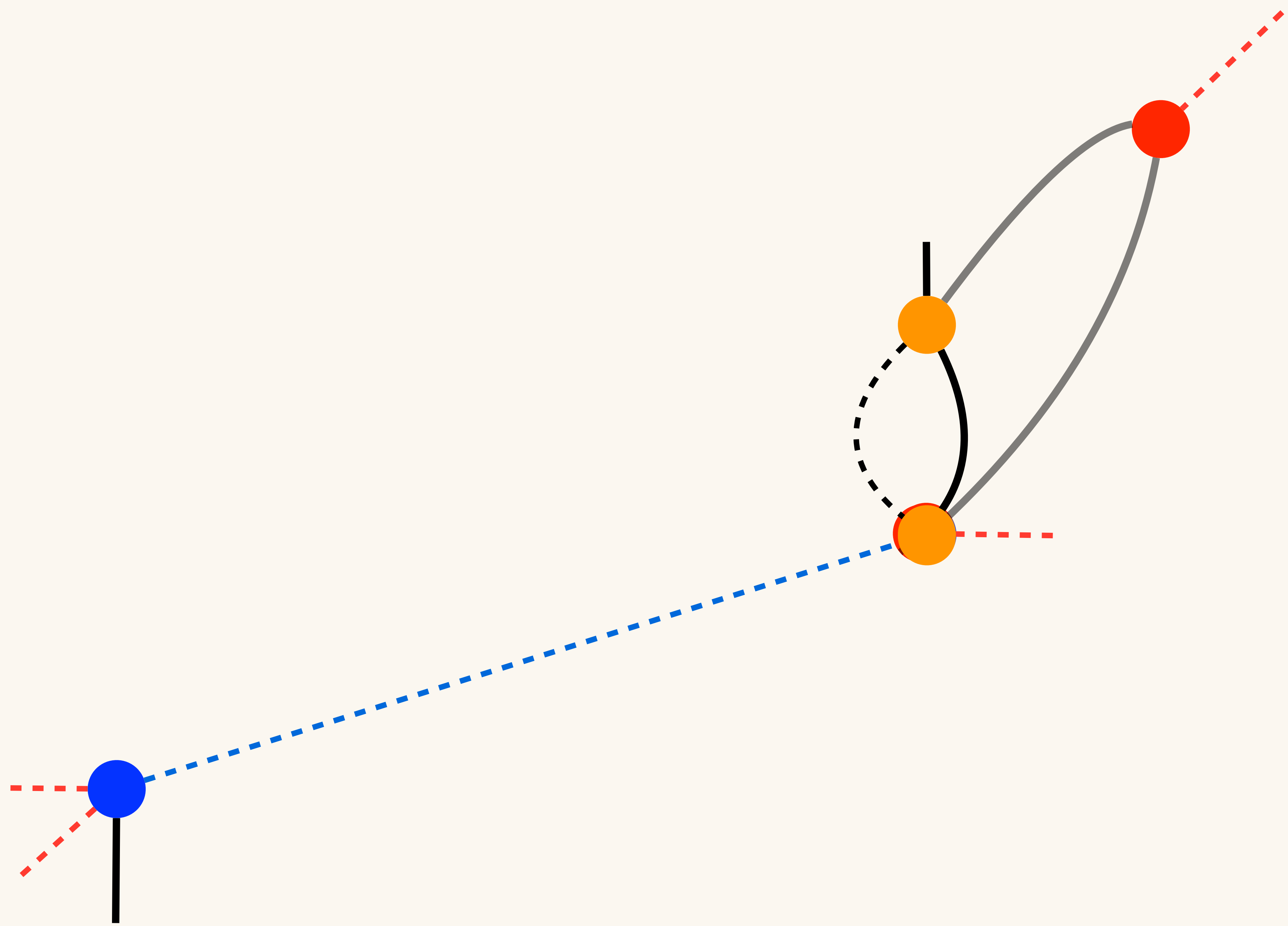
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



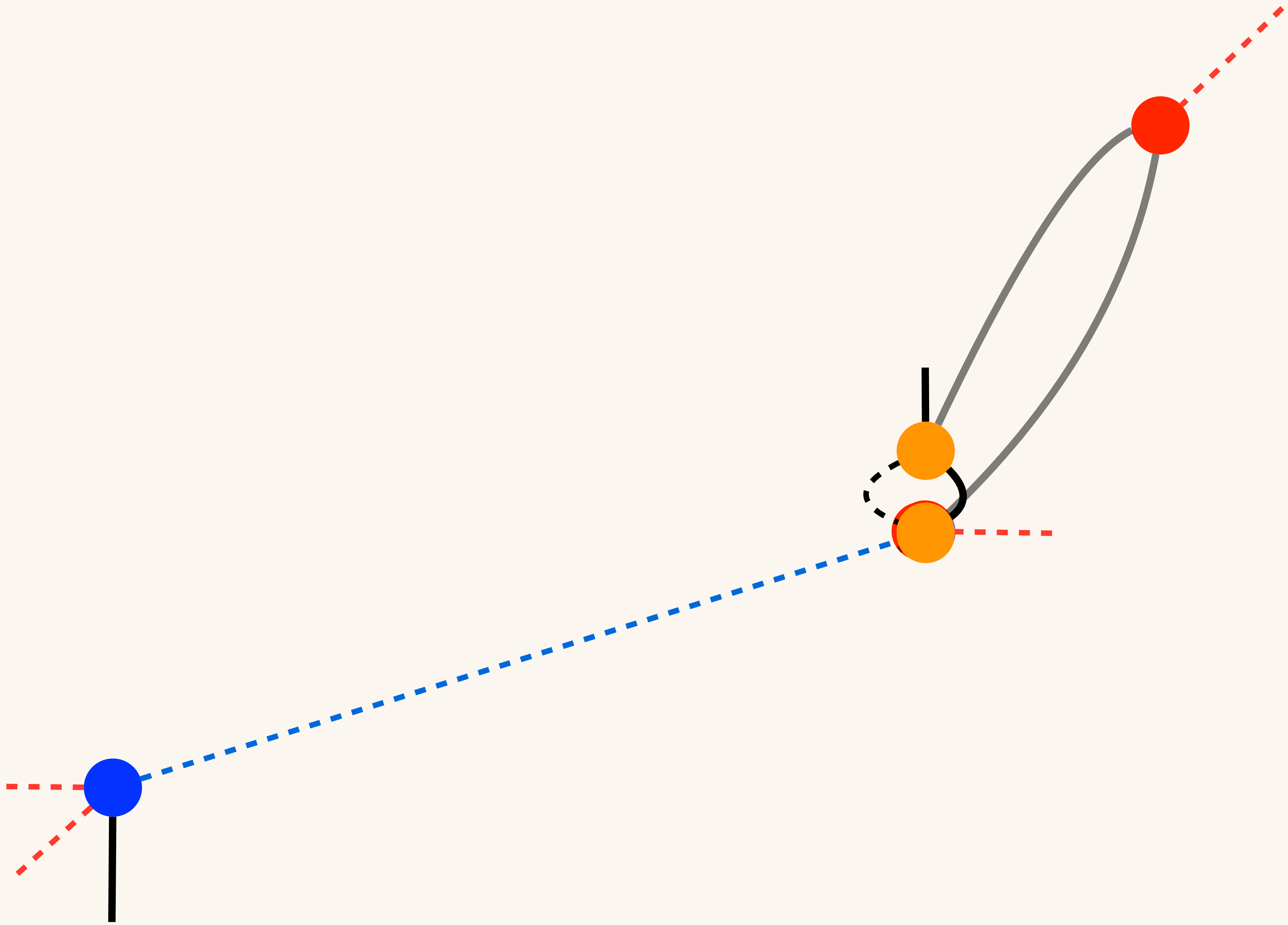
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

MDTRG: Contraction step



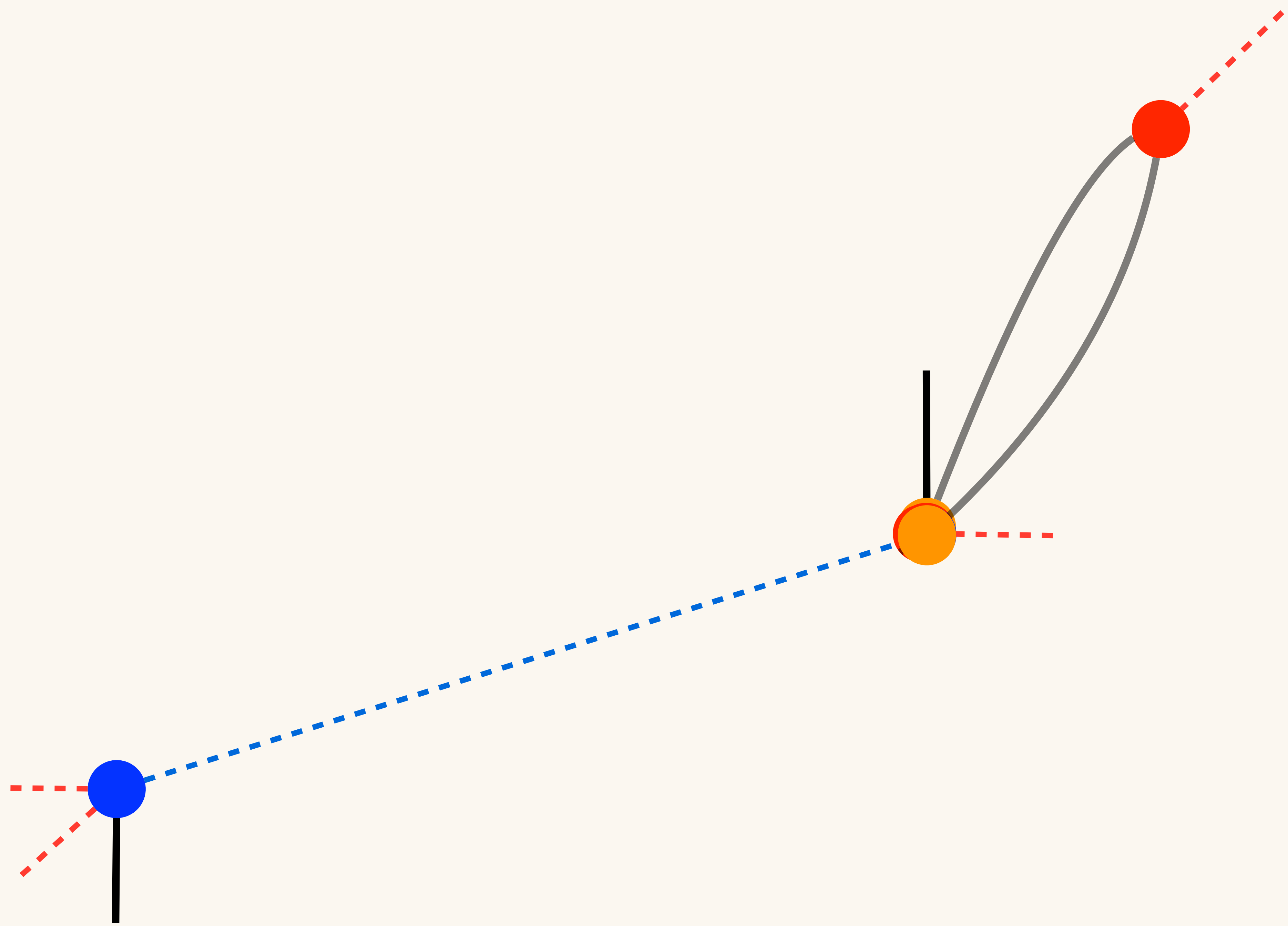
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



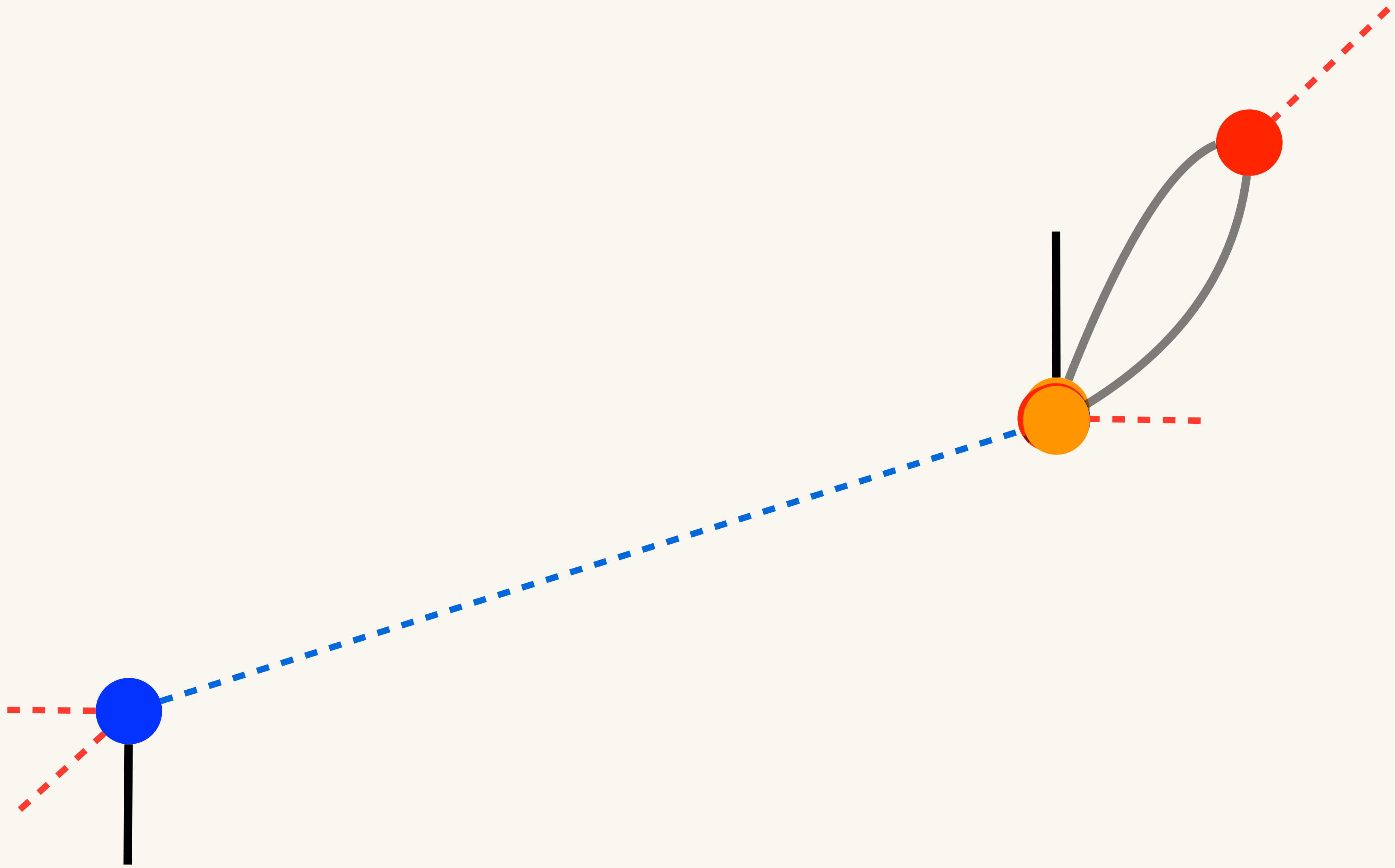
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



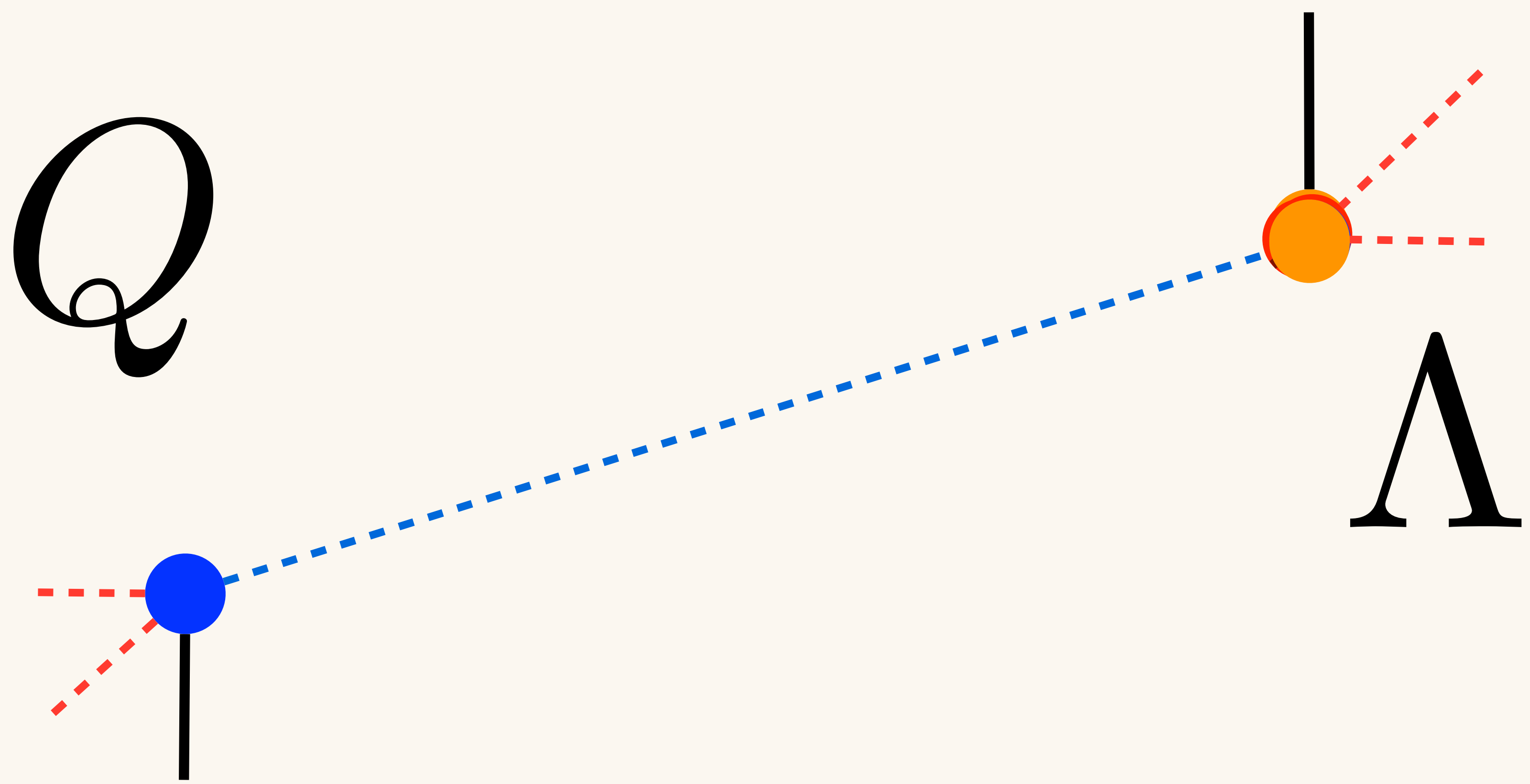
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ MDTRG: Contraction step



$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

MDTRG: Contraction step

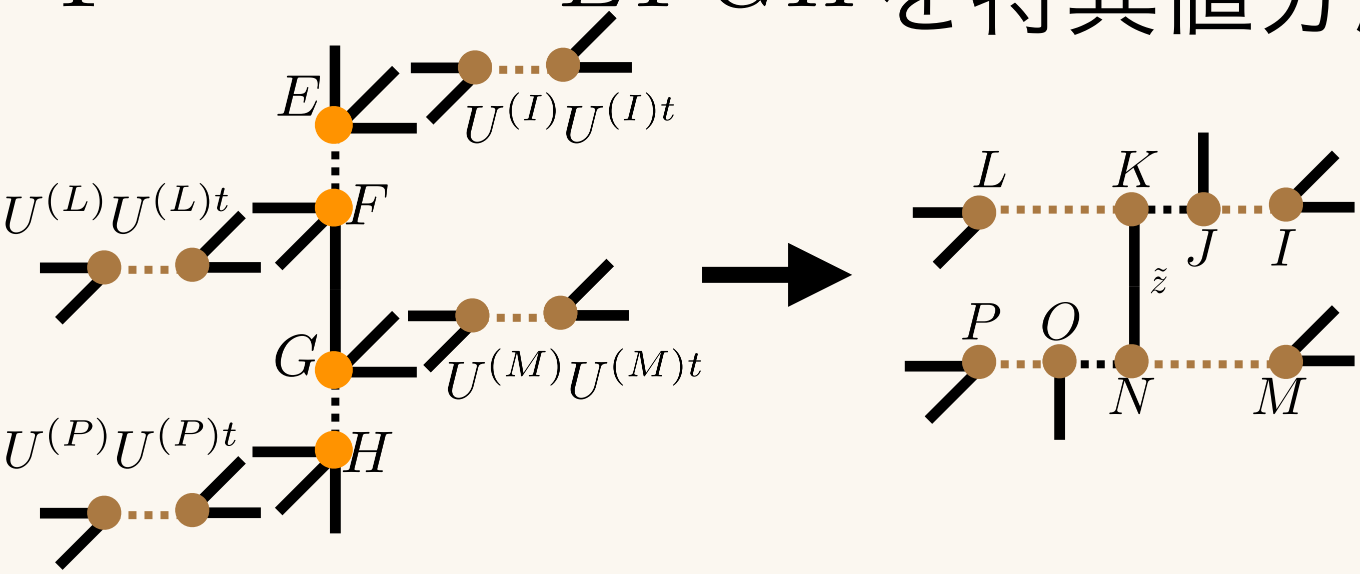


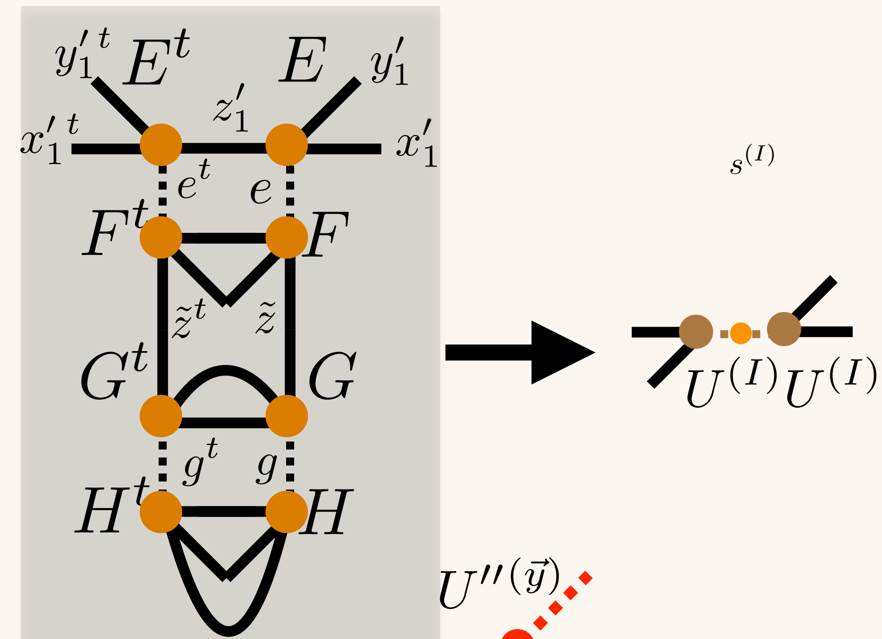
$$O(D^7) \to O(D^6) \to O(D^6) \to O(D^6) \to O(D^7) \to O(D^6)$$

◉ Minimally-decomposed TRG on triad rep.

◇ MDTRGをTriad表現。注目してるunit-cell tensor network

$\Gamma^{(EFGH)} = EFGH$を特異値分解.





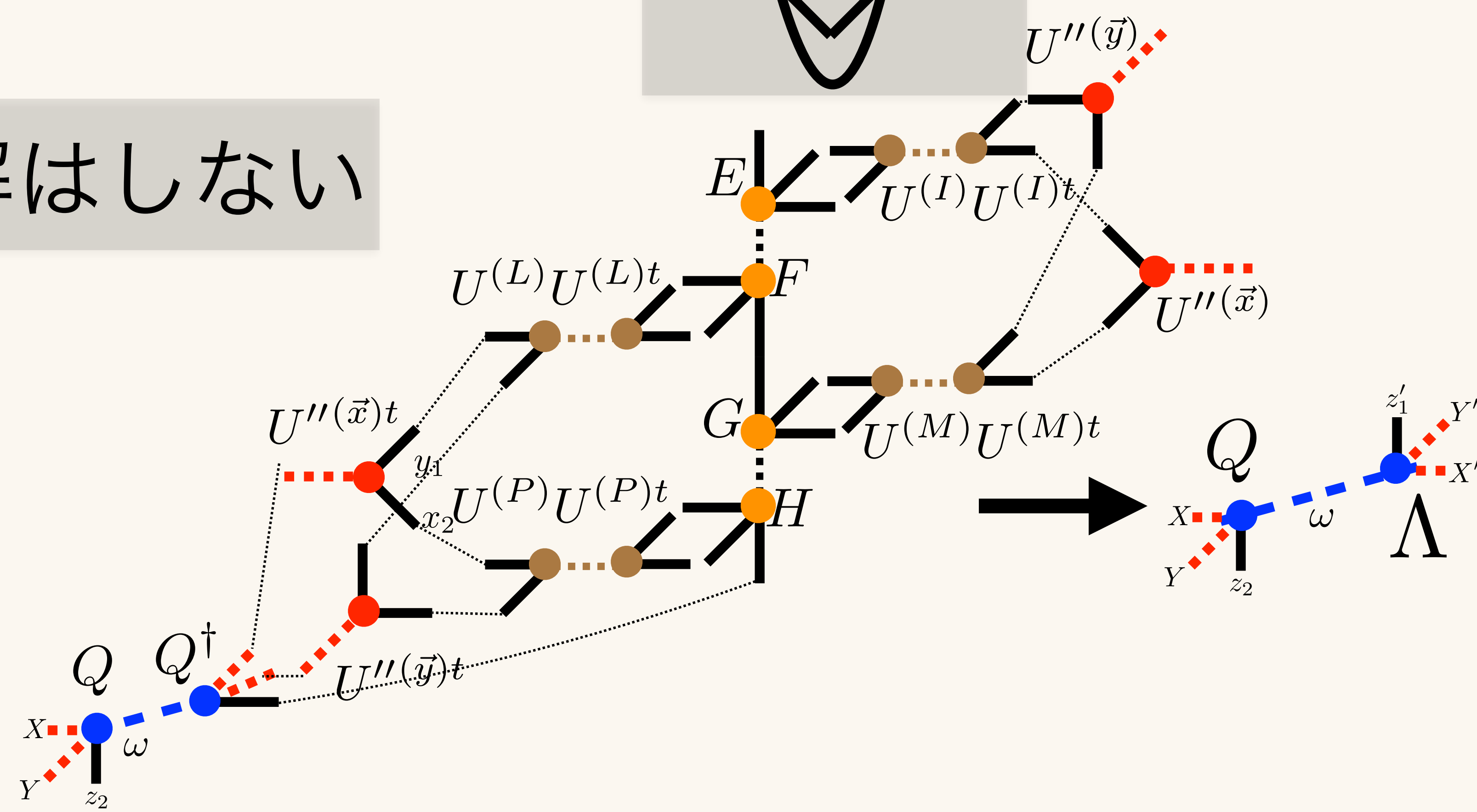
◇ E,F,G,Hを個別に分解はしない

✕ $E = U^{(0)} s^{(0)} V^{(0)}$

◇$\Gamma\Gamma^t$の分解で近似する

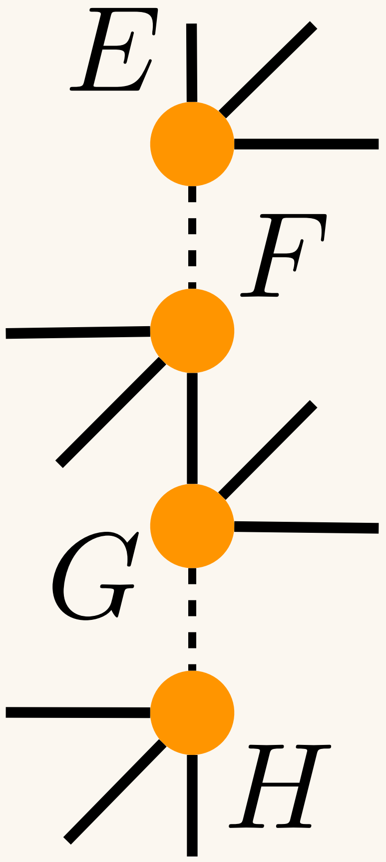
◇ 計算量削減

$O(D^{2d+1}) \to O(D^{d+3})$



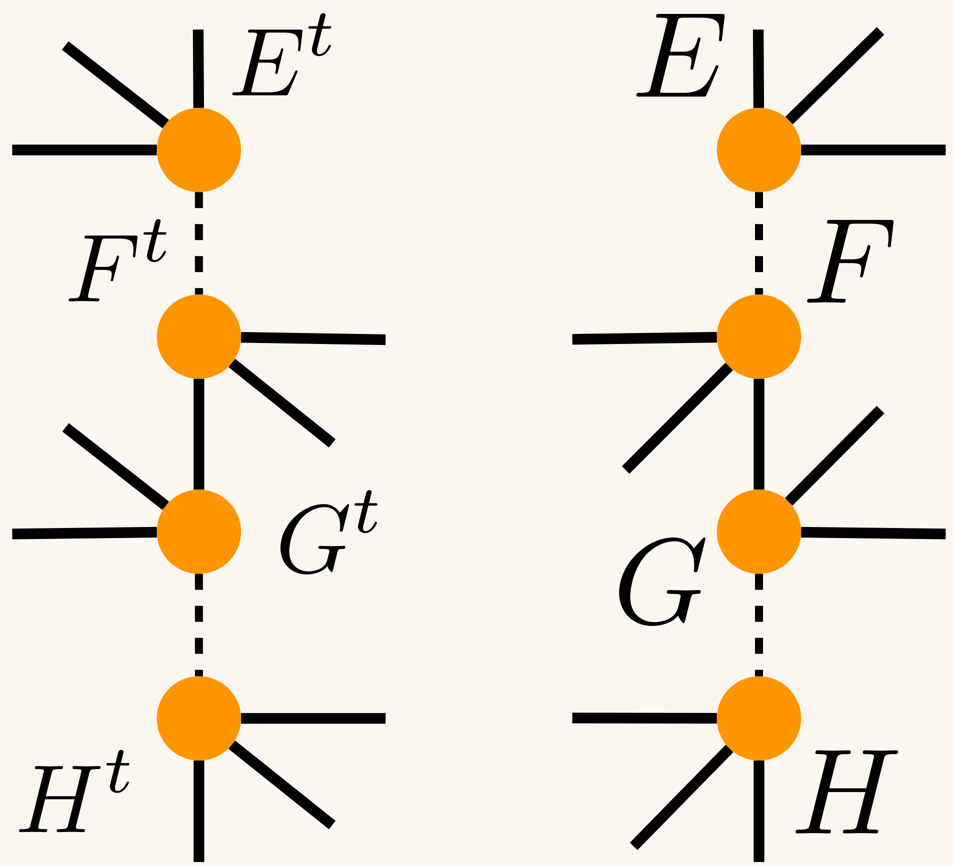
$QQ^\dagger U''^{(\vec{y})t} U''^{(\vec{x})t} U^{(LP)} U^{(LP)t} EFGH U^{(IM)} U^{(IM)t} U''^{(\vec{x})} U''^{(\vec{y})} = Q\Lambda \simeq A^{(\mathrm{next})}$

Triad-MDTRG: Isometry step



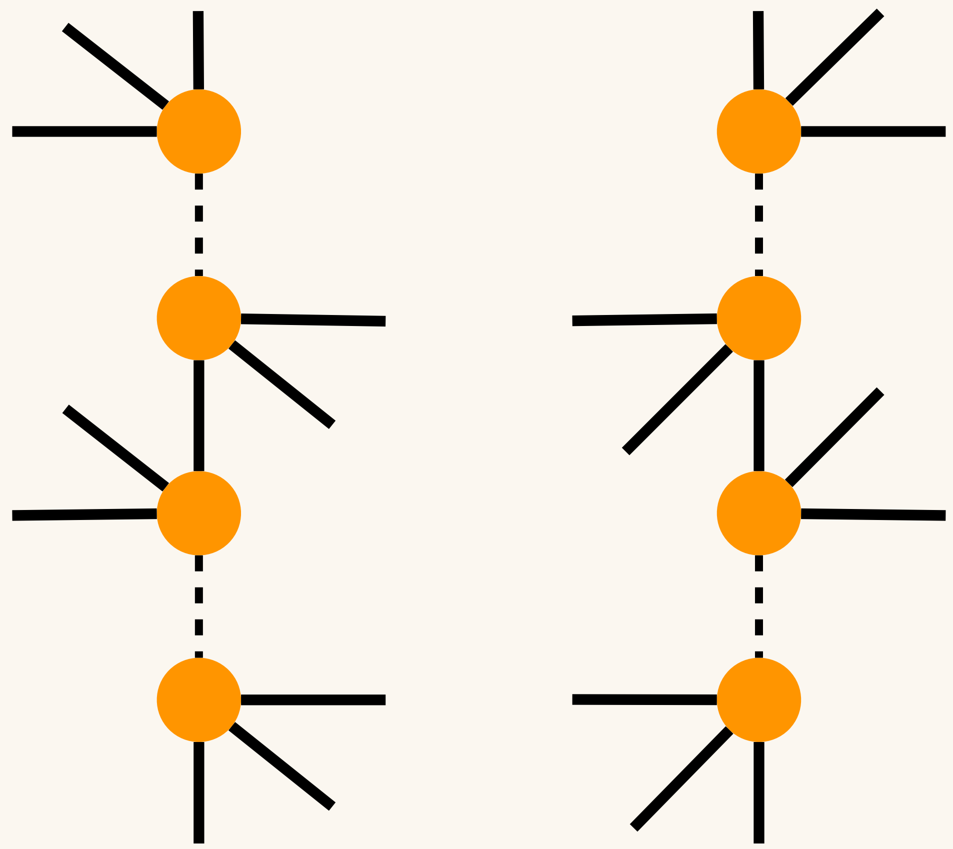
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



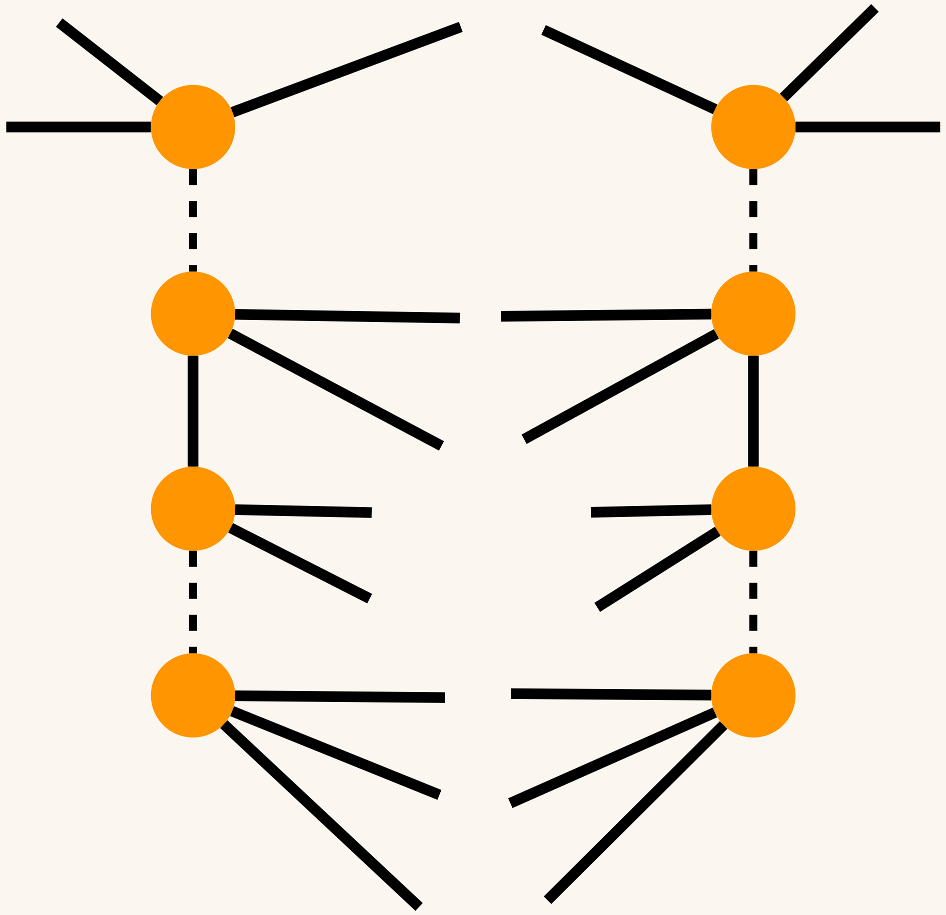
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

◉ Triad-MDTRG: Isometry step



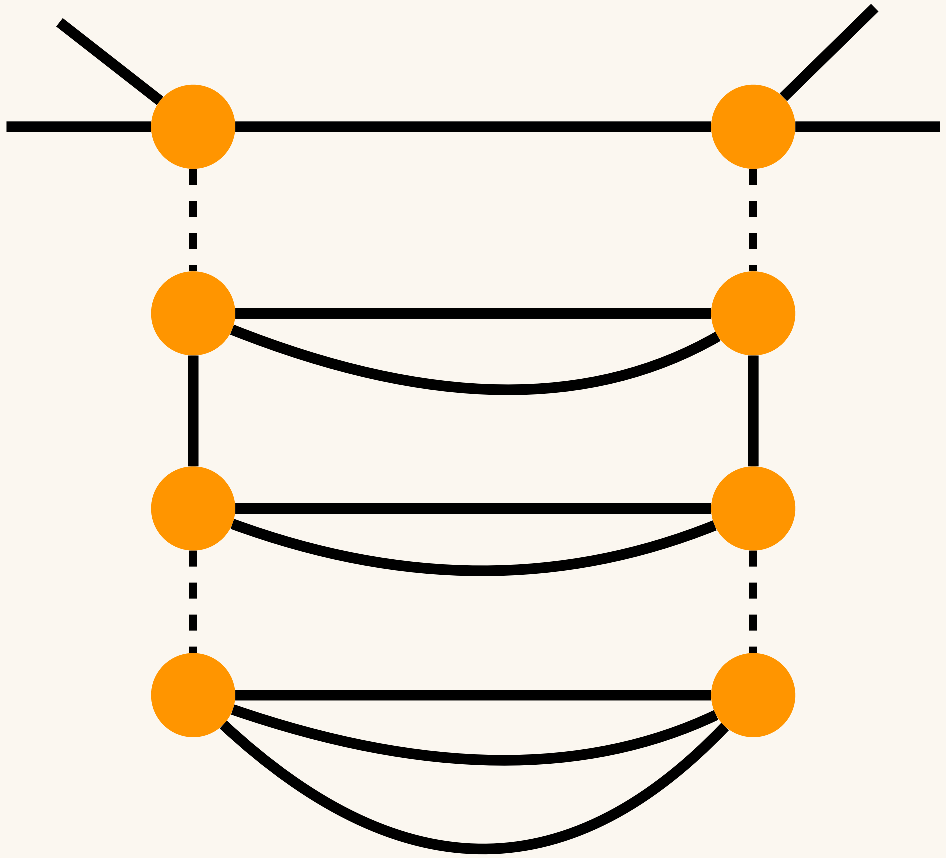
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



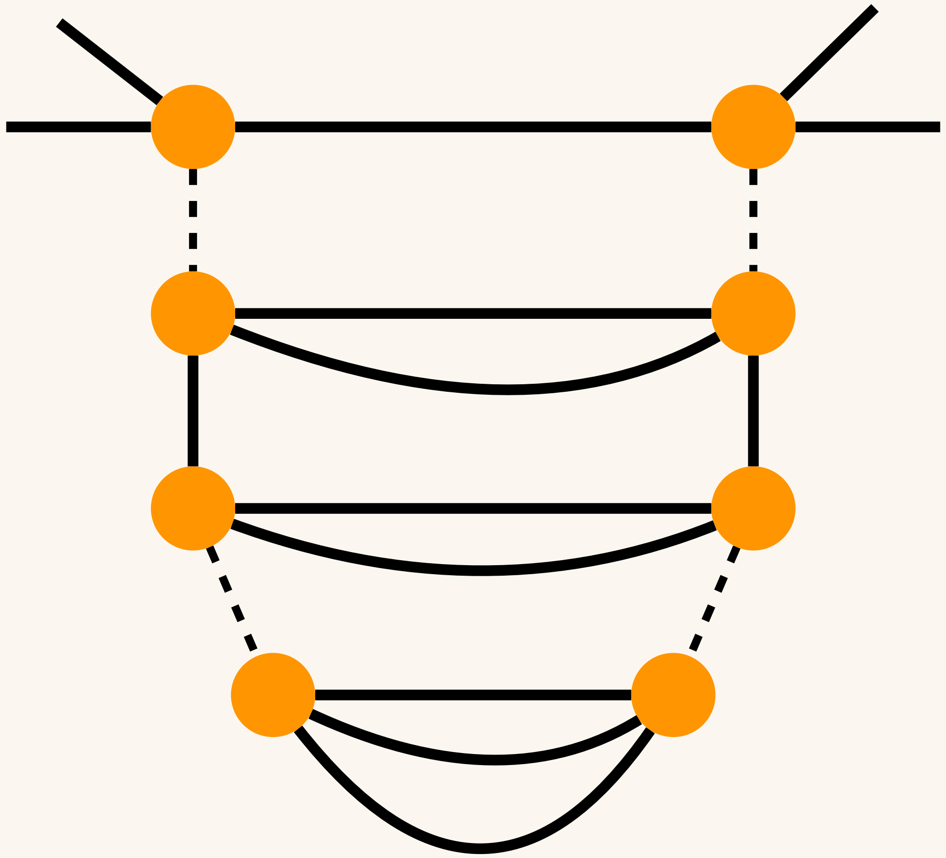
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

◉ Triad-MDTRG: Isometry step



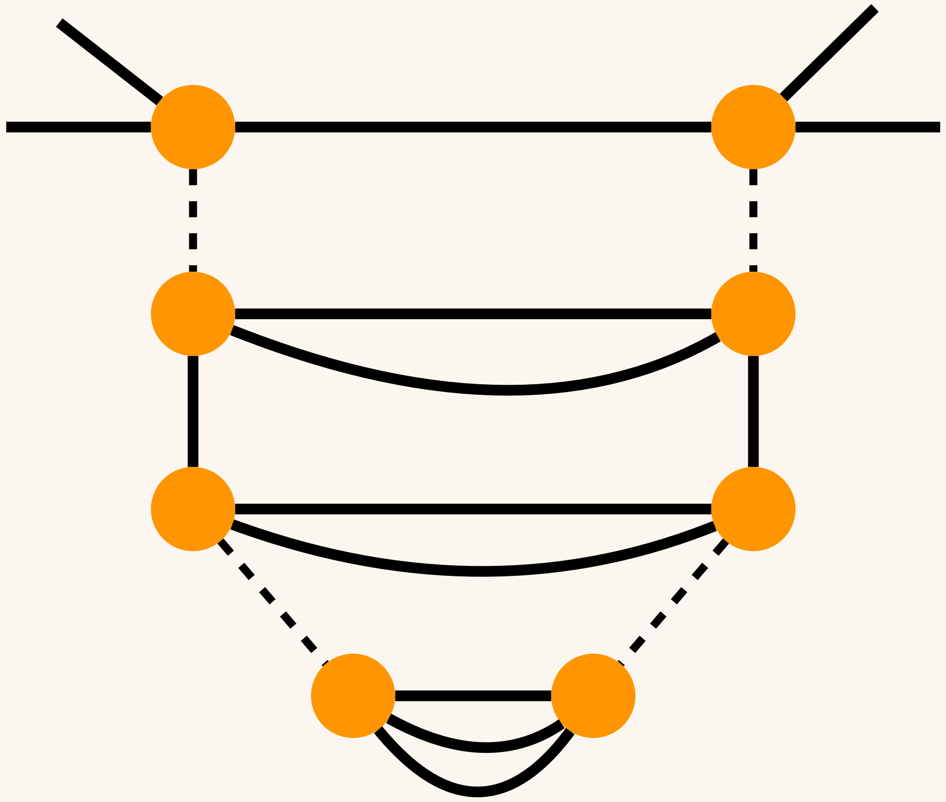
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



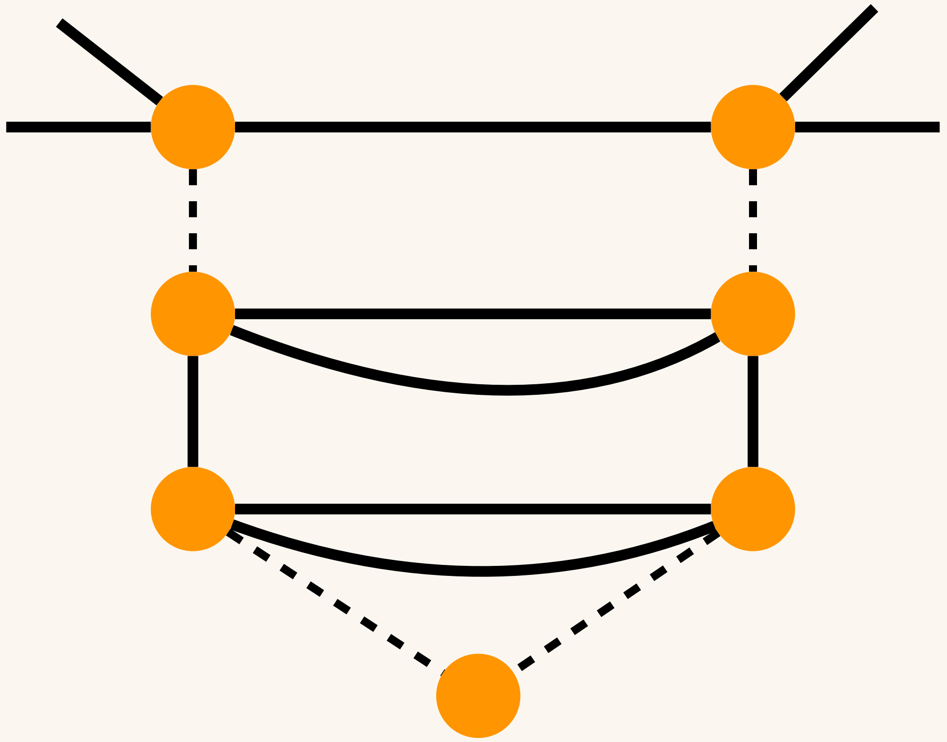
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



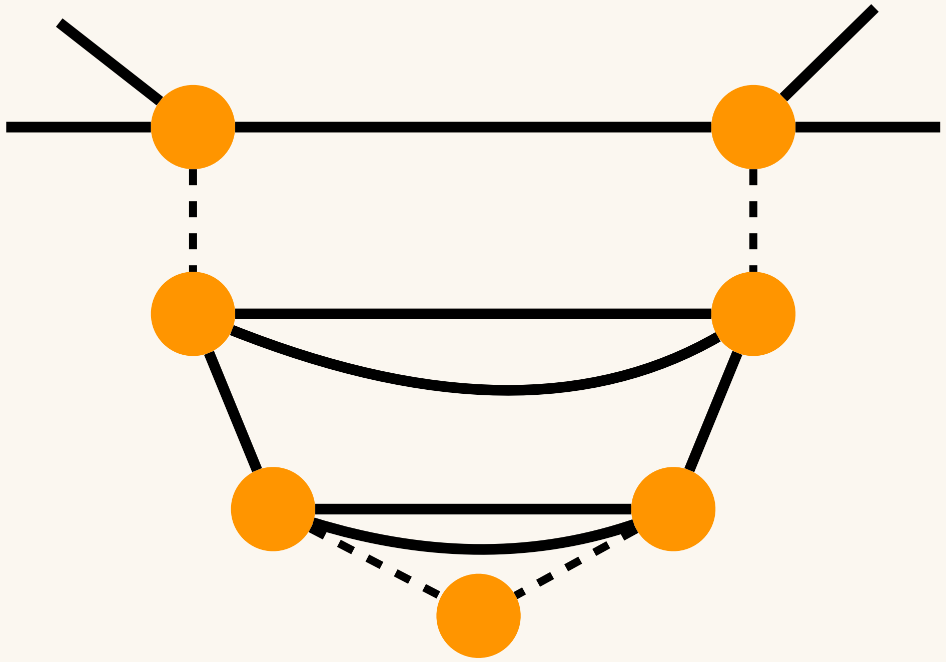
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

◉ Triad-MDTRG: Isometry step



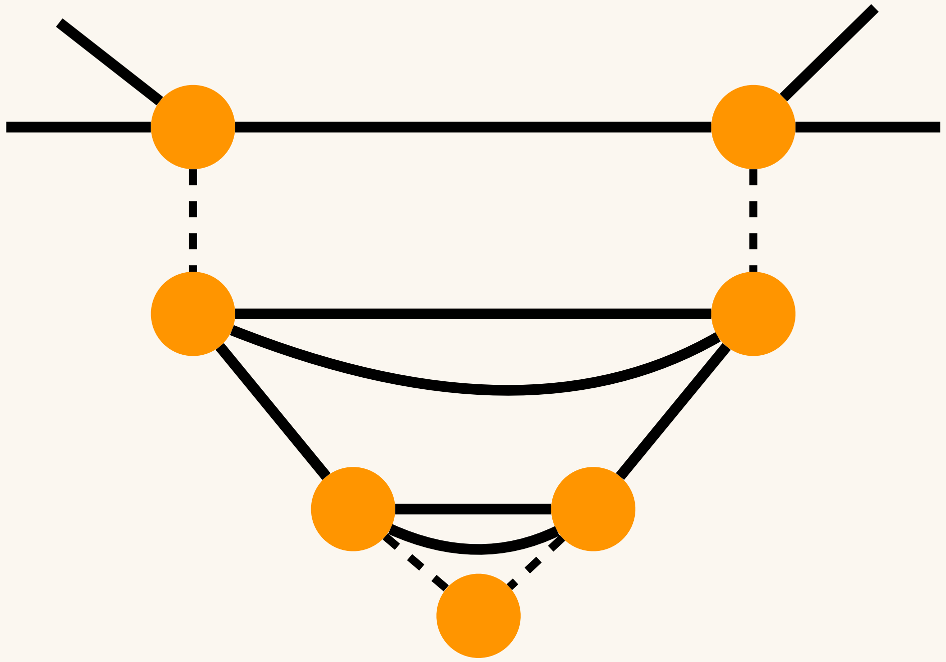
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



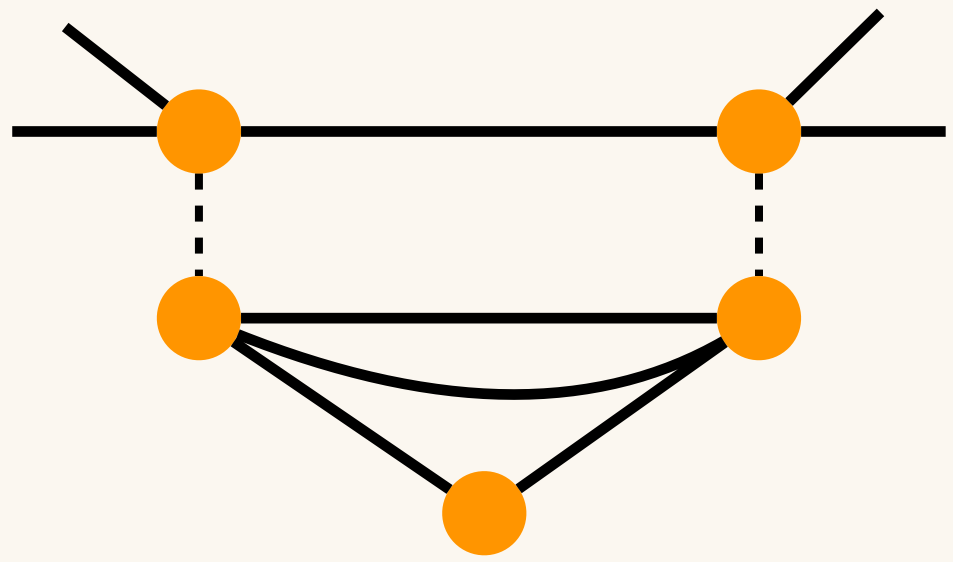
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



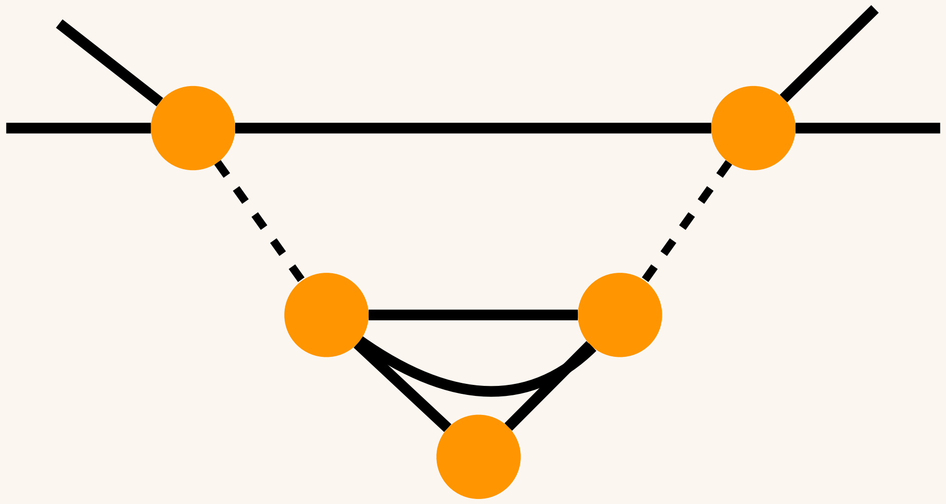
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



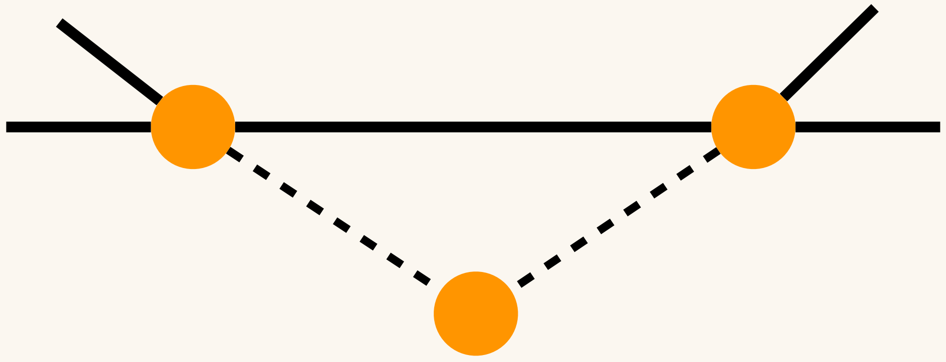
$$O(D^5) \rightarrow O(D^5) \rightarrow O(D^5) \rightarrow O(D^6) \rightarrow O(D^6)$$

Triad-MDTRG: Isometry step



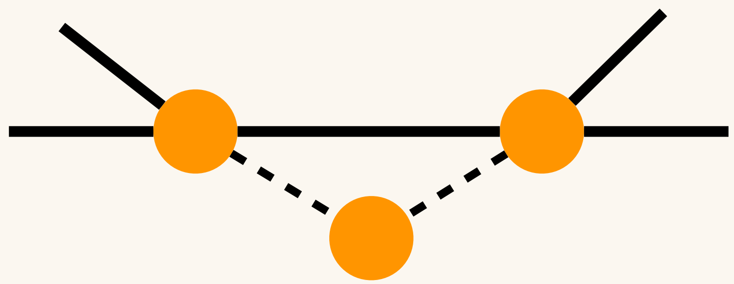
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



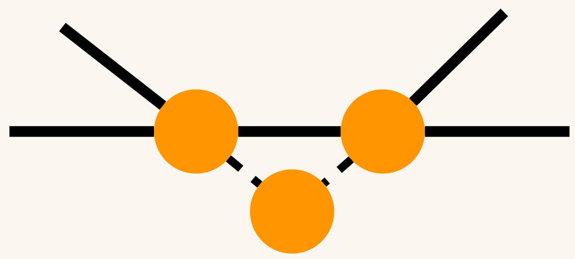
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



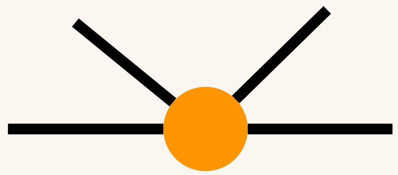
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

◉ Triad-MDTRG: Isometry step



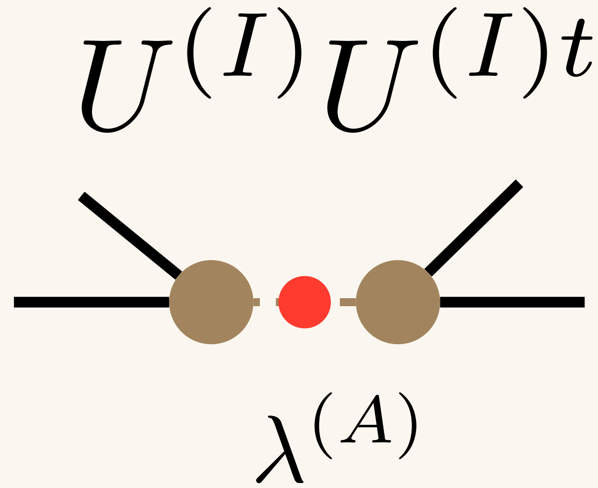
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step



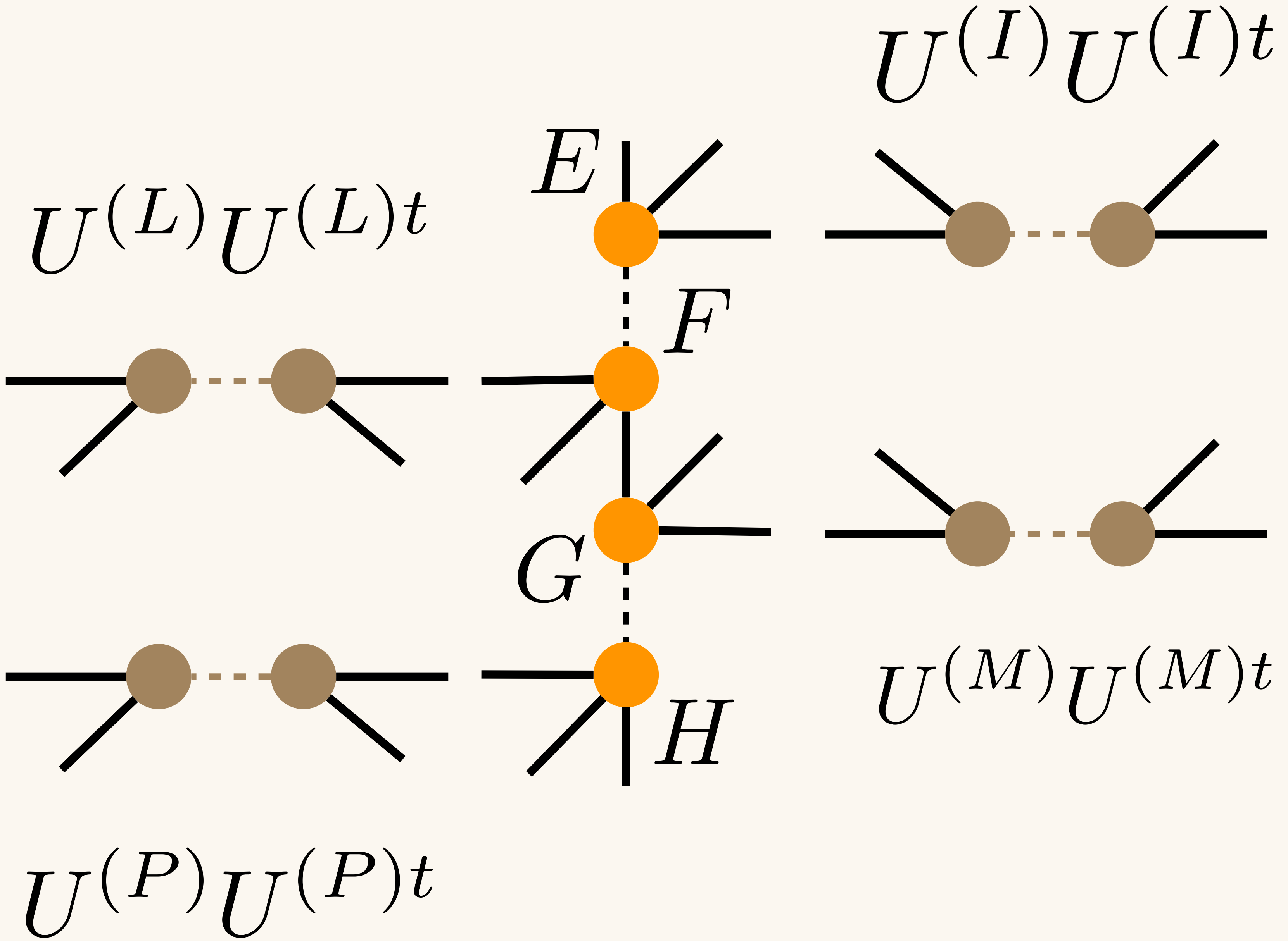
$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

Triad-MDTRG: Isometry step

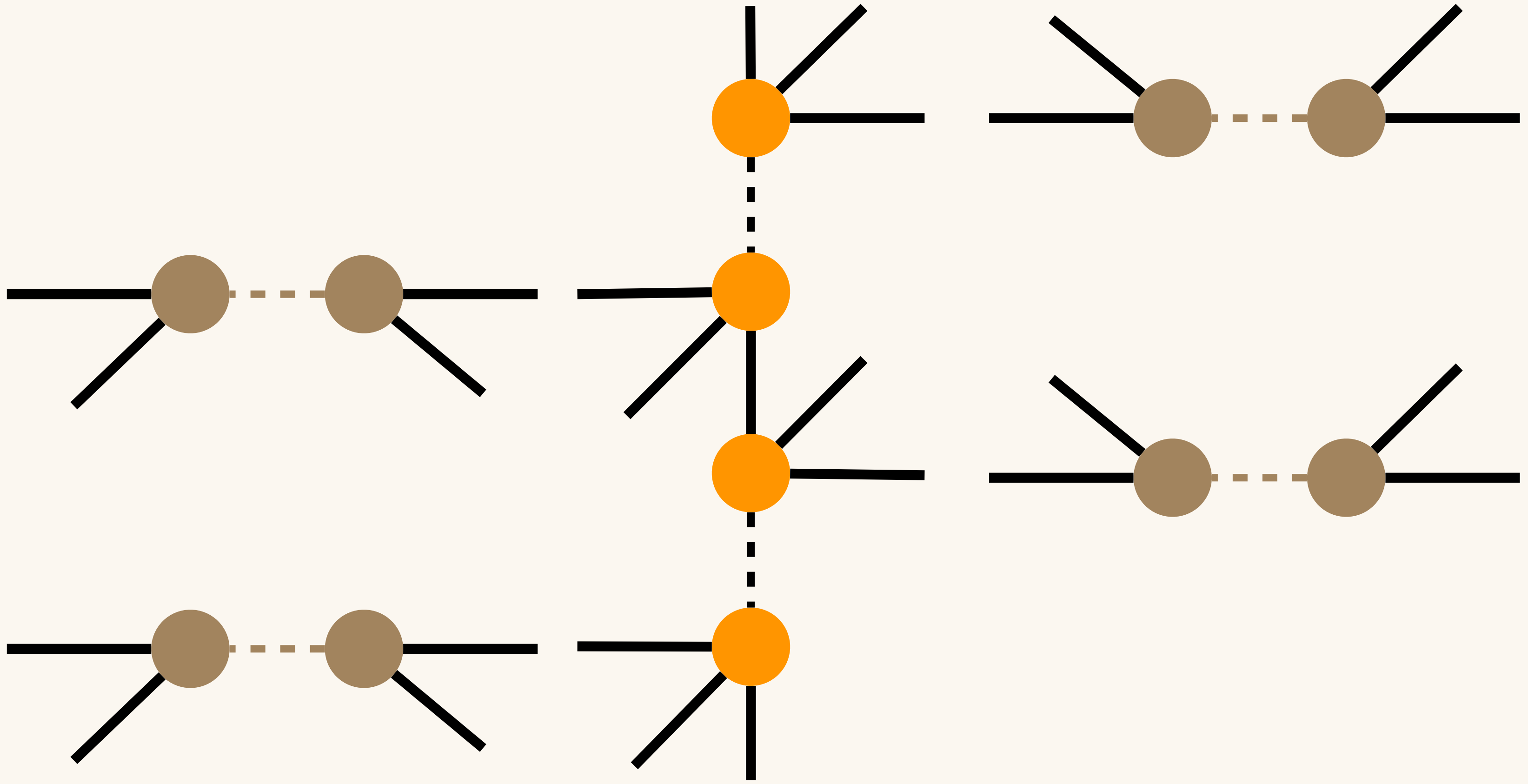


$$O(D^5) \to O(D^5) \to O(D^5) \to O(D^6) \to O(D^6)$$

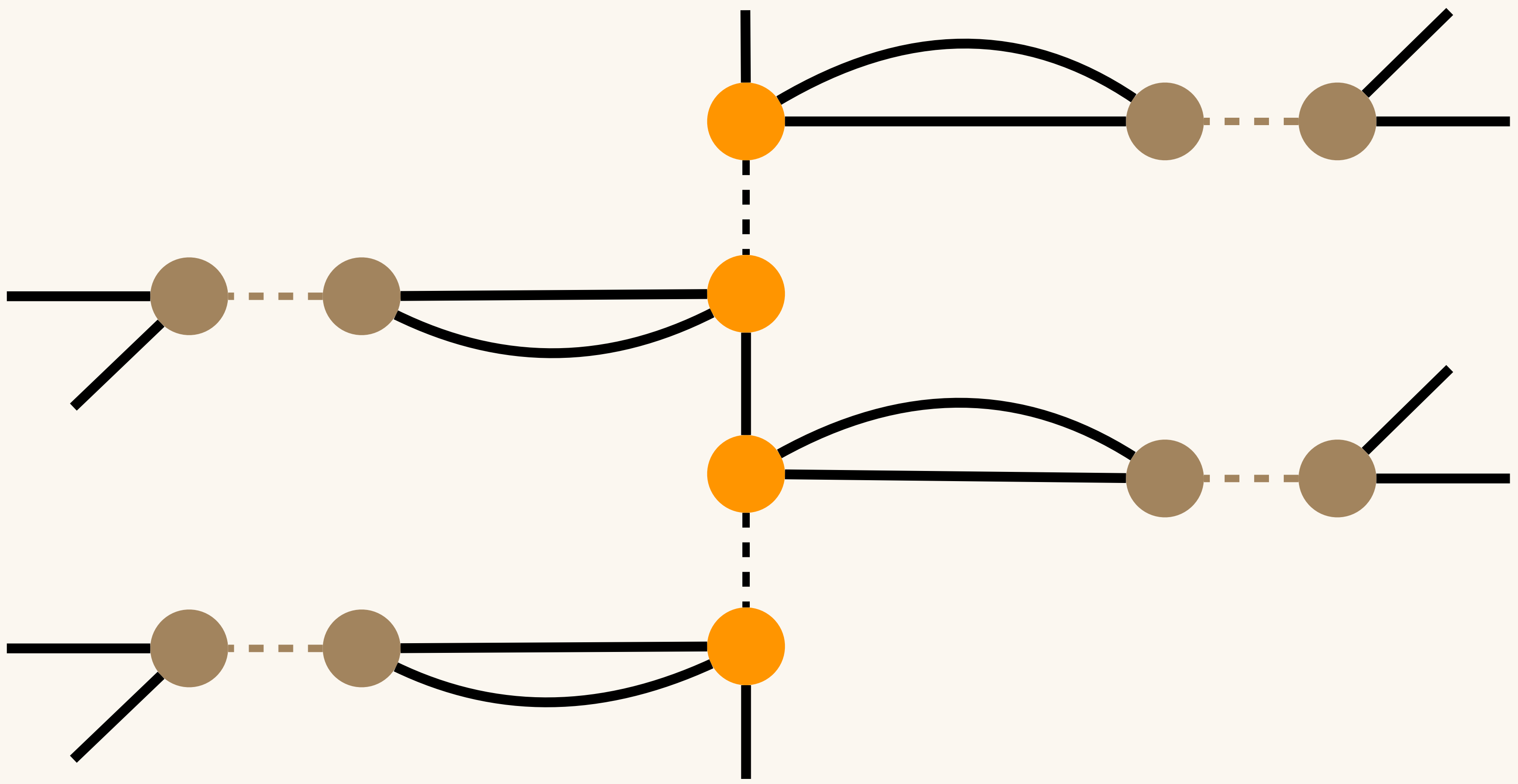
◉ Triad-MDTRG: Contraction step



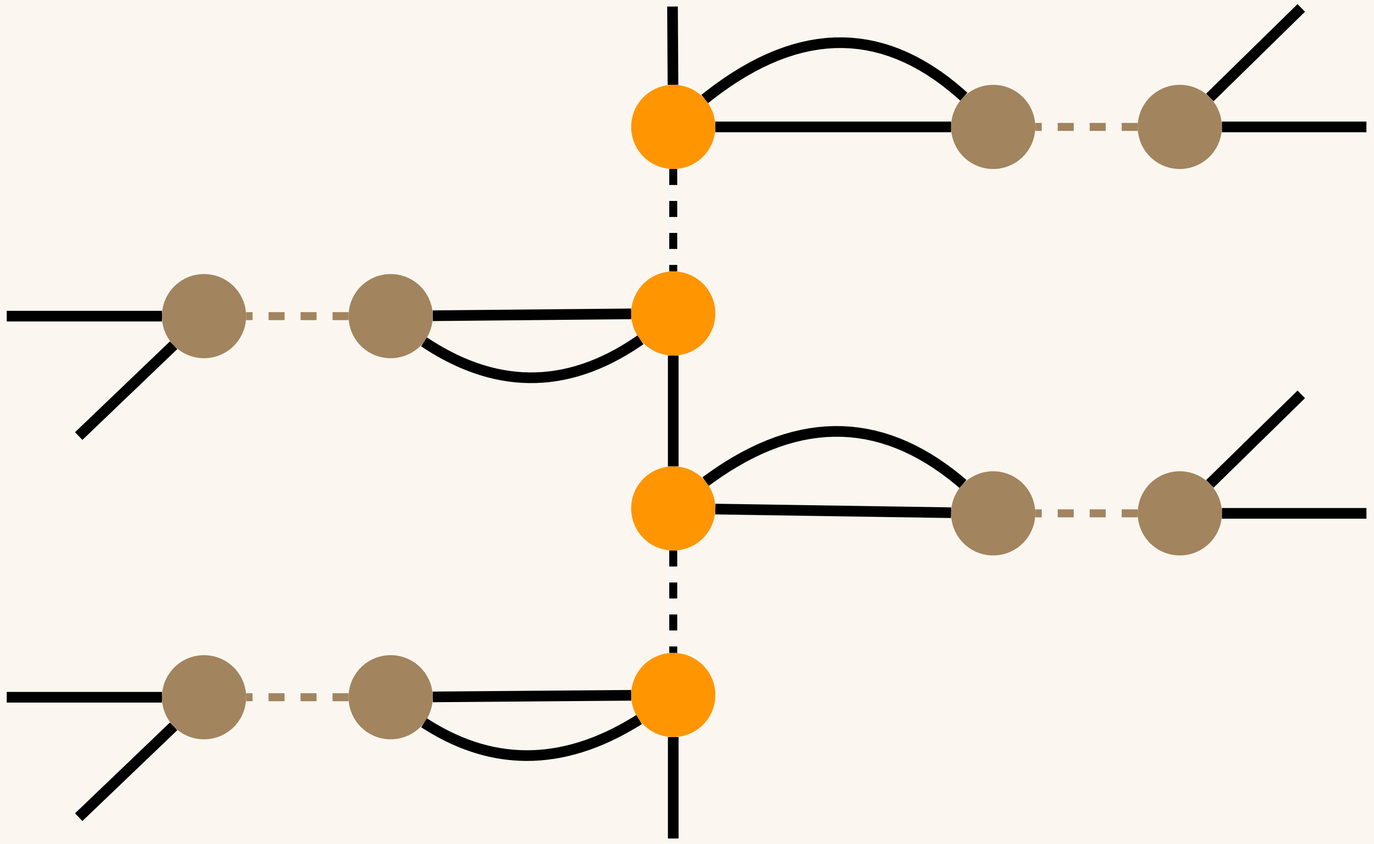
Triad-MDTRG: Contraction step



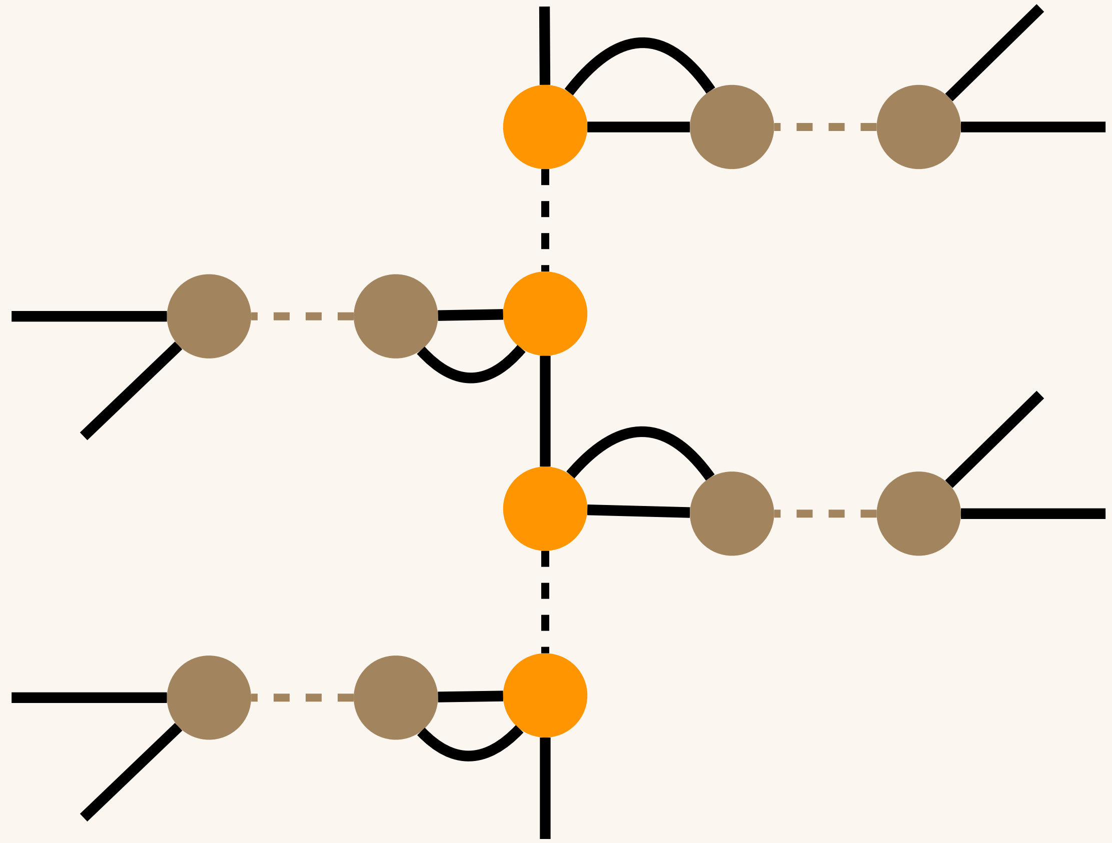
Triad-MDTRG: Contraction step



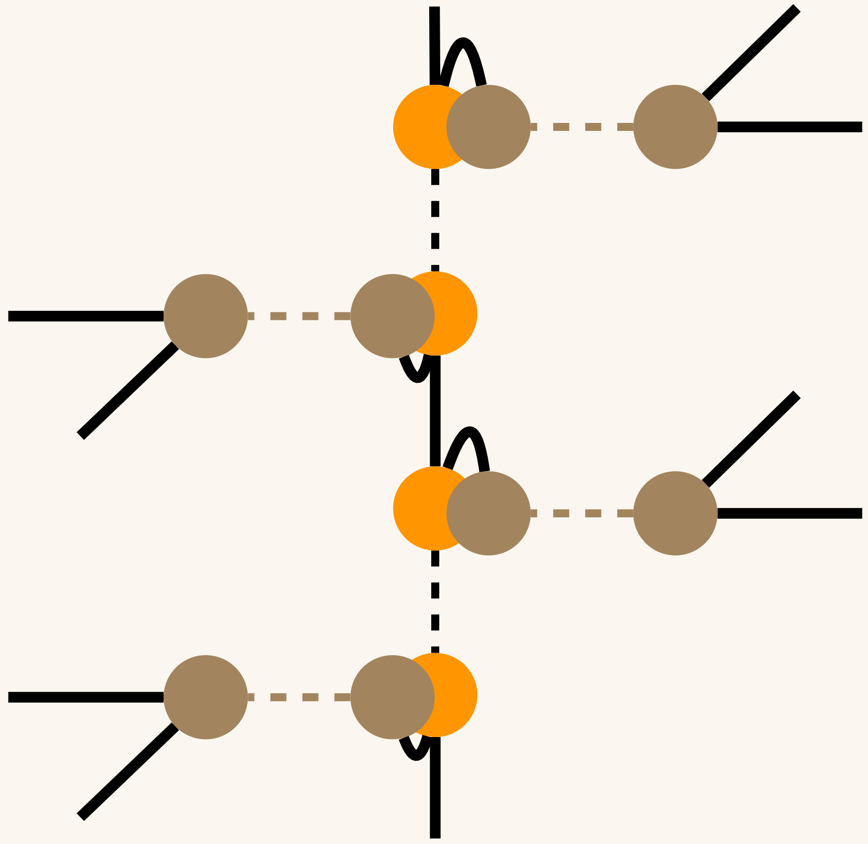
◉ Triad-MDTRG: Contraction step



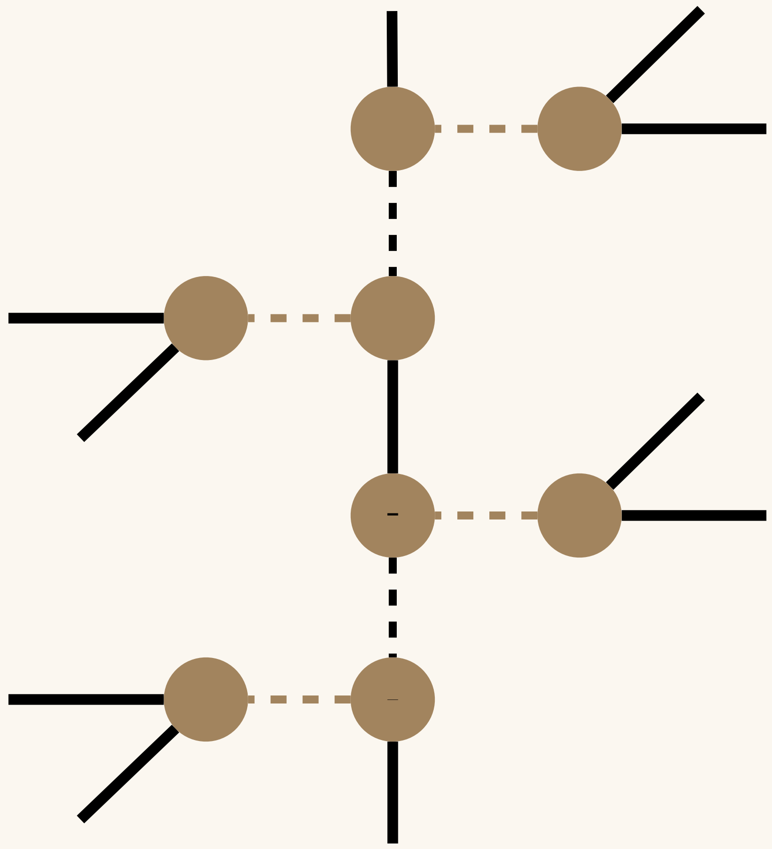
Triad-MDTRG: Contraction step



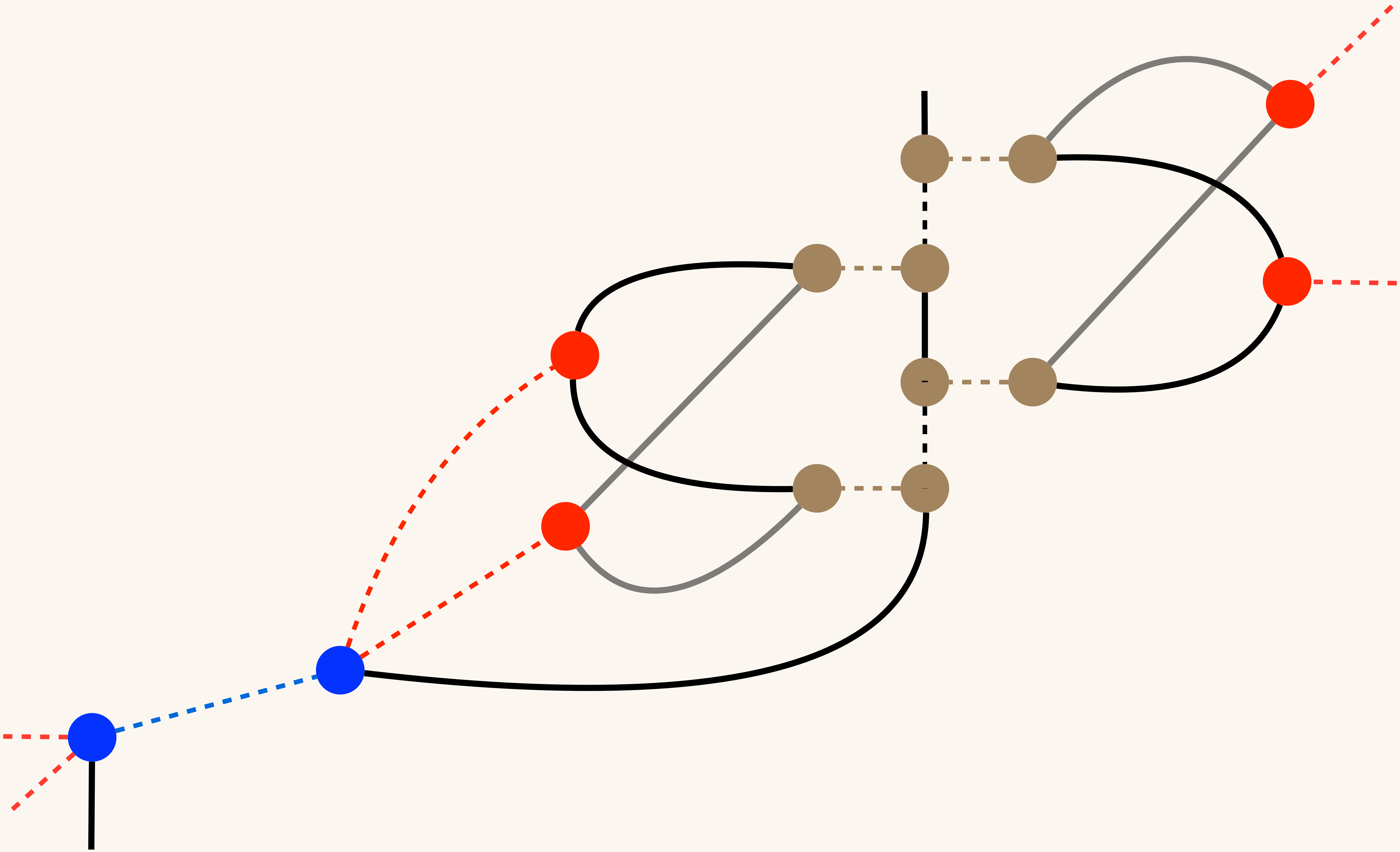
Triad-MDTRG: Contraction step



◉ Triad-MDTRG: Contraction step

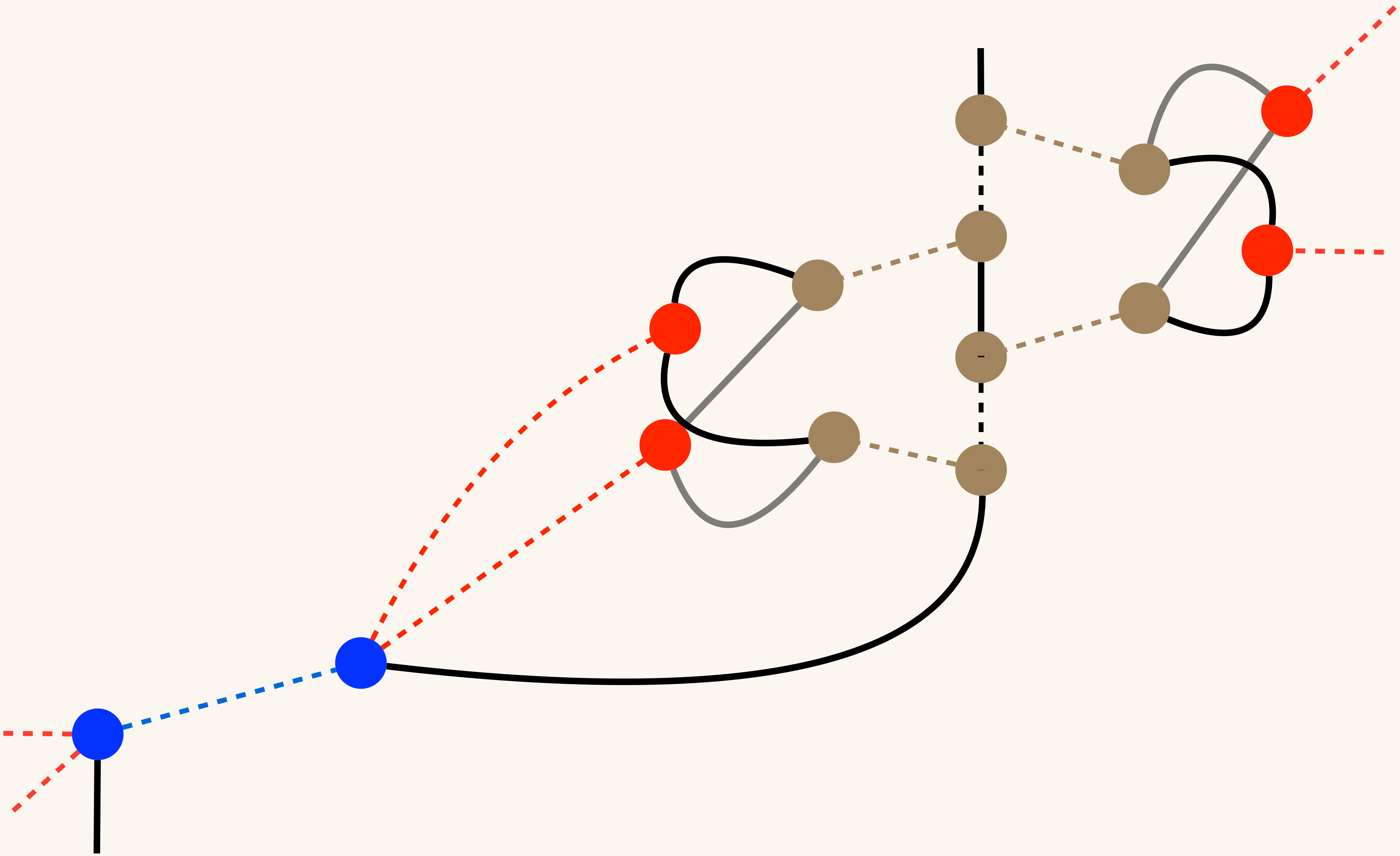


◉ Triad-MDTRG: Contraction step



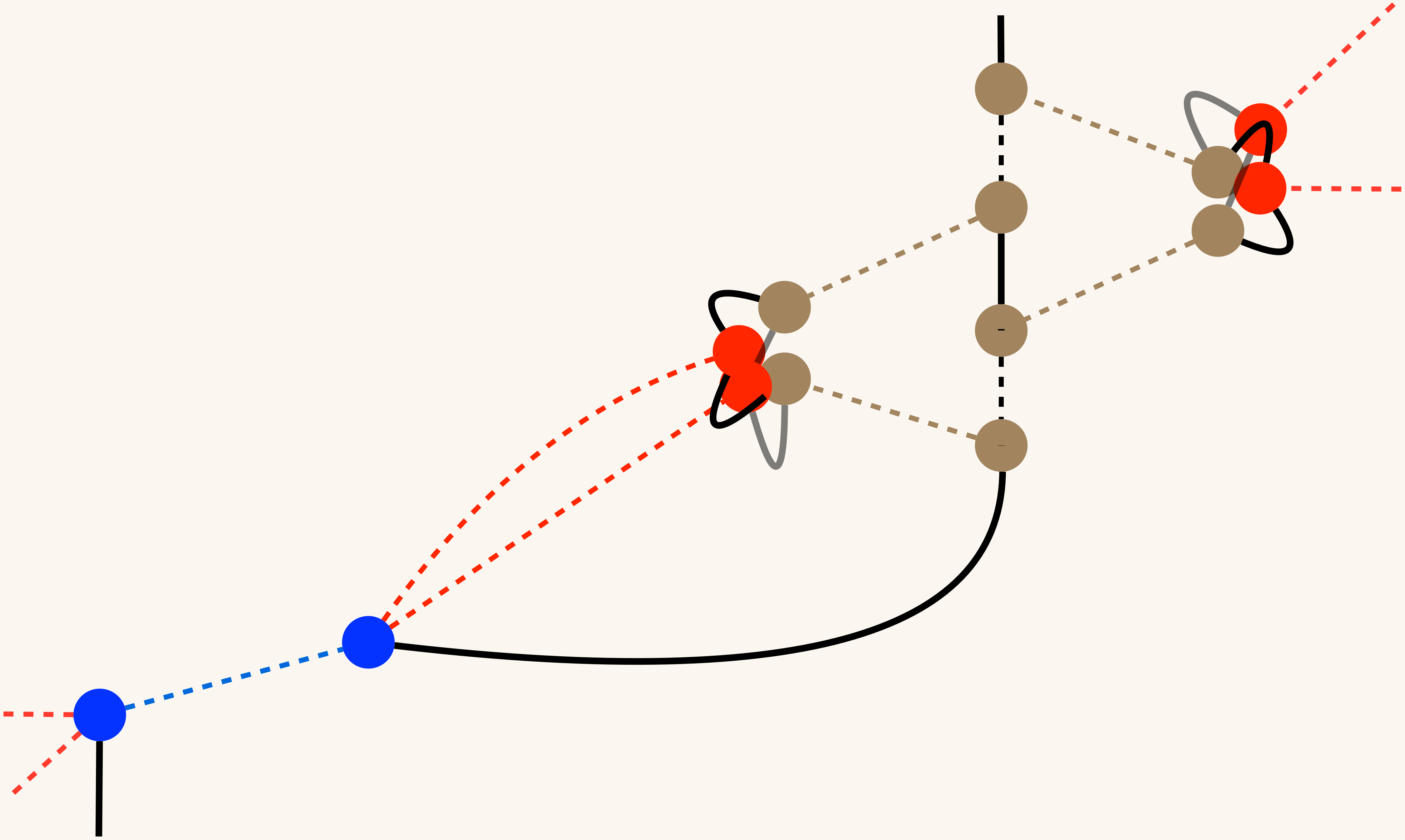
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

Triad-MDTRG: Contraction step



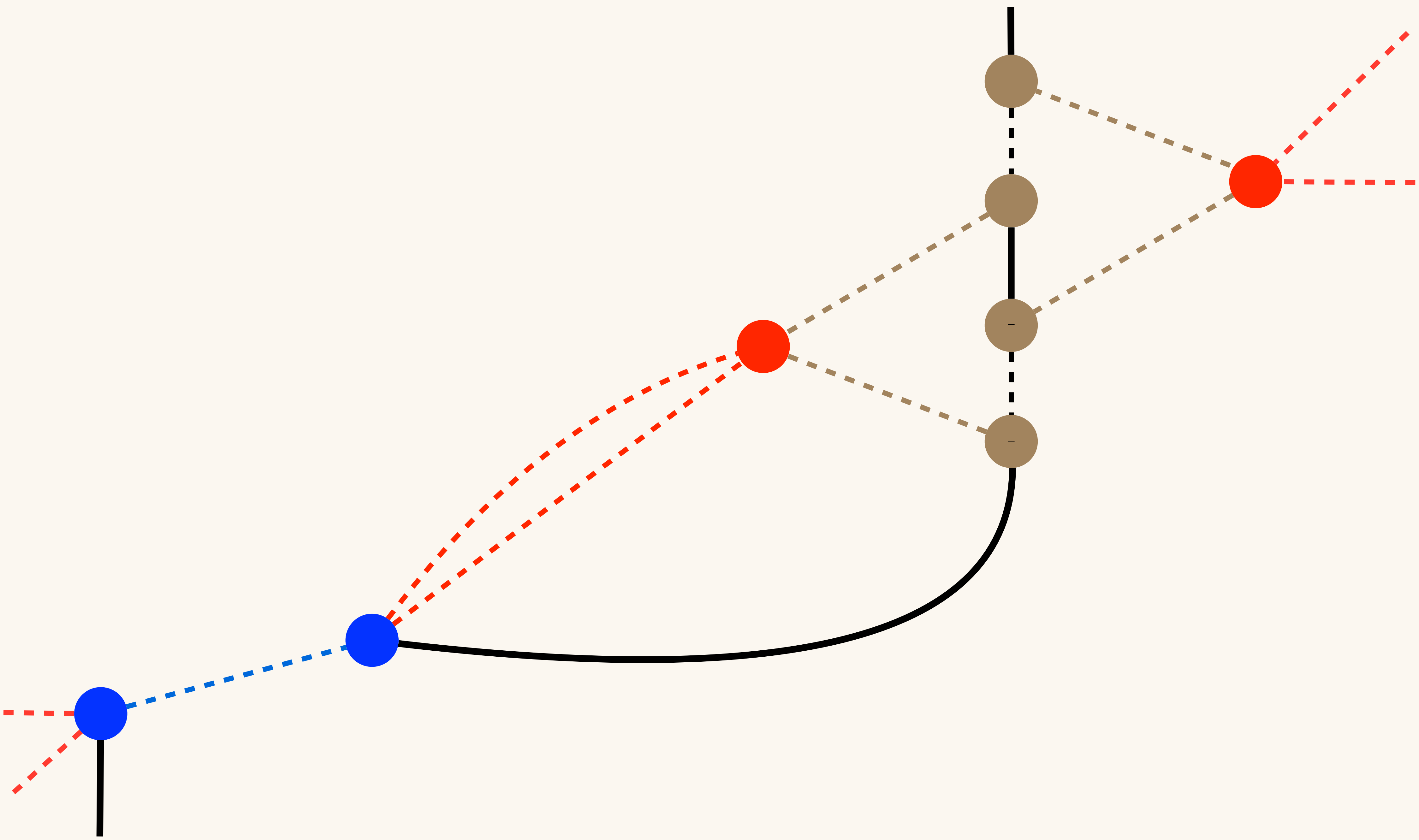
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

Triad-MDTRG: Contraction step



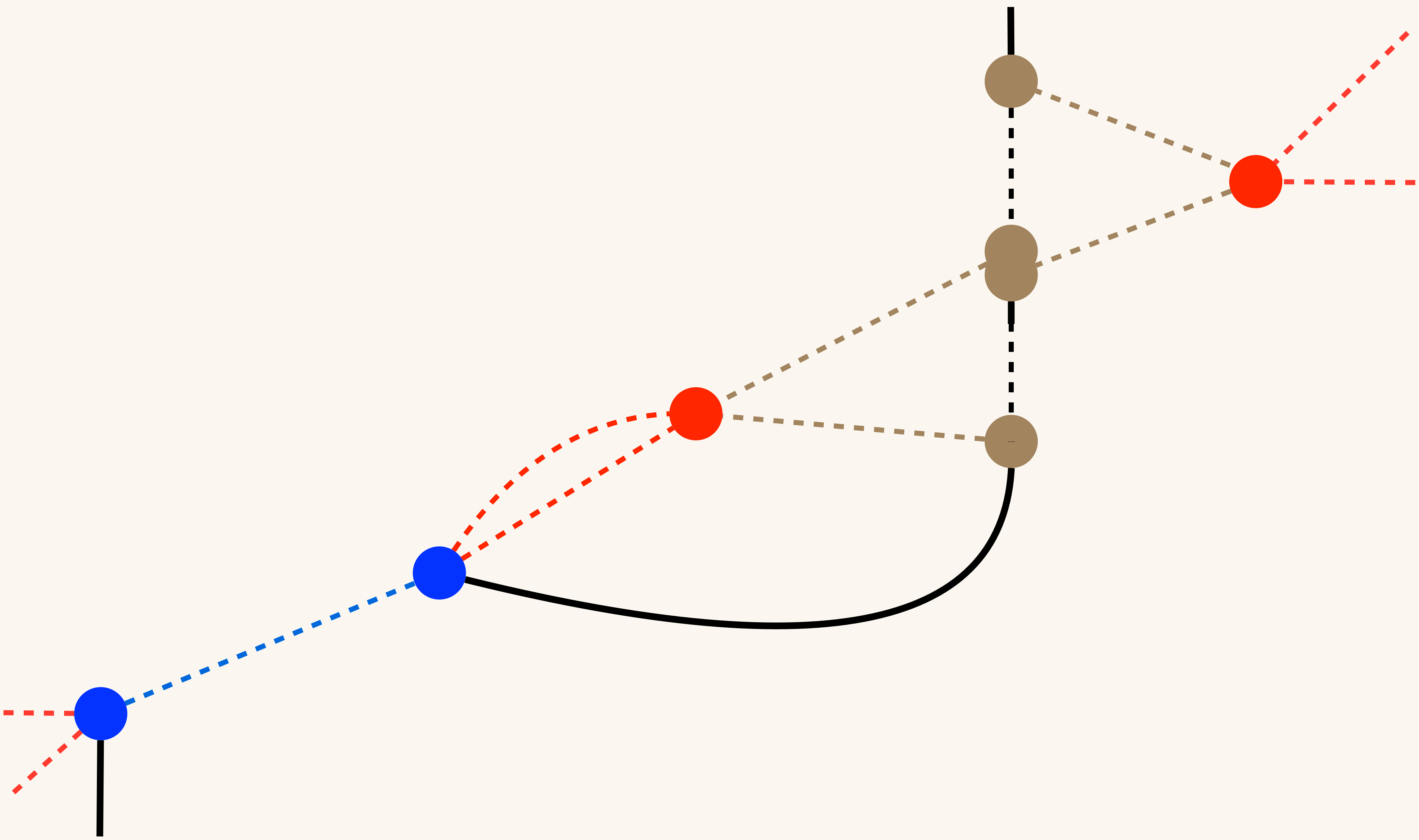
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

Triad-MDTRG: Contraction step



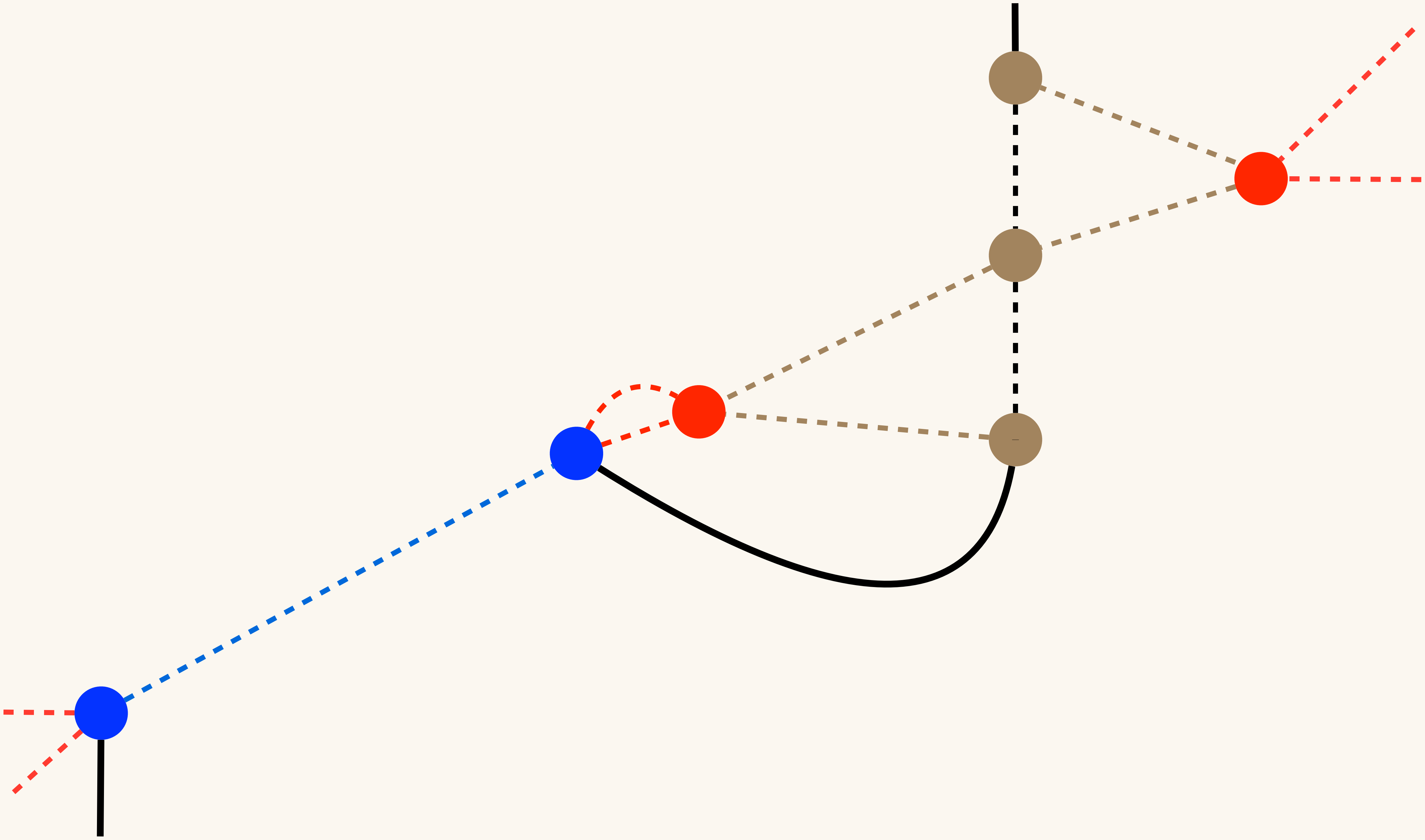
$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$

Triad-MDTRG: Contraction step



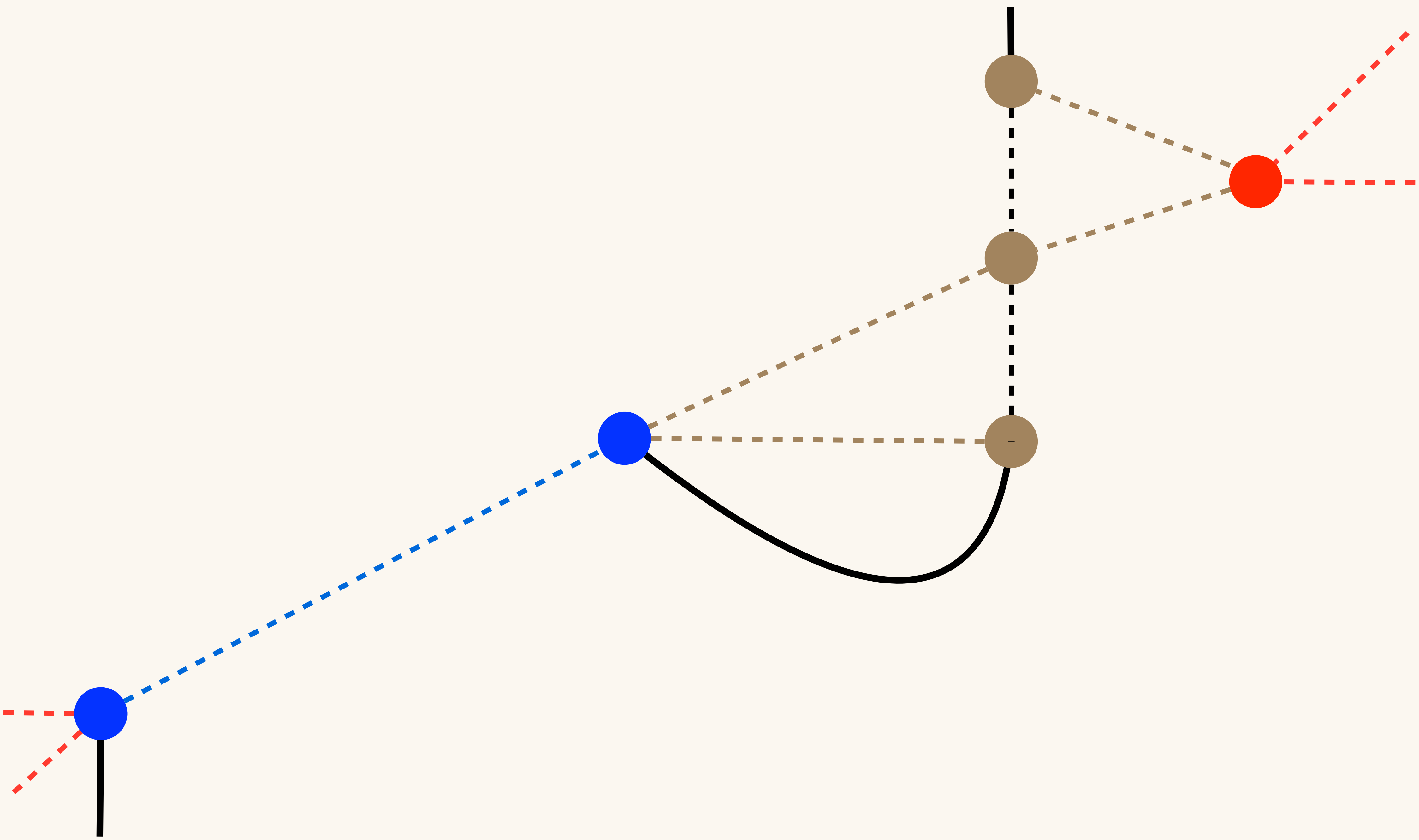
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

Triad-MDTRG: Contraction step



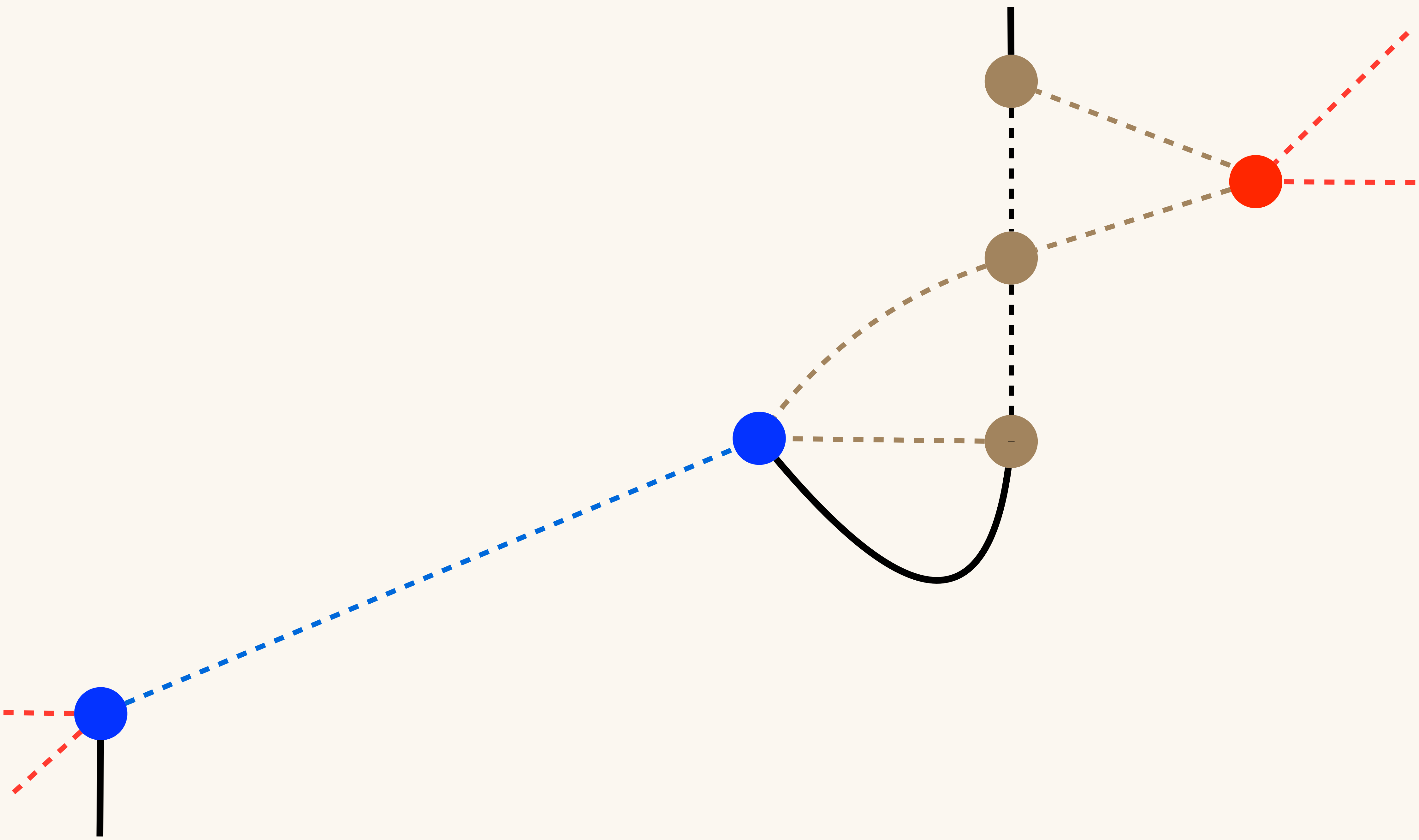
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

◉ Triad-MDTRG: Contraction step



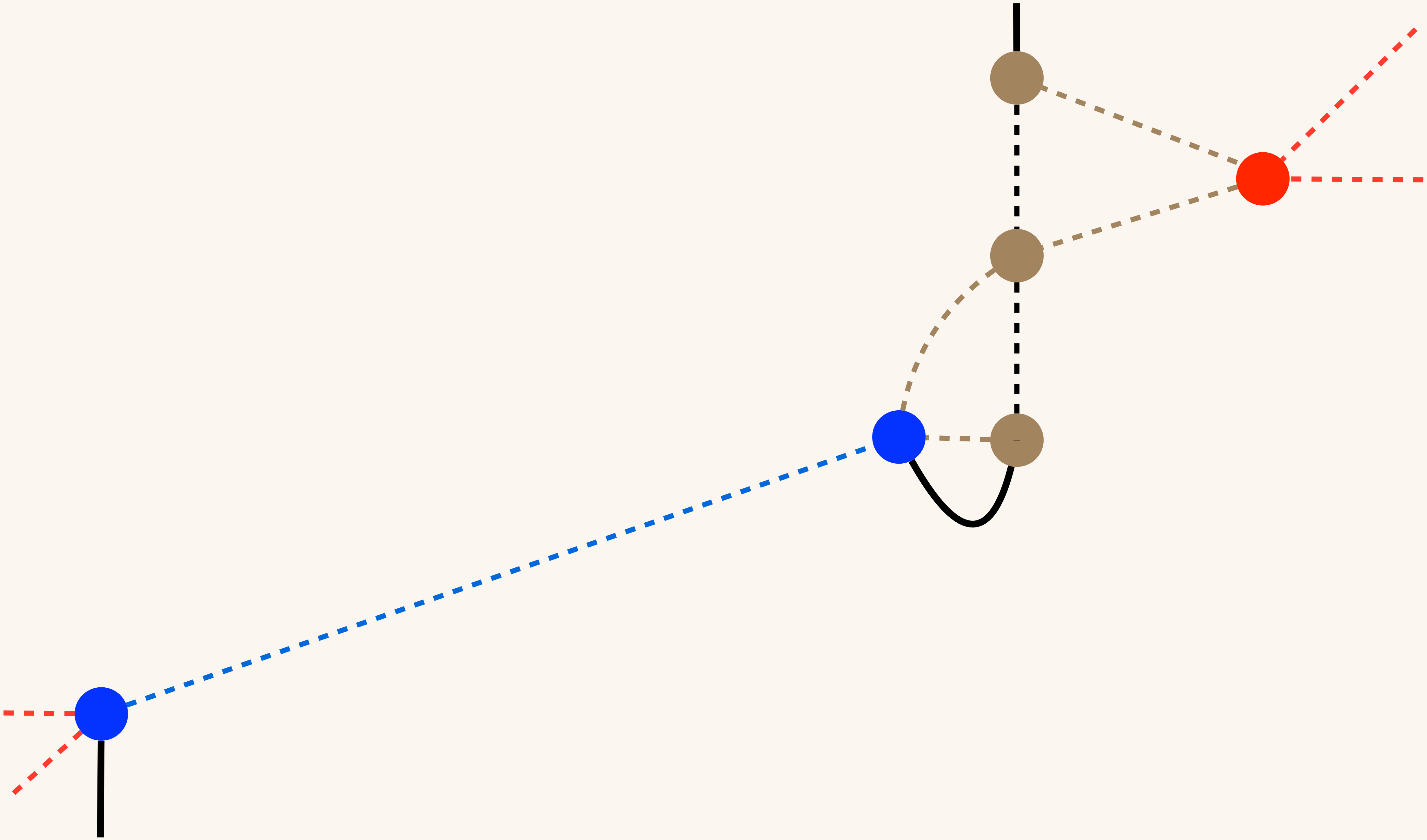
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

◉ Triad-MDTRG: Contraction step



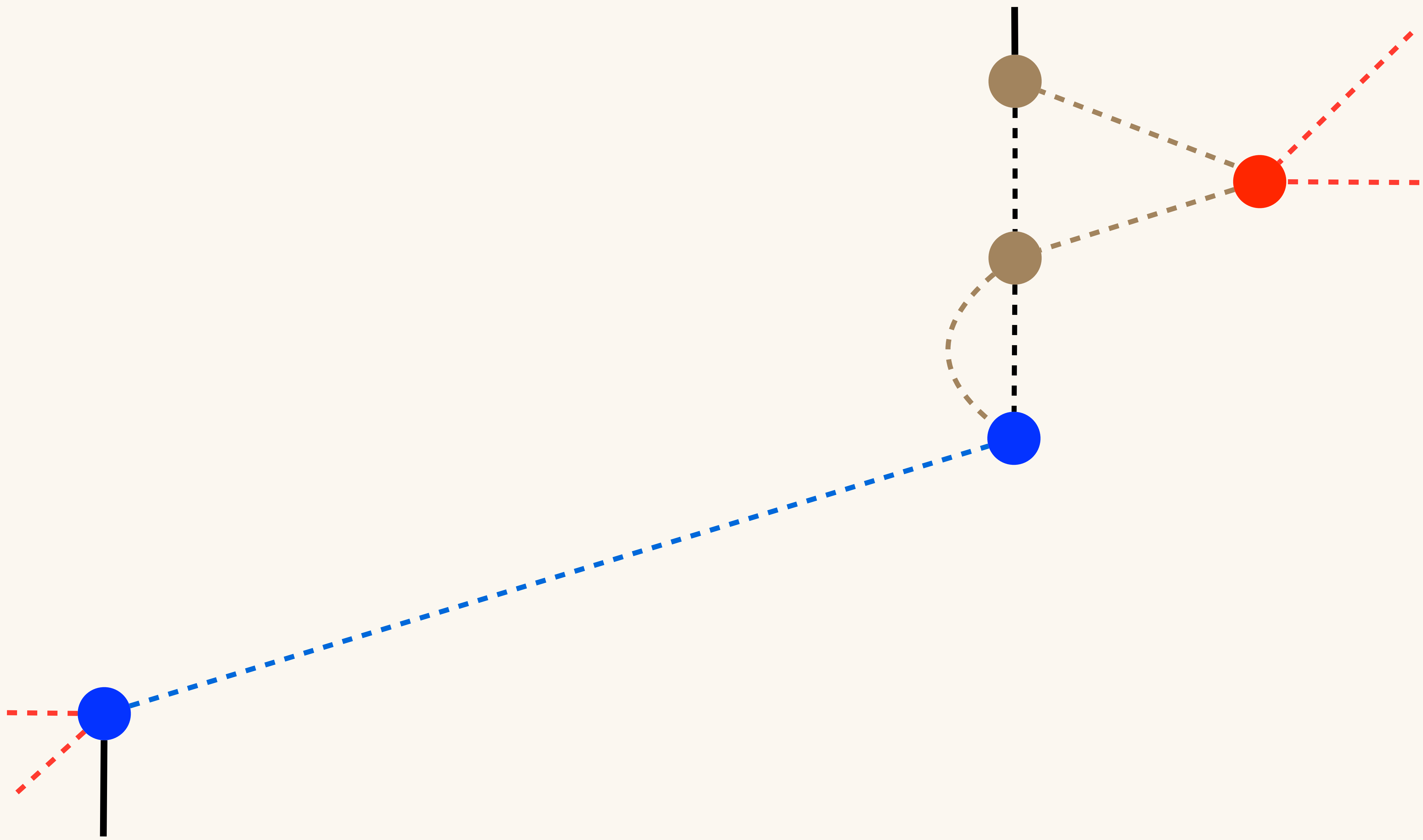
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

Triad-MDTRG: Contraction step



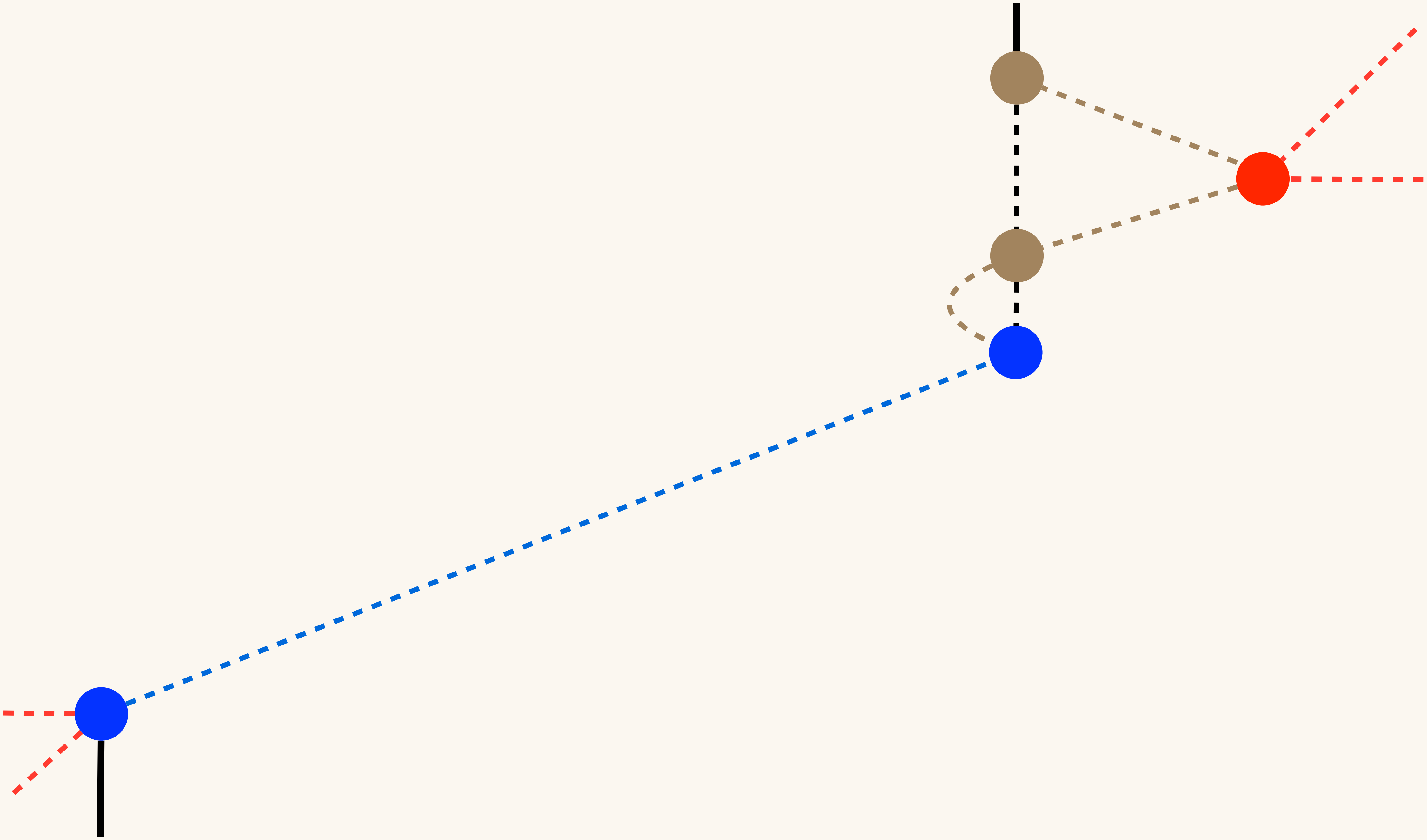
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

◉ Triad-MDTRG: Contraction step



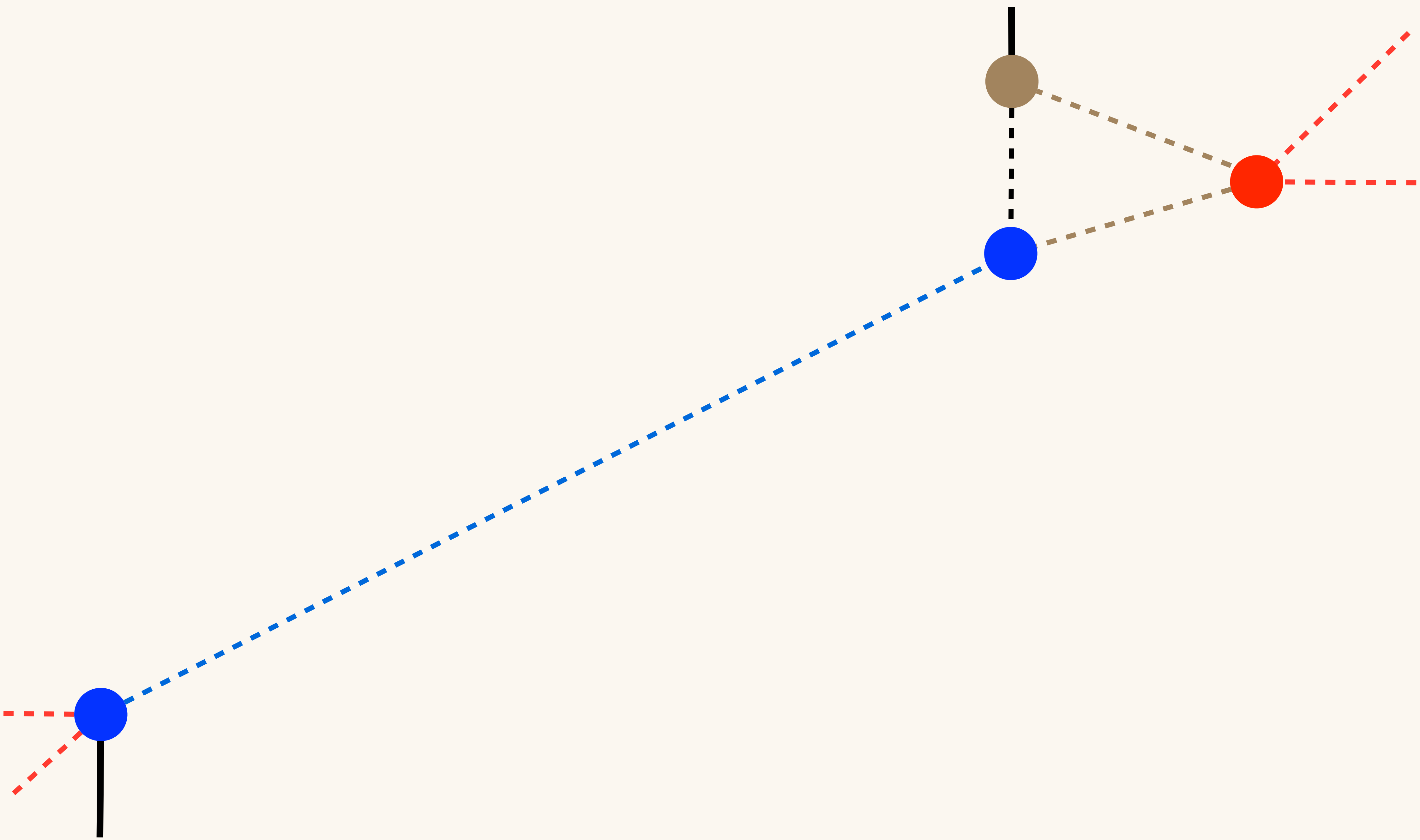
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

Triad-MDTRG: Contraction step



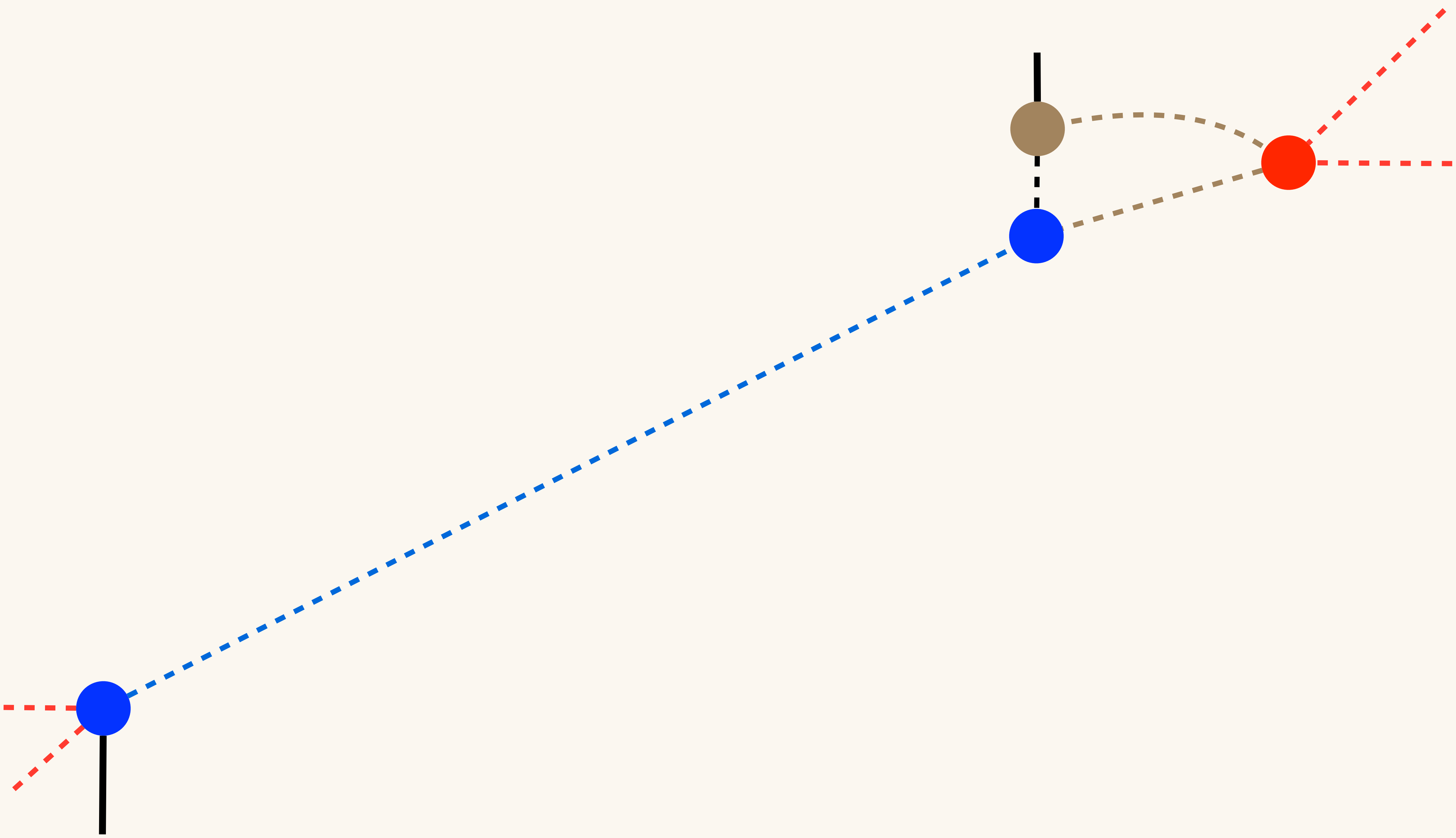
$$O(D^6) \rightarrow O(D^6) \rightarrow O(D^5) \rightarrow O(D^5) \rightarrow O(D^5) \rightarrow O(D^6)$$

◉ Triad-MDTRG: Contraction step



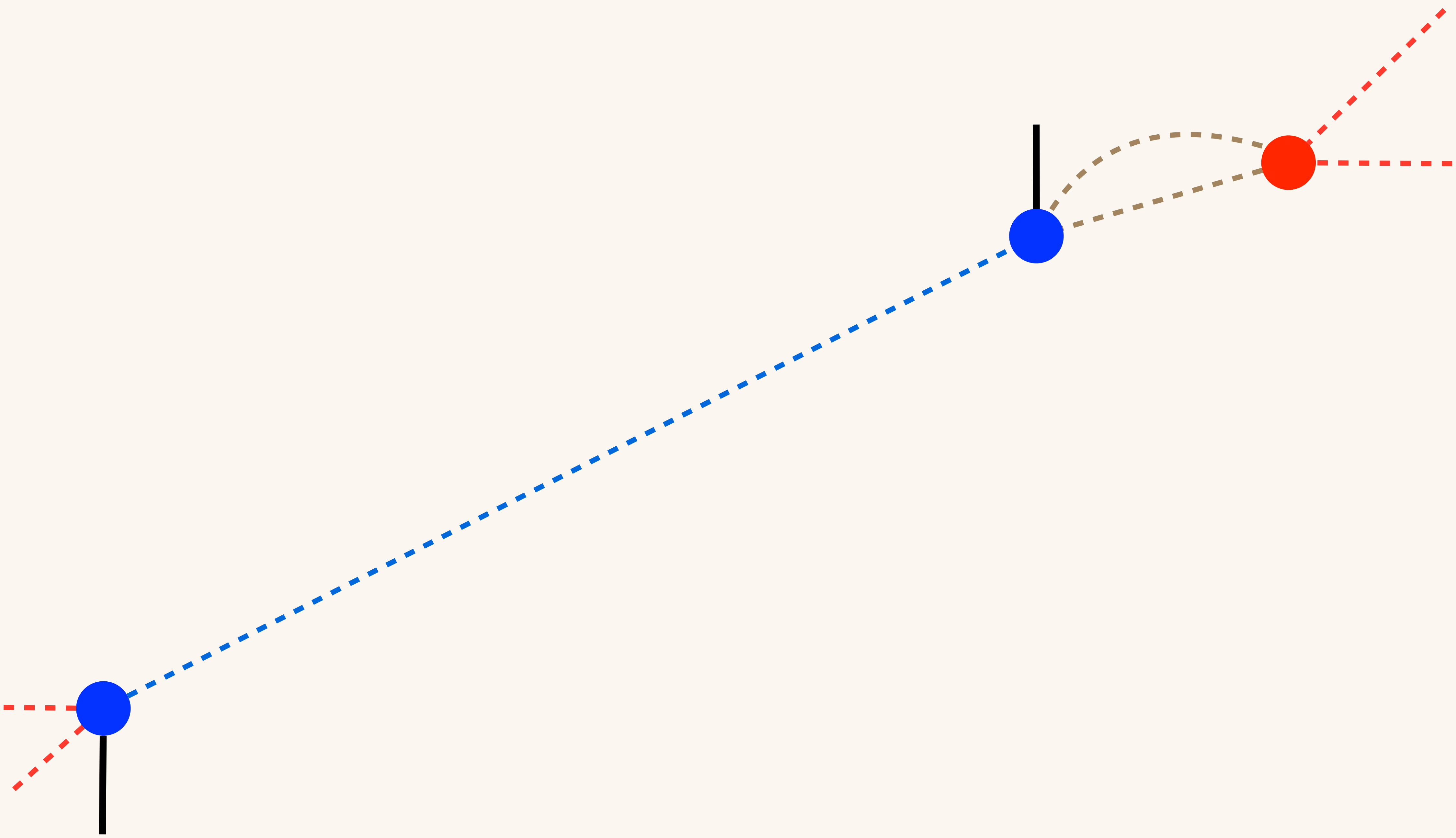
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

◉ Triad-MDTRG: Contraction step



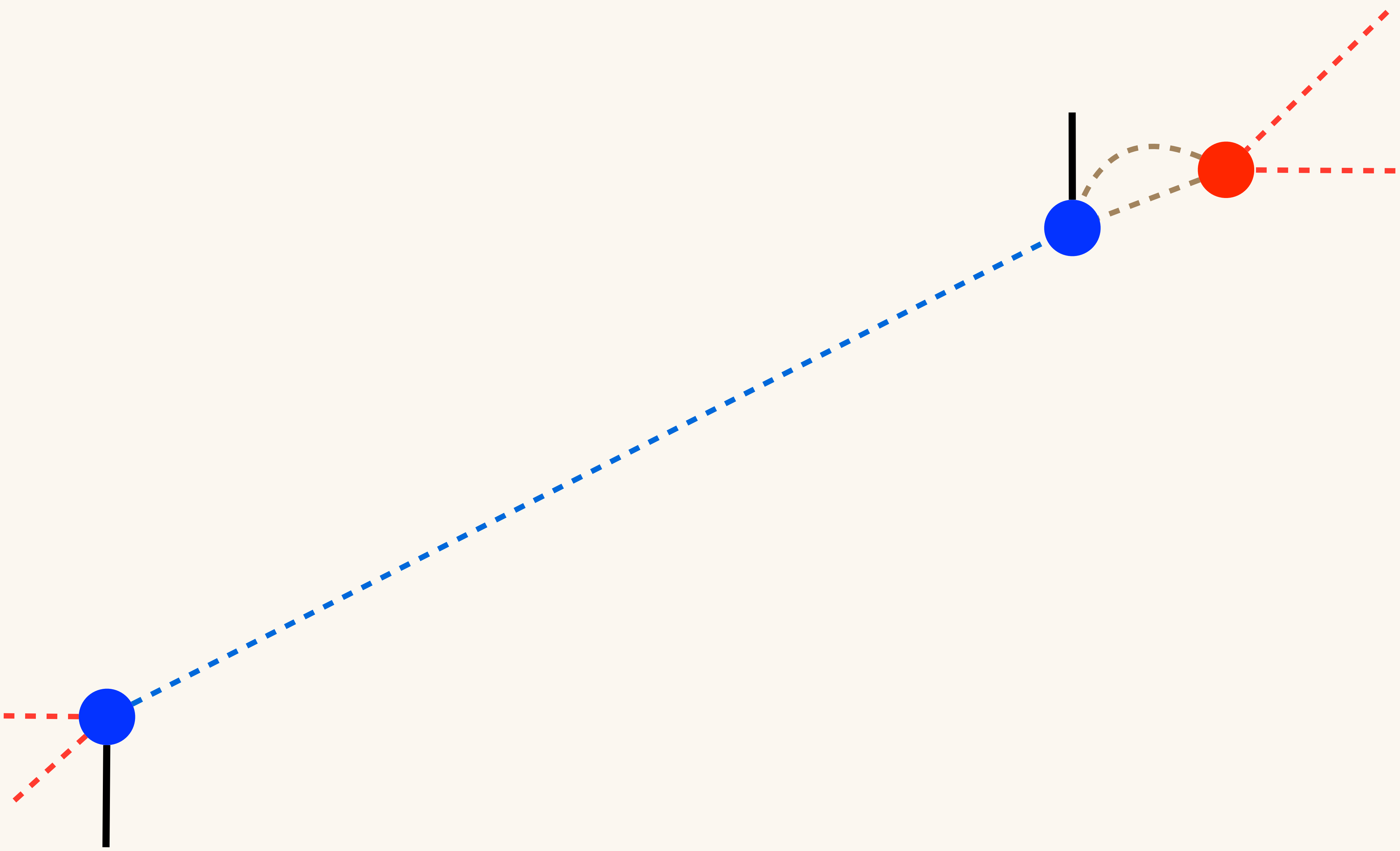
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

Triad-MDTRG: Contraction step



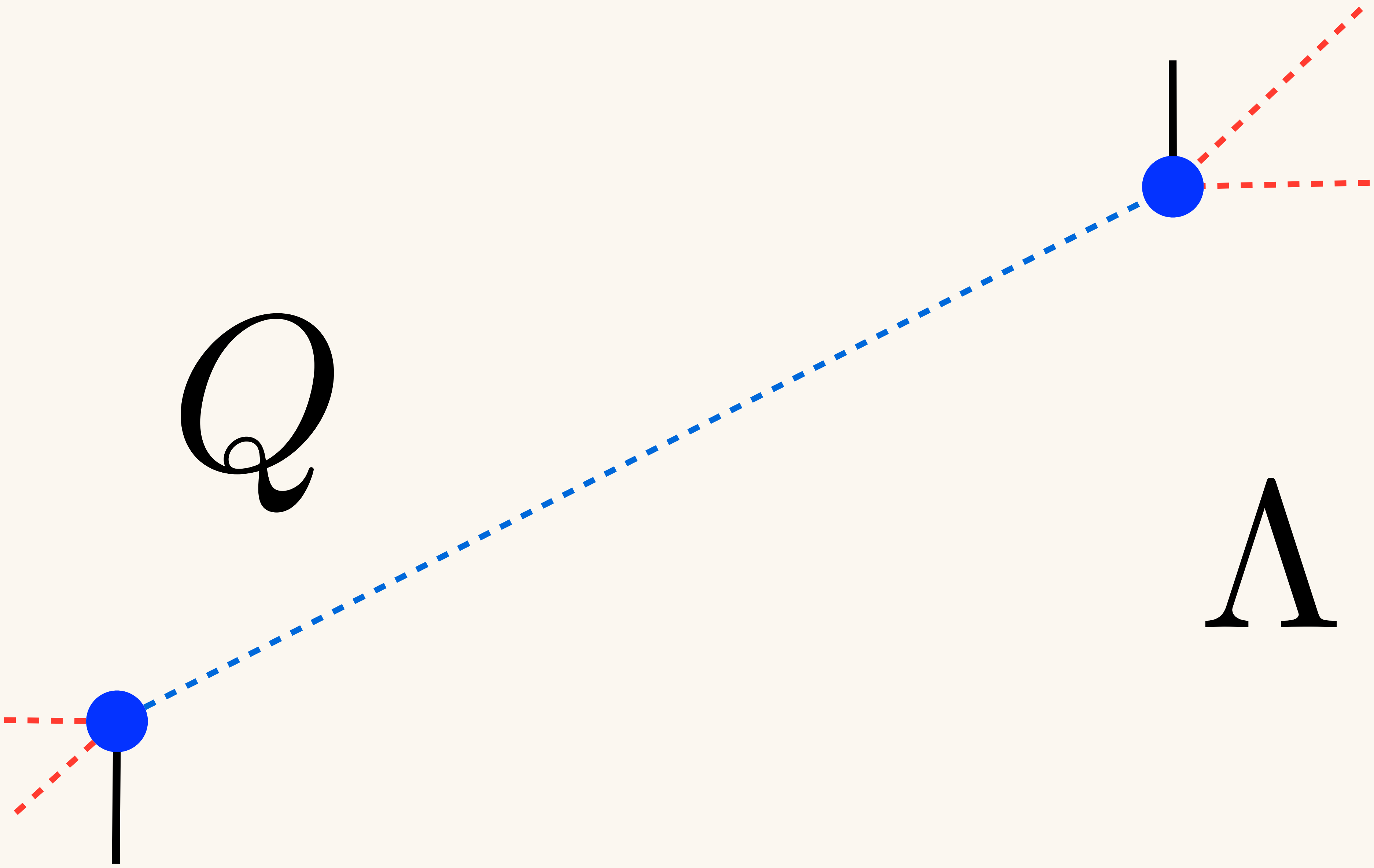
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

◉ Triad-MDTRG: Contraction step



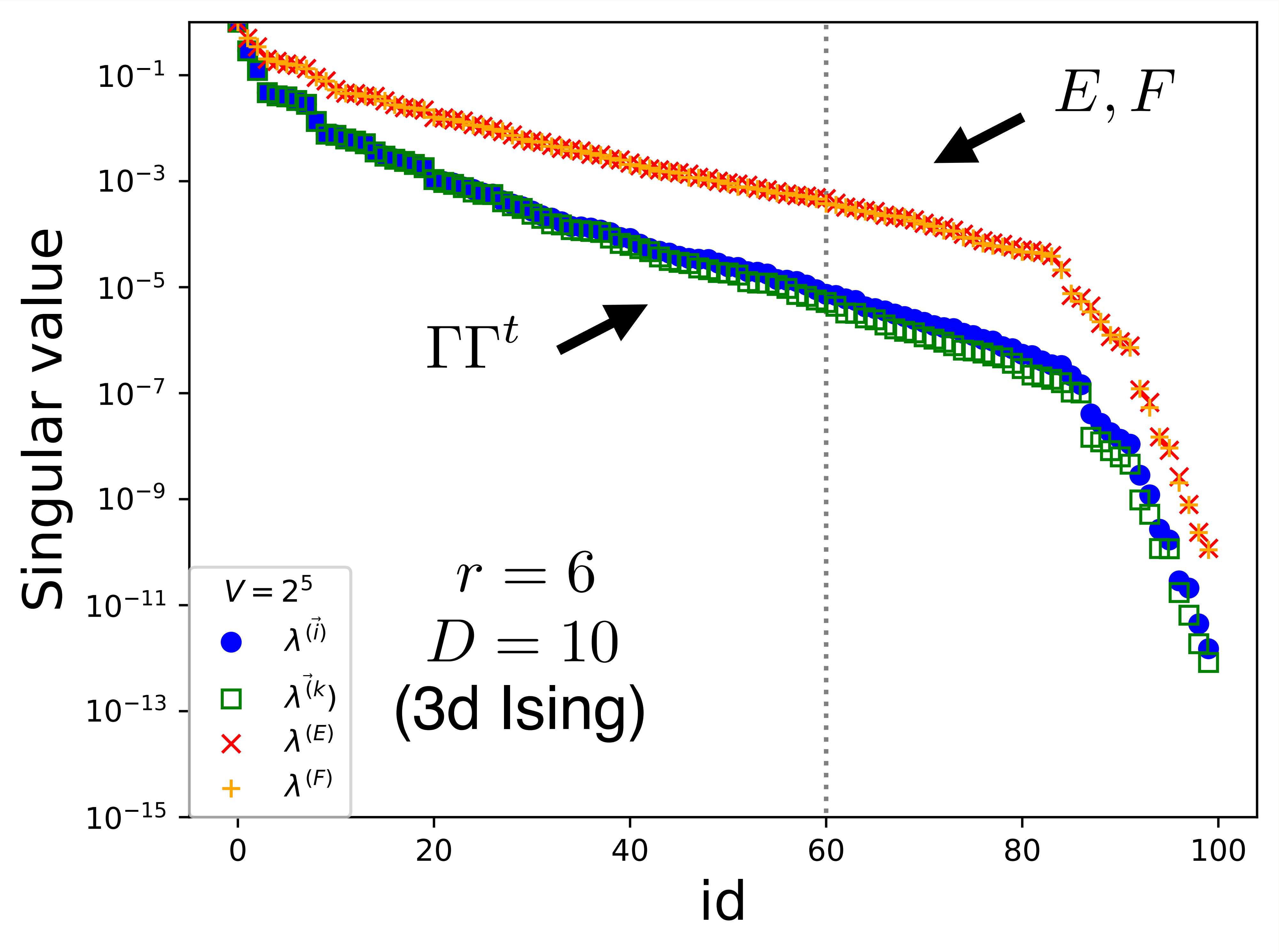
$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

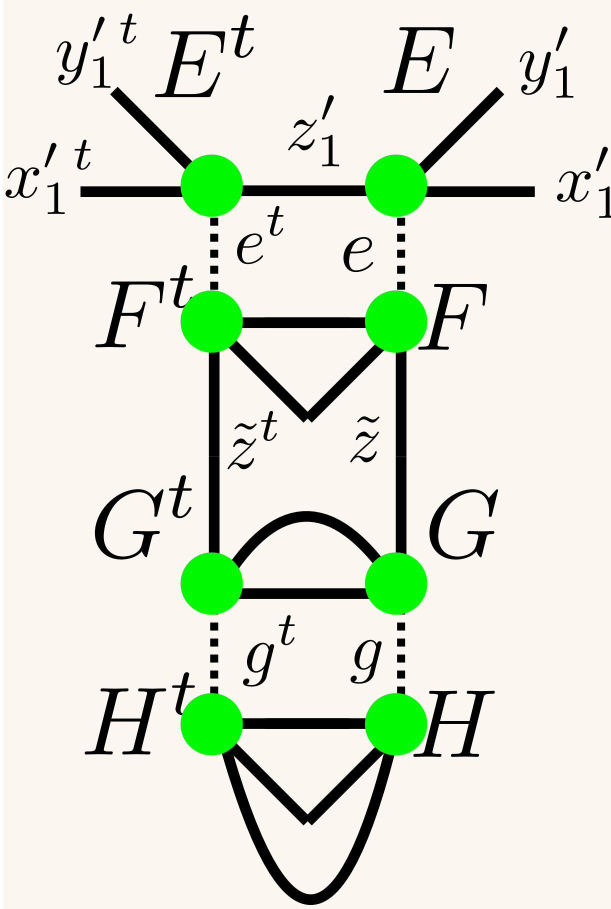
◉ Triad-MDTRG: Contraction step



$$O(D^6) \to O(D^6) \to O(D^5) \to O(D^5) \to O(D^5) \to O(D^6)$$

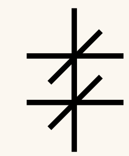
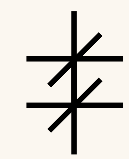
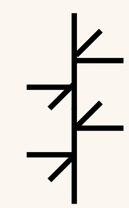
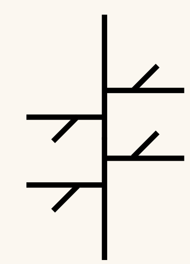
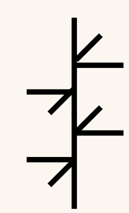
◉ Isometry for unit-cell tensor





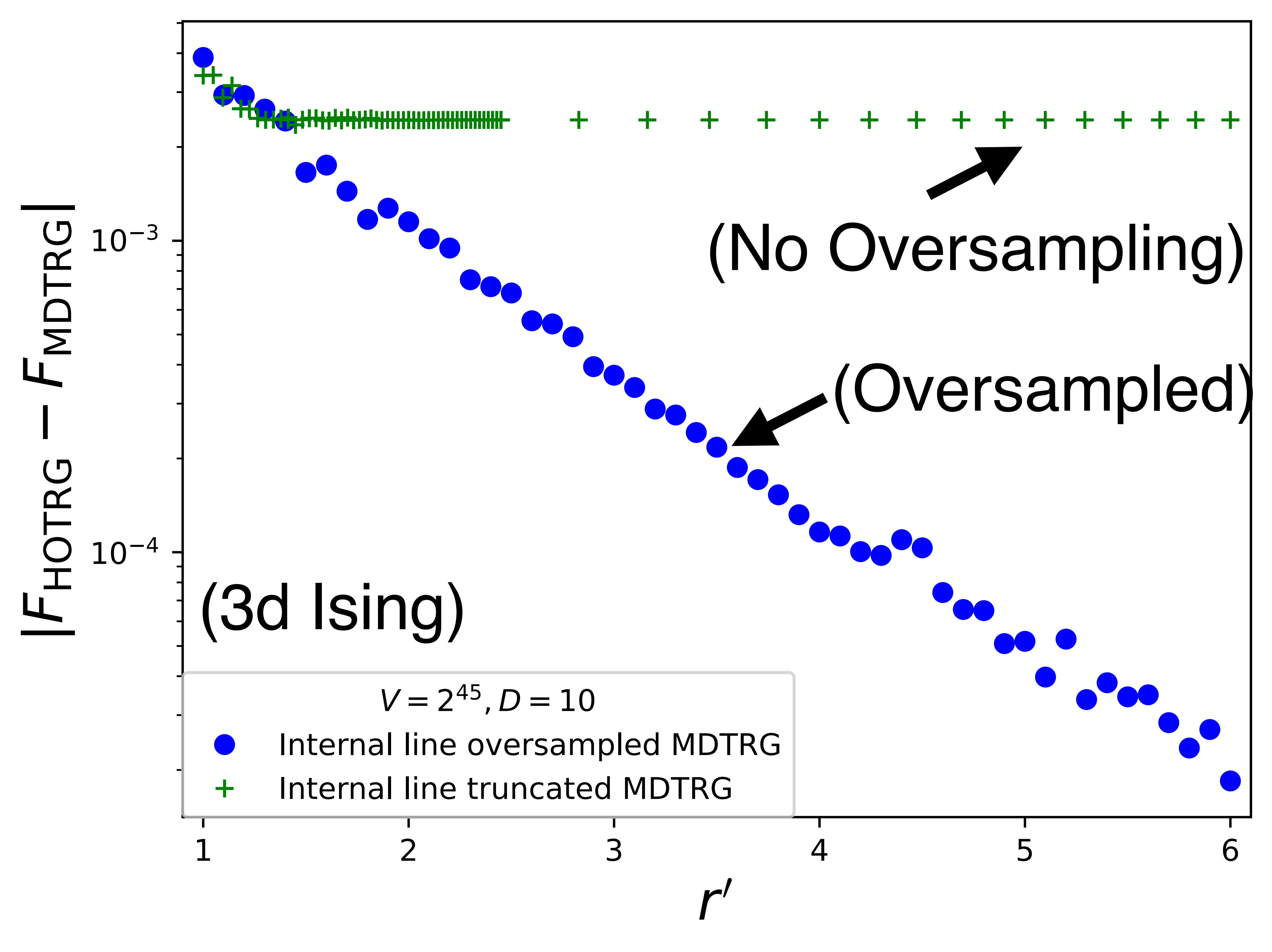
→ より広い範囲の近似は系統誤差を減らす

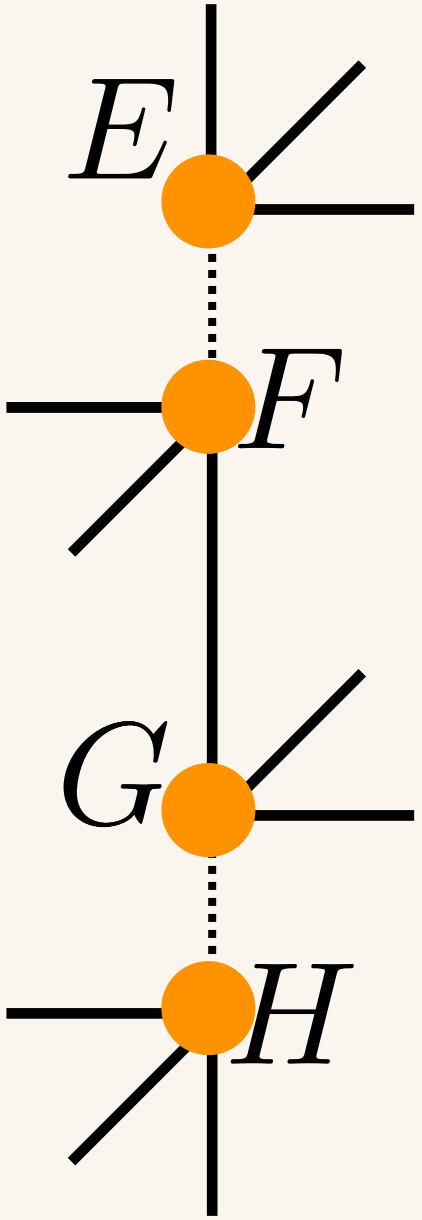
◉ 乱拓特異値分解を用いた比較

	with R-SVD	w/o R-SVD	各テンソルの足数	
◇ HOTRG	$O(D^{3d})$	$O(D^{4d-1})$		$2d$
◇ ATRG	$O(D^{2d+1})$	$O(D^{3d})$		$2d$
◇ MDTRG	$O(D^{2d+1})$	$O(D^{3d})$		$d+1$
◇ TTRG	$O(D^{d+3})$	$O(D^{d+4})$		3
◇ Triad-MDTRG	$O(D^{d+3})$	$O(D^{3d})$		$d+1$

→ 計算量は他の手法と同等にまで削減。系統誤差を見ていく

◉ 内線オーバーサンプリング

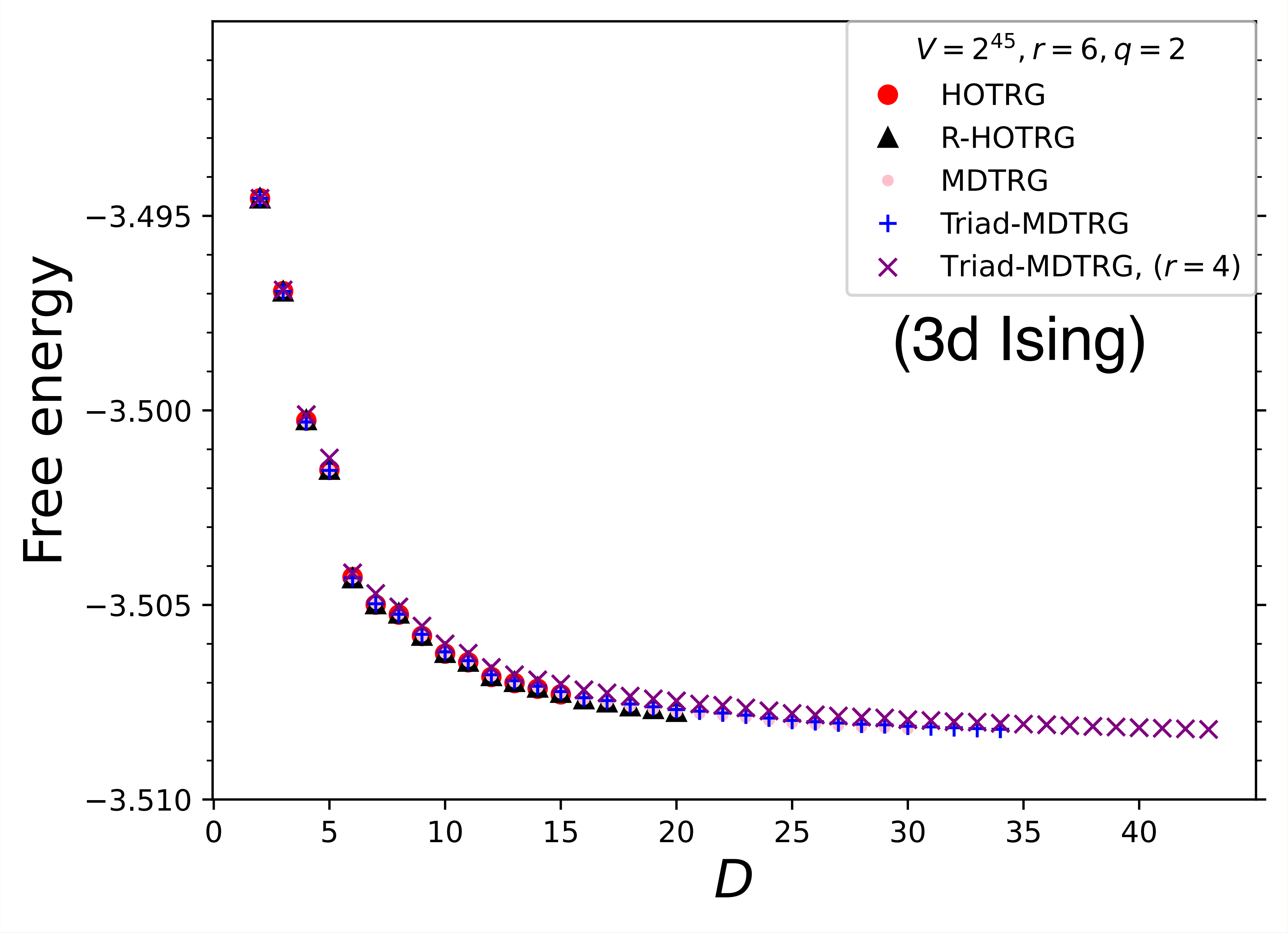




→ 内線(点線) をオーバーサンプリング$(D \to rD)$

しないとHOTRGと同じ精度へ収束しない $(r = \mathrm{Const.})$

◉ 3d-イジング模型でのテスト

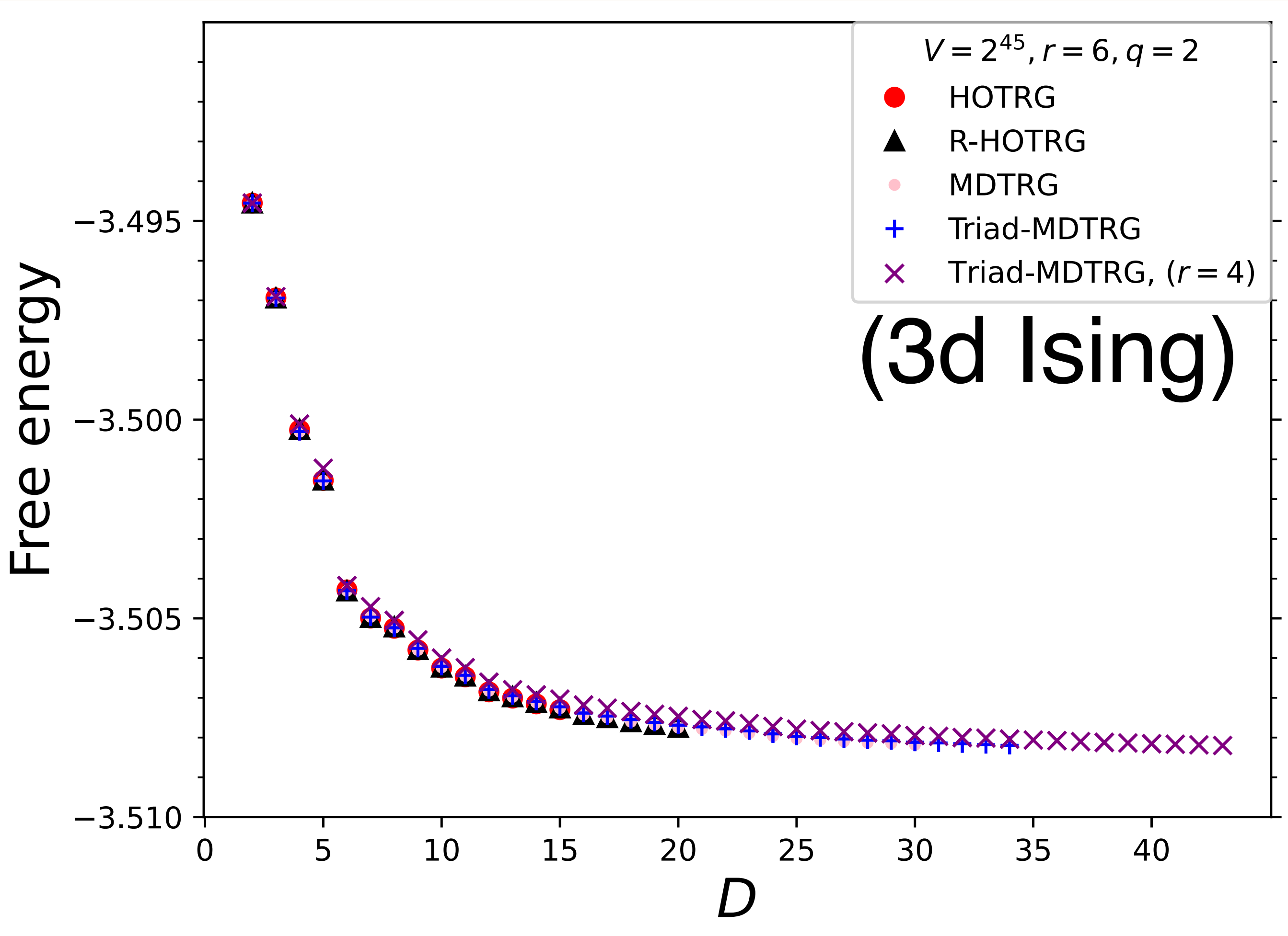


→ R-HOTRG, MDTRG, Triad-MDTRGはHOTRGに収束

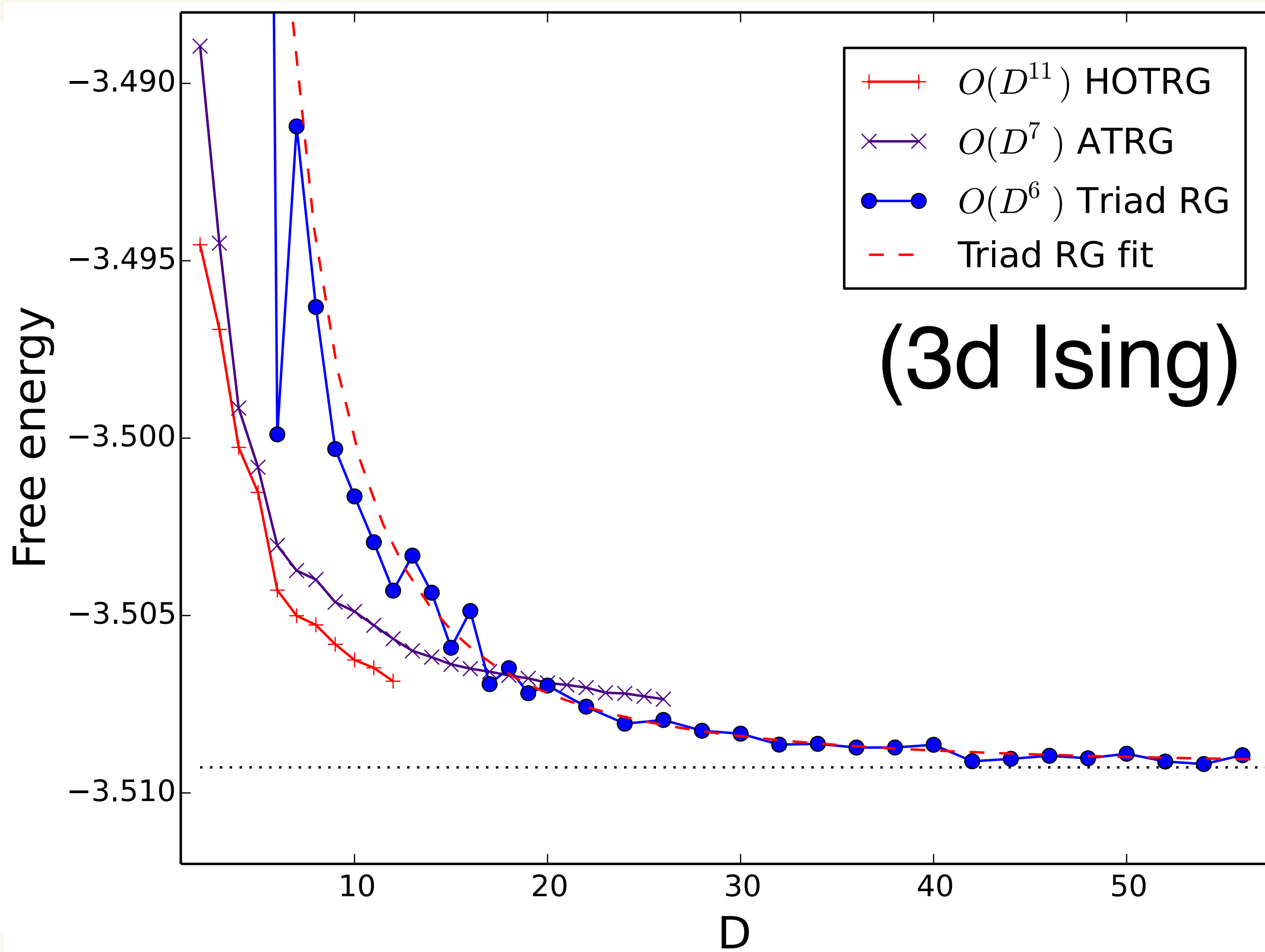
(追加の分解の誤差は全て支配的でない).

◉ 3d-イジング模型でのテスト

[K.N. arXiv:2307.14191]



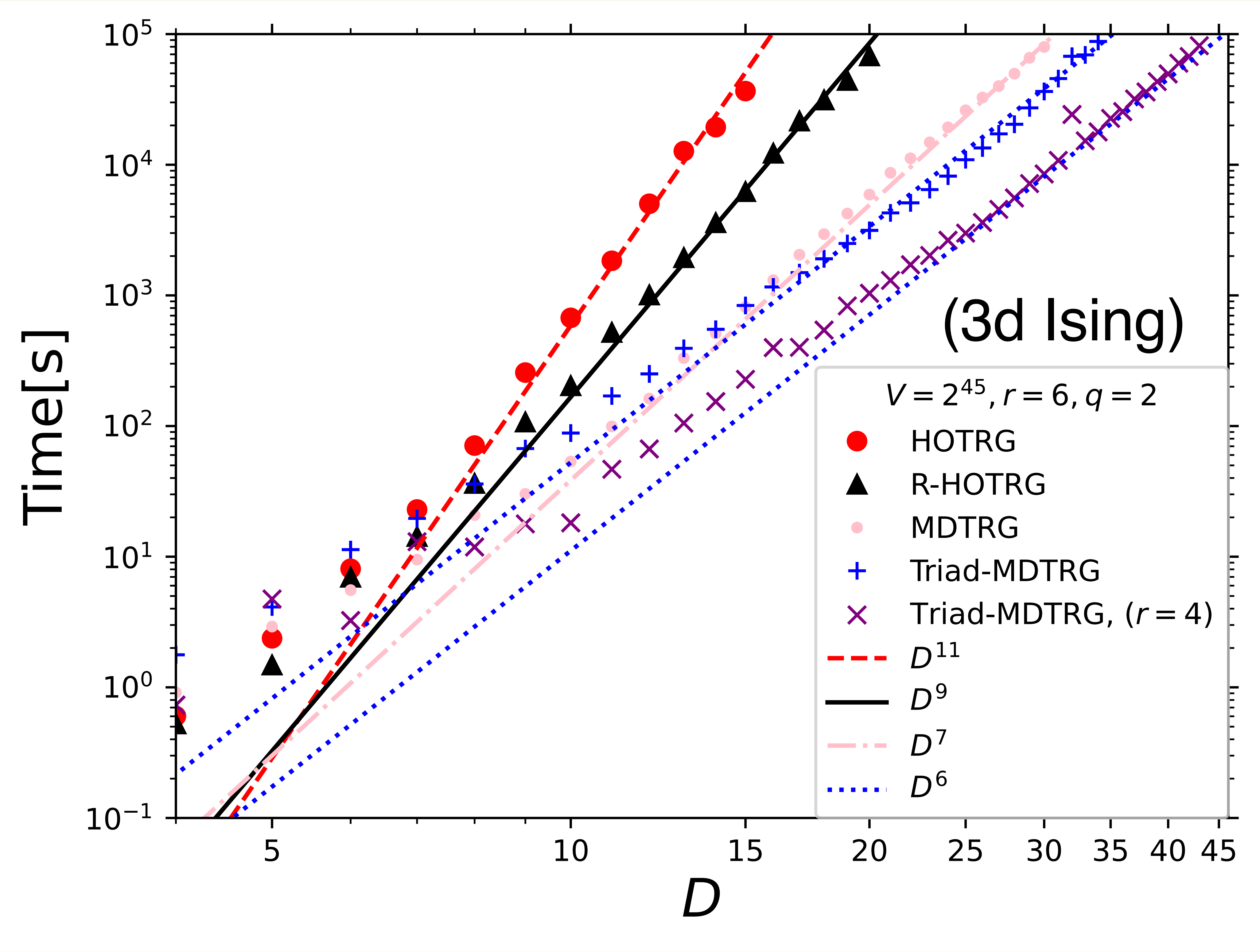
[D. Kadoh, K.N. arXiv:1912.02414]



→ R-HOTRG, MDTRG, Triad-MDTRGはHOTRGに収束

(追加の分解の誤差は全て支配的でない).

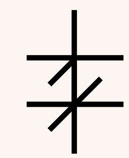
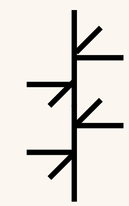
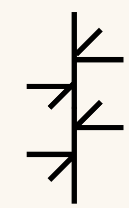
◉ 打ち切り添字サイズ D でのスケーリング



→ 想定通りのスケーリング

◉ まとめ

◇ HOTRGにRandomized-SVDを使うとどうなるのか？

	with R-SVD	w/o R-SVD	各テンソルの足数	
◇ HOTRG	$O(D^{3d})$	$O(D^{4d-1})$		$2d$
◇ MDTRG	$O(D^{2d+1})$	$O(D^{3d})$		$d+1$
◇ Triad-MDTRG	$O(D^{d+3})$	$O(D^{3d})$		$d+1$

◇ 追加の分解からくる系統誤差を減らせないか？

→ R-HOTRG, MDTRG, Triad-MDTRGはHOTRGと同精度。

支配的な系統誤差はどれもIsometryの打ち切りのみから。

Key ideas(MDTRG以外にも応用可能):

内線オーバーサンプリング unit-cellテンソルのIsometry