The six- and the eight-vertex models and counting perfect matchings

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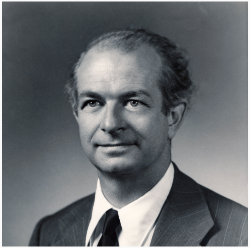
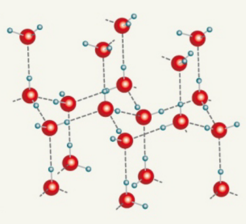
About the six-vertex model

History

Introduced by Linus Pauling (1935) to describe the properties of ice H_2O

- Each O has four nearest neighbors with O-H-O bonds
- Each H is in two possible positions (closer to one O or another)
- Each O must be surrounded by two H's near to it and two on the far side — the ice condition





Graphics by Mark Peplow

History

Elliott Lieb (1967a) considered “square ice”

- Two-dimensional version of real ice
- Defined by the same ice condition applied to the *square lattice*

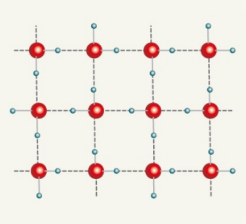
Lieb’s square ice constant

N — number of O’s

Z — the *partition function*

Lieb found the *exact solution* as

$$W = \lim_{N\to\infty} Z^{1/N} = \left(\frac{4}{3}\right)^{3/2} \approx 1.5396007\ldots$$



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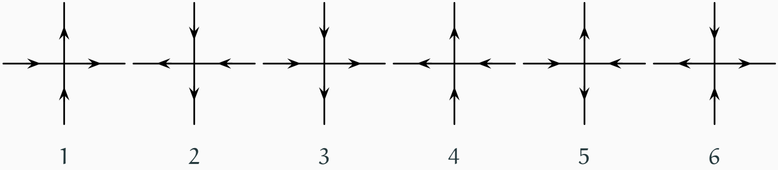
Definition



- States are Eulerian orientations on 4-regular graphs
  O — vertices, H — arrows
- Six permitted types of local configurations around a vertex — six possible weights $w_1, \dots, w_6$
- Under arrow reversal symmetry,
  $w_1 = w_2 = a, w_3 = w_4 = b, w_5 = w_6 = c$
- Partition function $Z(G; a, b, c) = \sum_{\tau \in \mathcal{EO}(G)} a^{n_1+n_2} b^{n_3+n_4} c^{n_5+n_6}$

Original motivation

In addition to water ice with $(a, b, c) = (1, 1, 1)$, several other real crystals with hydrogen bonds satisfy the ice model.

The KDP model

{ a = b > 1, c = 1 }

The Rys F model

{ a = b = 1, c > 1 }

Exact solutions for these models (Elliott Lieb 1967b, 1967c) and some other generalized models (Sutherland 1967, Yang 1967, Nagle 1969, etc.) have been obtained.

Exact computational complexity

Computing (unweighted) #Eulerian orientations is #P-COMPLETE on

- general Eulerian graphs (Mihail and Winkler, 1992)
- even degree regular graphs (Huang and Lu, 2012)
- planar 4-regular graphs (Guo and Williams, 2013)

For the six-vertex model under complex weights

- Cai, Fu, and Xia (2018) proved a *complexity dichotomy* for general 4-regular graphs
- Cai, Fu, and Shao (2017) proved a *complexity trichotomy* for planar 4-regular graphs

In both two works, cancellation plays an important role for P-time computable cases.

Exact computational complexity

Under our setting with arrow reversal symmetry and a, b, c being nonnegative

- TRACTABLE $\begin{cases} \text{two of } a, b, c \text{ are } 0\text{'s} \\ \text{one of } a, b, c \text{ is } 0 \text{ and the other two are equal} \end{cases}$
- PLANAR TRACTABLE $\begin{cases} c^2 = a^2 + b^2 \\ \text{one of } a, b \text{ is } 0 \end{cases}$
- #P-HARD otherwise

We study the approximate computational complexity of calculating $Z(a, b, c)$ on general 4-regular graphs for nonnegative a, b, c.

Approximate counting and sampling

All previous results are on the unweighted point $(a, b, c) = (1, 1, 1)$

- Mihail and Winkler (1992): an FPRAS for #EULERIAN ORIENTATIONS on general Eulerian graphs
- Luby, Randall, and Sinclair (1995): rapid mixing of a Markov chain that leads to a FPAUS for Eulerian orientations on rectangular regions of the square lattice with fixed boundaries
- Randall and Tetali (1998): improve to the rapid mixing of the single-site Glauber dynamics
- Goldberg, Martin, and Paterson (2002): improve to the free boundary case

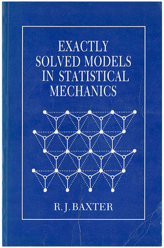
We give the first results for weighted cases.
Our results conform to the phase transition phenomenon in physics.

Phase transition and approximate complexity

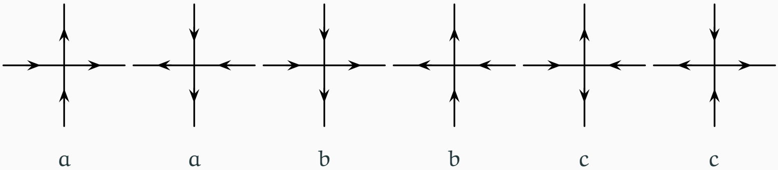
Phase transition

Described by Rodney Baxter (1982) in his famous book “Exactly Solved Models in Statistical Mechanics” —

On the square lattice, the weights (a, b, c) determine the relative probabilities of states, and thus can influence the macroscopic behavior of the system.

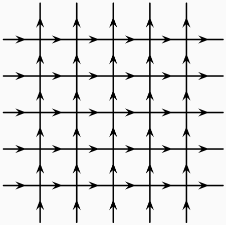


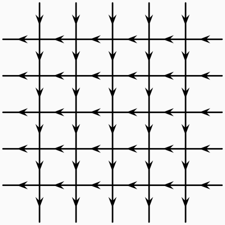
Phase transition



On a square lattice region with its side length approaching infinity

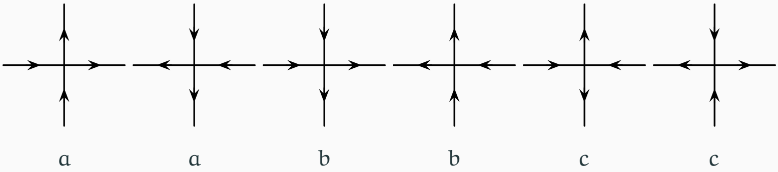
$a > b + c$ (FE: ferroelectric phase)



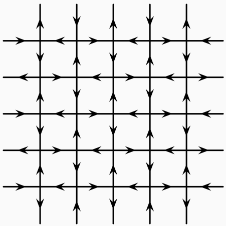


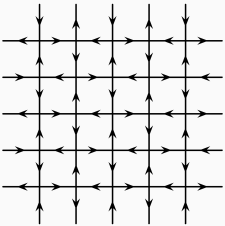
$b > a + c$ (also FE) — symmetric to the above case

Phase transition



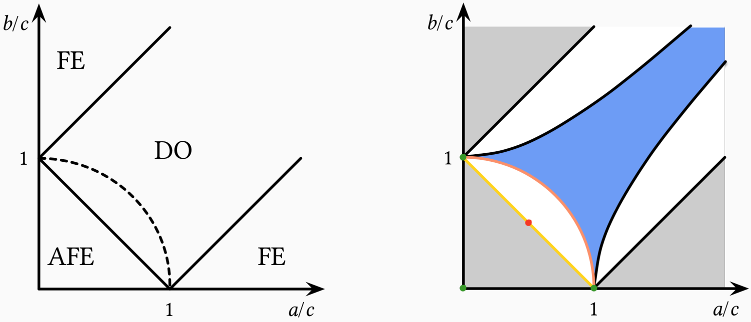
$c > a + b$ (AFE: anti-ferroelectric phase)
two types of "saddle" configurations alternate





$c \leqslant a + b$, $b \leqslant a + c$, and $a \leqslant b + c$ (DO: disordered phase)
the system is disordered

Our results



Theorem (Jin-Yi Cai, L., and Pinyan Lu, 2017)

There is an FPRAS for $Z(G; a, b, c)$ *if* $a^2 \leqslant b^2 + c^2$, $b^2 \leqslant a^2 + c^2$, *and* $c^2 \leqslant a^2 + b^2$ *(the blue region).*

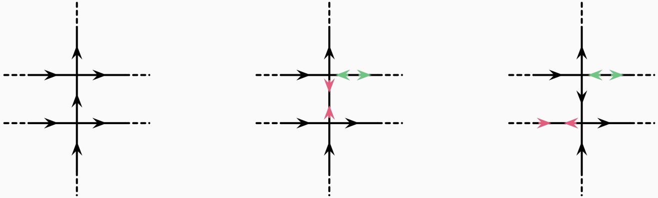
There is no FPRAS for $Z(G; a, b, c)$ *if* $a > b + c$ *or* $b > a + c$ *or* $c > a + b$ *(the FE/AFE region), unless* $\mathsf{RP} = \mathsf{NP}$.

Proof sketch — fpras

Counting via sampling: Markov chain Monte Carlo

Directed-loop algorithm ($\mathcal{M}_\mathrm{D}$)

State space: Eulerian orientations and near-Eulerian orientations
Transitions: *Metropolis moves* between neighboring states — creating, shifting, and merging of two "defects" on the edges



Used by Rahman and Stillinger (1972), Yanagawa and Nagle (1979), Barkema and Newman (1998), Syljuåsen and Zvonarev (2004), etc.

Depicts the *Bjerrum defects* happening in real ice (BN'98).

Technical lemma

$\mathcal{Z}_0$: total weight of Eulerian orientations (the partition function)
$\mathcal{Z}_2$: total weight of near-Eulerian orientations

Lemma

If $\frac{\mathcal{Z}_2}{\mathcal{Z}_0}$ *is polynomially upper bounded, then* $\mathcal{M}_D$ *is rapidly mixing when* $a^2 \leqslant b^2 + c^2$, $b^2 \leqslant a^2 + c^2$, *and* $c^2 \leqslant a^2 + b^2$ *(the blue region).*

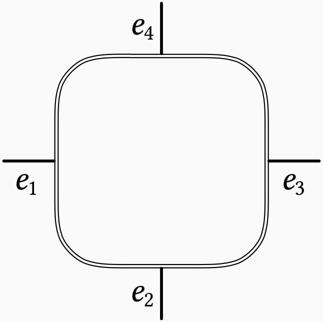
- Proved by a *canonical path argument*
- Can also be derived by techniques of McQuillian (2013) (windable framework)

We show that $\frac{\mathcal{Z}_2}{\mathcal{Z}_0}$ is polynomially upper bounded in the whole DO phase $(a \leqslant b + c, b \leqslant a + c, c \leqslant a + b)$
and the following structural lemma plays a crucial role.

Closure properties — a structural lemma

A 4-ary construction: a 4-regular graph having 4 "external" edges

- defines a constraint function — for a particular input, the value is the weighted sum of all valid internal configurations consistent with the input
- also satisfies the ice rule and the arrow reversal symmetry for some a', b', c' — can be viewed as a virtual vertex



Closure properties — a structural lemma

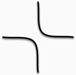
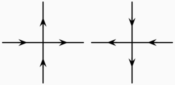
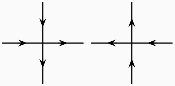
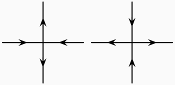
Lemma

The set of 4-ary constraint functions lying in the DO phase ($a \leqslant b + c, b \leqslant a + c, c \leqslant a + b$) is closed under 4-ary constructions.

The lemma is important not only for its crucial role in giving the FPRAS, but also reveals a structural difference between the two sides of the phase transition threshold.

Decomposition of Eulerian orientations

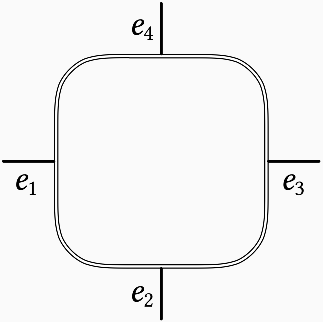
Decompose one Eulerian orientation of G into $2^{|V|}$ circuit partitions by pairing incoming edges to outgoing edges in two possible ways.

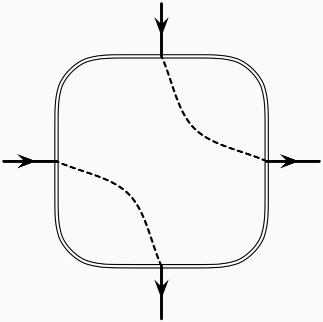
Configurations	Weight			
	a	0	1	1
	b	1	0	1
	c	1	1	0

Decomposition of Eulerian orientations

The idea of decomposition also works for 4-ary constructions

- We can put weight $w(\cdot)$ on local pairings at vertices
- Define the weight of a circuit decomposition to be the product of weights on vertices
- Define the weight $W(\cdot)$ of global pairings for the 4-ary construction as a virtual vertex, e.g. $W(\neg\llcorner) =$ weighted sum of all circuit decompositions where $\{e_1, e_2\}\{e_3, e_4\}$ are paired up





Closure properties — proof idea

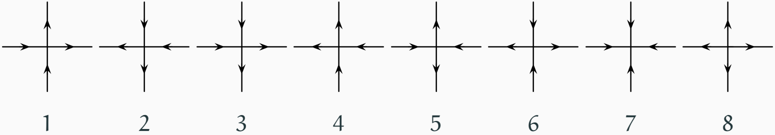
Under weighted decomposition $\begin{cases} a = w(\,) + w(\,) \\ b = w(\,) + w(\,) \\ c = w(\,) + w(\,) \end{cases}$

- Constraint function $(a, b, c) \in$ DO at every vertex $\Longleftrightarrow$
- Weights of pairings $w(\,), w(\,), w(\,) \geqslant 0$ at every vertex $\Longleftrightarrow$
- Weights of circuit partitions of the 4-ary construction are nonnegative $\Longrightarrow$
- Induced weight function $W(\cdot)$ of the global pairings of the 4-ary construction are nonnegative $\Longleftrightarrow$
- Constraint function of the 4-ary construction $(a', b', c') \in$ DO

Proof sketch — hardness (skipped)

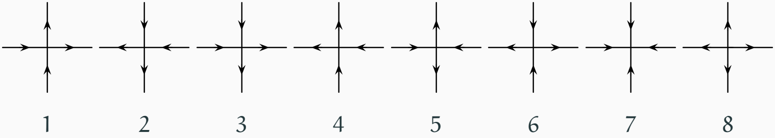
The eight-vertex model

Definition



- Allows “sink” and “source” with weight $w_7 = w_8 = d$
- The six-vertex model is the special case when $d = 0$
- States are even orientations
- $Z(G; a, b, c, d) = \sum_{\tau \in \mathcal{O}_e(G)} a^{n_1+n_2} b^{n_3+n_4} c^{n_5+n_6} d^{n_7+n_8}$

Phase transition



On a square lattice region with its side length approaching infinity

- Ferroelectric/Anti-ferroelectric phase (FE/AFE):
  $a > b + c + d$, $b > a + c + d$, $c > a + b + d$, or $d > a + b + c$
- Disordered phase (DO): $\begin{cases} a \leqslant b + c + d \\ b \leqslant a + c + d \\ c \leqslant a + b + d \\ d \leqslant a + b + c \end{cases}$

Our results (Cai, L., Lu, and Yu, 2018)

FE/AFE: NP-**hard**

DO

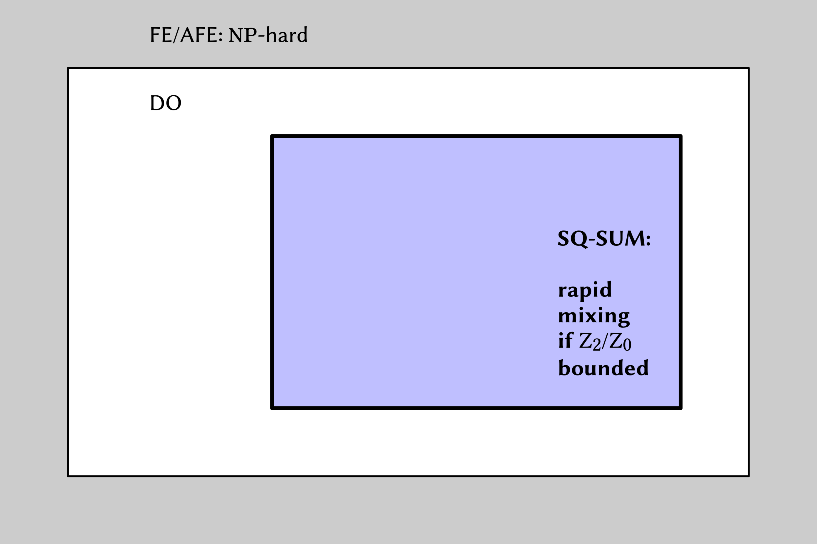
Notation

$$\text{SQ-SUM} = \left\{ (a, b, c, d) \mid \begin{cases} a^2 \leqslant b^2 + c^2 + d^2 \\ b^2 \leqslant a^2 + c^2 + d^2 \\ c^2 \leqslant a^2 + b^2 + d^2 \\ d^2 \leqslant a^2 + b^2 + c^2 \end{cases} \right\}.$$

Remark

SQ-SUM $\subset$ DO.

Our results (Cai, L., Lu, and Yu, 2018)



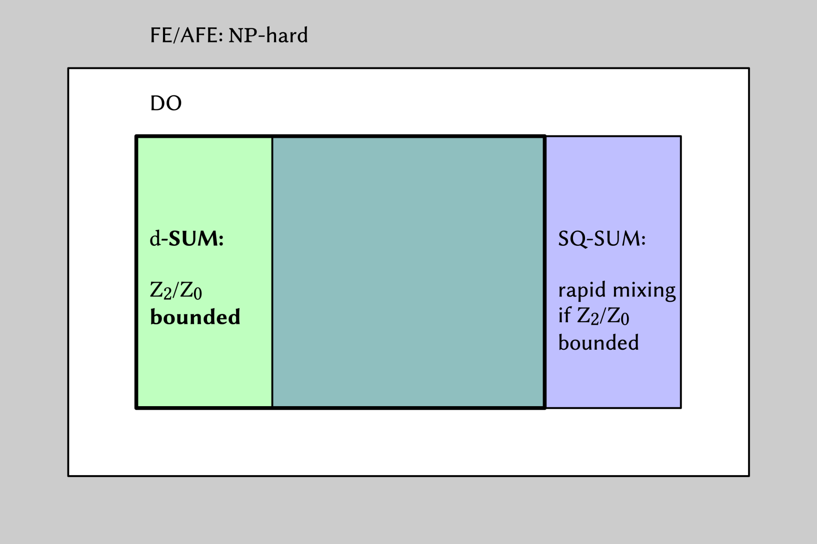
Notation

$$\mathrm{d\text{-}SUM} = \left\{ (a, b, c, d) \mid \begin{cases} a + d \leqslant b + c \\ b + d \leqslant a + c \\ c + d \leqslant a + b \end{cases} \right\}.$$

Remark

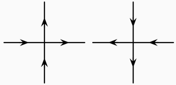
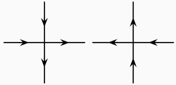
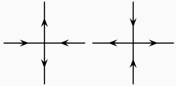
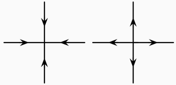
$\mathrm{d\text{-}SUM} \subset \mathrm{DO}$.

Our results (Cai, L., Lu, and Yu, 2018)

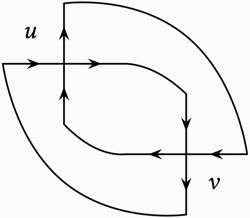
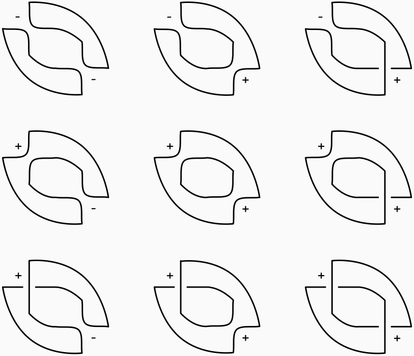


Decomposition of even orientations

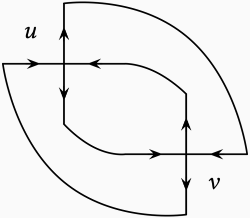
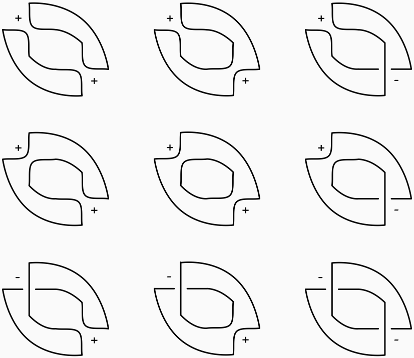
Decompose one even orientation into $3^{|V|}$ annotated circuit partitions by pairing edges in all three possible ways (instead of two!).

Configurations	Weight	Sign		
				
	a	−	+	+
	b	+	−	+
	c	+	+	−
	d	−	−	−

An even orientation and its decomposition

τ	$\Phi(\tau)$
	

Another even orientation and its decomposition

τ	$\Phi(\tau)$
	

Closure properties for the eight-vertex model

Lemma

The set of 4-ary constraint functions lying in the **DO** *phase is closed under 4-ary constructions.*

— again reveals a structural difference between the two sides of the phase transition threshold.

Proof idea: Under weighted decomposition
$$\begin{cases} a = w(\asymp_{-}) + w()\!(_{+}) + w(\dashv\!\vdash_{+}) \\ b = w(\asymp_{+}) + w()\!(_{-}) + w(\dashv\!\vdash_{+}) \\ c = w(\asymp_{+}) + w()\!(_{+}) + w(\dashv\!\vdash_{-}) \\ d = w(\asymp_{-}) + w()\!(_{-}) + w(\dashv\!\vdash_{-}) \end{cases}$$

- $(a, b, c, d) \in \mathrm{DO} \iff$ there exists a nonnegative $w(\cdot) \implies$
- Induced weight function $W(\cdot)$ of pairings of the 4-ary construction as a virtual vertex are nonnegative $\iff$
- Constraint function $(a', b', c', d') \in \mathrm{DO}$

Closure properties for the eight-vertex model

Lemma

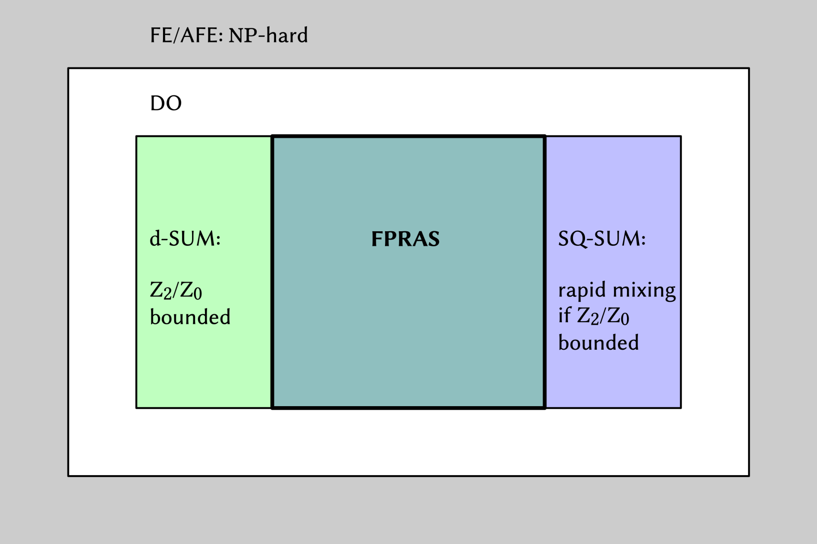
The set of 4-ary constraint functions lying in the d*-SUM region is closed under 4-ary constructions.*

— directly indicates that $\frac{Z_2}{Z_0}$ is polynomially upper bounded.

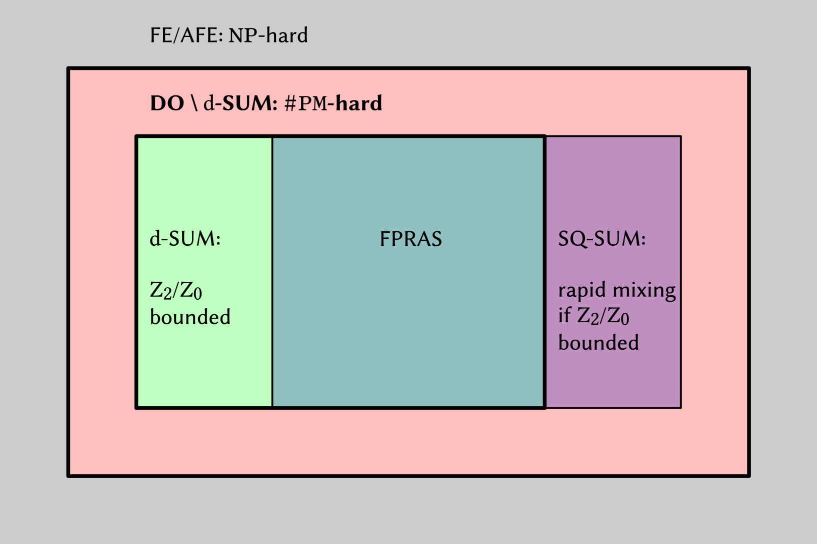
Proof idea: Under weighted decomposition $\begin{cases} a = w(\urcorner\llcorner_{-}) + w(\lrcorner\ulcorner_{+}) + w(\dashv\vdash_{+}) \\ b = w(\urcorner\llcorner_{+}) + w(\lrcorner\ulcorner_{-}) + w(\dashv\vdash_{+}) \\ c = w(\urcorner\llcorner_{+}) + w(\lrcorner\ulcorner_{+}) + w(\dashv\vdash_{-}) \\ d = w(\urcorner\llcorner_{-}) + w(\lrcorner\ulcorner_{-}) + w(\dashv\vdash_{-}) \end{cases}$

- $(a, b, c, d) \in d$-SUM $\Longleftrightarrow \begin{cases} w(\urcorner\llcorner_{+}) \geqslant w(\urcorner\llcorner_{-}) \\ w(\lrcorner\ulcorner_{+}) \geqslant w(\lrcorner\ulcorner_{-}) \\ w(\dashv\vdash_{+}) \geqslant w(\dashv\vdash_{-}) \end{cases} \Longrightarrow$
- Induced weight function $W(\cdot)$ has $\begin{cases} W(\urcorner\llcorner_{+}) \geqslant W(\urcorner\llcorner_{-}) \\ W(\lrcorner\ulcorner_{+}) \geqslant W(\lrcorner\ulcorner_{-}) \\ W(\dashv\vdash_{+}) \geqslant W(\dashv\vdash_{-}) \end{cases} \Longleftrightarrow$
- Constraint function $(a', b', c', d') \in d$-SUM

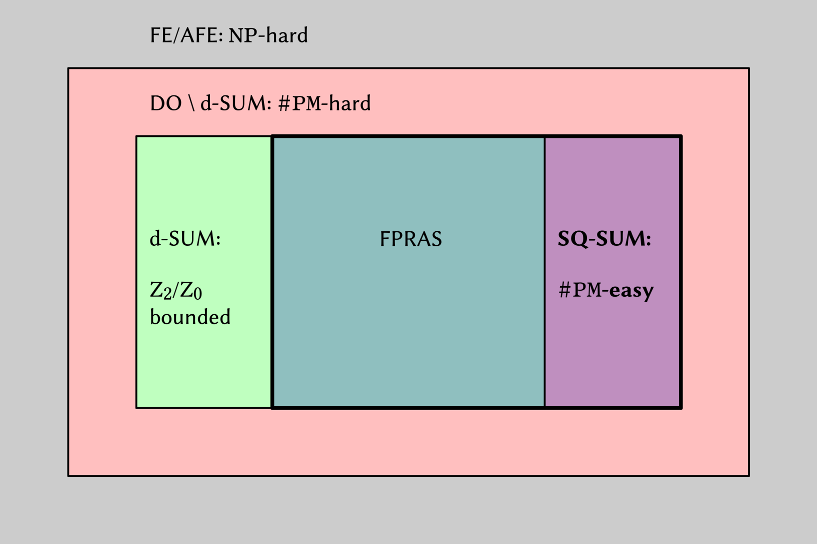
Our results (Cai, L., Lu, and Yu, 2018)



Our results (Cai and L., 2019a)



Our results (Cai and L., 2019a)



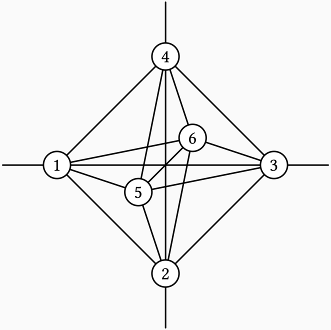
Counting Perfect Matchings and Matchgates

A k-ary matchgate: a graph with k external edges

- external edges are labelled $i_1, \ldots, i_k$
- each non-external edge e has a nonnegative weight w_e
- defines a constraint function f on the k external edges, where $f(b_1, \ldots, b_k)$ for $(b_1, \ldots, b_k) \in \{0,1\}^k$ is the sum, over perfect matchings, of the product of the weight of edges with assignment 1, where the dangling edge i_j is assigned b_j, and the empty product has weight 1

In order to show #PM-easiness, we show that every eight-vertex constraint function represented by $(a, b, c, d) \in$ SQ-SUM can be implemented by a 4-ary matchgate.

A 4-ary matchgate for the eight-vertex model

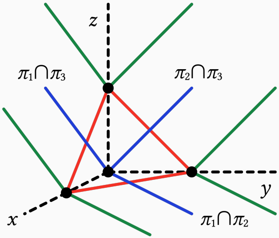


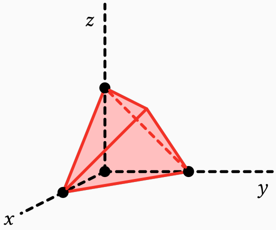
$$
\begin{aligned}
a_1' &= w_{12} + w_{15}w_{26} + w_{25}w_{16}, \\
a_2' &= w_{34} + w_{35}w_{46} + w_{45}w_{36}, \\
b_1' &= w_{14} + w_{15}w_{46} + w_{45}w_{16}, \\
b_2' &= w_{23} + w_{25}w_{36} + w_{35}w_{26}, \\
c_1' &= w_{13} + w_{15}w_{36} + w_{35}w_{16}, \\
c_2' &= w_{24} + w_{25}w_{46} + w_{45}w_{26}, \\
d_1' &= (w_{12}w_{34} + w_{14}w_{23} + w_{13}w_{24}) + \\
&\quad (w_{35}w_{46} + w_{45}w_{36})w_{12} + (w_{15}w_{26} + w_{25}w_{16})w_{34} + \\
&\quad (w_{25}w_{36} + w_{35}w_{26})w_{14} + (w_{15}w_{46} + w_{45}w_{16})w_{23} + \\
&\quad (w_{25}w_{46} + w_{45}w_{26})w_{13} + (w_{15}w_{36} + w_{35}w_{16})w_{24} \\
d_2' &= w_{56}.
\end{aligned}
$$

A geometric lemma

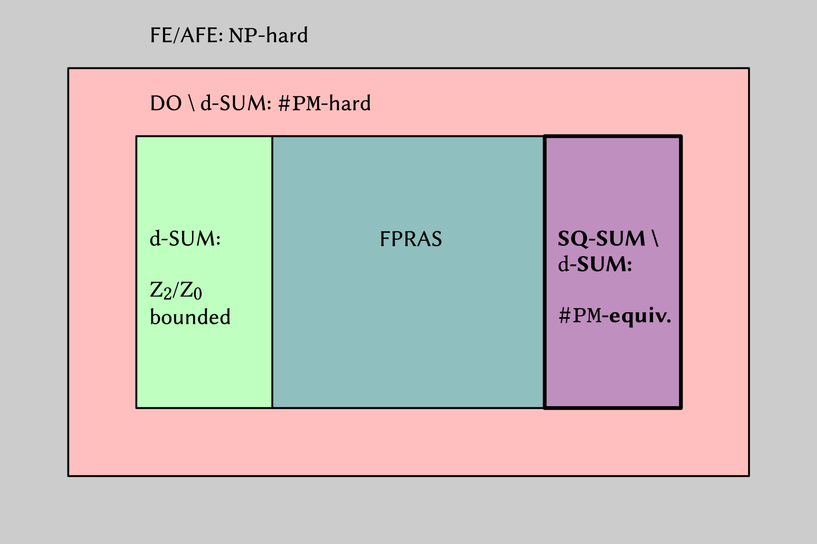
Lemma

Let
$U = \{(x,y,z) \in \mathbb{R}^3_{>0} \mid x \leqslant y+z+1, y \leqslant x+z+1, z \leqslant x+y+1, 1 \leqslant x+y+z\}$,
$V = \{(x,y,z) \in \mathbb{R}^3_{>0} \mid x+y+z = 1\}$, *and*
$W = \{(x,y,z) \in \mathbb{R}^3_{>0} \mid x \leqslant y+z, y \leqslant x+z, z \leqslant x+y\}$. *Then* U *is the Minkowski sum of* V *and* W*, namely,* U *consists of precisely those points* $\mathbf{u} \in \mathbb{R}^3$*, such that* $\mathbf{u} = \boldsymbol{v} + \boldsymbol{w}$ *for some* $\boldsymbol{v} \in V$ *and* $\boldsymbol{w} \in W$*.*





Our results (Cai and L., 2019a)



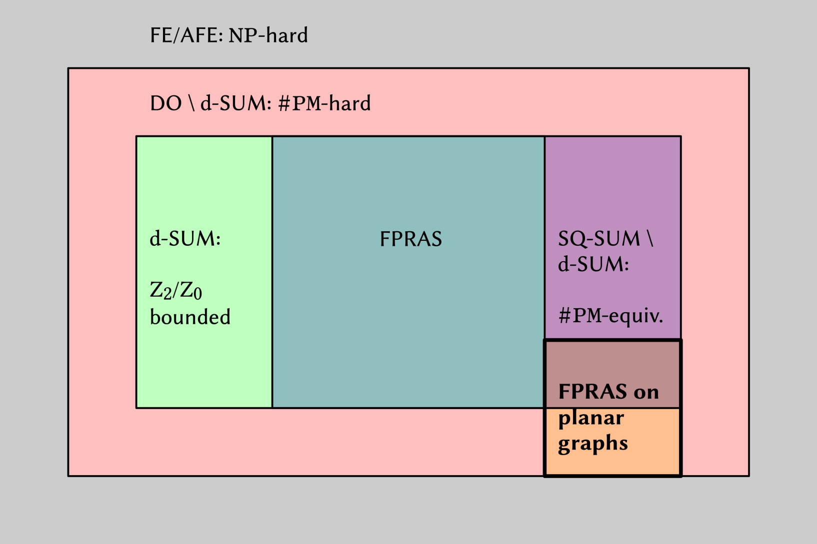
Our results (Cai and L., 2019a)

Our result is tight: no (a, b, c, d) outside SQ-SUM can be implemented by a matchgate (Bulatov, Goldberg, Jerrum, Richerby, and Živný, 2017).

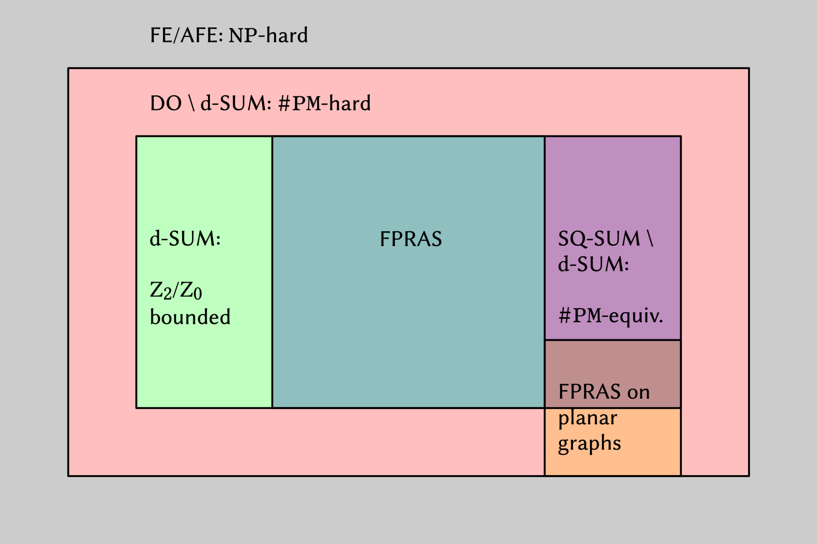
In fact, we have a theorem of independent interest

- It is open for several years what are the constraint functions that can be implemented by nonnegatively weighted k-ary matchgates for $k > 3$.
- We give the characterization for 4-ary matchgates (they are essentially those satisfying $\begin{cases} a_1 a_2 \leqslant b_1 b_2 + c_1 c_2 + d_1 d_2 \\ b_1 b_2 \leqslant a_1 a_2 + c_1 c_2 + d_1 d_2 \\ c_1 c_2 \leqslant a_1 a_2 + b_1 b_2 + d_1 d_2 \\ d_1 d_2 \leqslant a_1 a_2 + b_1 b_2 + c_1 c_2. \end{cases}$)

Our results (Cai, L., Lu, and Yu, 2018) and (Cai and L., 2019b)



Open problems



Thank you!