



On the complexity of quantum partition functions

David Gosset

Based on:

Sergey Bravyi, Anirban Chowdhury, DG, Pawel Wocjan. *Nature Physics*, 18(11):1367-1370, 2022 Sergey Bravyi, Anirban Chowdhury, DG, Vojtech Havlicek, Guanyu Zhu. arXiv:2302.11454, 2023 Sergey Bravyi, DG. *Phys. Rev. Lett*. 119, 100503, 2017









Complexity of many-body systems

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Interactions between particles (qubits, bosons, fermions,)







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How hard is it to compute their physical properties?

Ground energy problems are intractable optimization problems

Computing the **ground energy** of **classical** locally interacting systems is an NP-hard (intractable) optimization problem

e.g. 3-SAT
$$H = \sum_{z \in \{0,1\}^n} C(z) |z\rangle \langle z| \qquad C(z) = \text{Number of clauses violated by } z$$

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e.g. 2D Ising with
magnetic field
[Barahona 1982]
$$H = \sum_{(i,j) \in E(G)} J_{ij} Z_i Z_j + h_i Z_i$$



Quantum Cook-Levin theorem (informal):

Computing the ground energy of an n particle quantum system with local interactions to precision 1/poly(n) is an **intractable quantum optimization problem.**

Input: An *n*-qubit local Hamiltonian *H*, a number $a \in \mathbb{R}$, a precision $\epsilon = 1/n^{\alpha}$

Output: (YES) The ground energy of *H* is $\leq a$ (NO) The ground energy of *H* is $\geq a + \epsilon$

а + є а

(promised one of these conditions is satisfied)

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Theorem (Kitaev 1999) The local Hamiltonian problem is **QMA-complete.**

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The local Hamiltonian problem is QMA-complete. Quantum analogue of NP

The local Hamiltonian problem remains QMA-complete even for systems with 2-qubit interactions [Kempe Kitaev Regev 2004]



2-local Hamiltonian on a 2D grid [Oliveira Terhal 2008]



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Hubbard model on a 2D grid with site-dependent magnetic field [Schuch Verstraete 2009].



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There is also an important class of ground energy problems associated with **stoquastic** Hamiltonians that lies in between NP and QMA... [Bravyi Divincenzo Oliveira Terhal 2006]

	$H = \sum h(i,j)$		
	1≤ <i>ī</i> < <i>j</i> ≤n	LH problem	
Ising model	$h(i,j) = \alpha_{ij} Z_i Z_j$	NP-complete	(Classical)
XY model	$h(i,j) = \alpha_{ij}(X_iX_j + Y_iY_j)$	QMA-complete [Cubitt Montanaro 2013]	(Quantum)

$$H = \sum_{1 \le i < j \le n} h(i, j)$$

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Ising model	$h(i,j) = \alpha_{ij} Z_i Z_j$	NP-complete	(Classical)
Transverse-field Ising model	$h(i,j) = \alpha_{ij}X_iX_j - \gamma_iZ_i - \gamma_jZ_j$	StoqMA-complete [Bravyi, Hastings 2014]	(Stoquastic)
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These examples illustrate all nontrivial possibilities within the framework of [Cubitt Montanaro 2013])

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There are also some very special examples where local Hamiltonian problems are easy.

Beyond ground energy

How hard is it to compute physical properties in thermal equilibrium?





Vojta M. Quantum phase transitions. Reports on Progress in Physics. 2003 Nov 3;66(12):2069. Bitko, D., T. F. Rosenbaum, and G. Aeppli. *PRL* 77.5 (1996): 940.

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Complexity of partition functions

$$Z = \mathrm{Tr}[e^{-\beta H}]$$

Partition function

Exact computation as hard as #P

e.g., can count the number of solutions to a 3-SAT formula

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We are interested in relative-error approximation...

QPF problem: Given H, β and $\delta > 0$, compute an estimate \widetilde{Z} satisfying $(1 - \delta) \operatorname{Tr}[e^{-\beta H}] \le \widetilde{Z} \le (1 + \delta) \operatorname{Tr}[e^{-\beta H}]$

Defines a robust class of computational problems that are equivalent under polynomial-time reductions.

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Why? Partition function of L noninteracting copies of *H* is $(Tr[e^{-\beta H}])^{L}$ Compute this to constant error and then take the Lth root.

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General case is equivalent to special case with 2-local Hamiltonians T. S. Cubitt, A. Montanaro, and S. Piddock, "Universal quantum Hamiltonians" PNAS 115, no. 38, pp. 9497–9502, 2018.

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Estimating thermal mean values (additive error)

Estimating density of states of a local Hamiltonian (relative error)

Quantum approximate counting

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QPF is polynomial time equivalent to:

Estimating thermal mean values (additive error)

Given *H*, β , $\epsilon > 0$, and a Pauli operator *P*, compute an estimate μ satisfying

$$\left|\mu - \frac{\operatorname{Tr}[Pe^{-\beta H}]}{Z}\right| \le \epsilon$$

QPF problem: Given H, β and $\delta > 0$, compute an estimate \widetilde{Z} satisfying $(1 - \delta) \operatorname{Tr}[e^{-\beta H}] \le \widetilde{Z} \le (1 + \delta) \operatorname{Tr}[e^{-\beta H}]$

b

a

QPF is polynomial time equivalent to:

Let $m_{[a,b]}$ be the number of eigenvalues of H in an interval [a,b]

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Why relative-error approximation?

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QPF is polynomial time equivalent to:

Let $m_{[a,b]}$ be the number of eigenvalues of H in an interval [a,b]

Estimating density of states (relative error)

Given *H* and two thresholds a < b and precision parameters ϵ, δ output an estimate *m* satisfying

$$(1-\delta)m_{[a,b]} \le m \le (1+\delta)m_{[a-\epsilon,b+\epsilon]}$$



QPF problem: Given
$$H,\beta$$
 and $\delta > 0$, compute an estimate \widetilde{Z} satisfying
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...which is directly related to our lack of understanding of quantum approximate counting more generally...

Counting : classical, quantum, exact, approximate



Consider a classical (NP) verifier circuit



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#P is the class of problems (functions) of the form: Given a verifier circuit, count the number of accepting witnesses.

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Can also think of #*P* as describing those mathematical quantities which admit a **combinatorial interpretation:** counting a set where membership is efficiently checkable.

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Examples:

Permanent of a {0,1} matrix (counts perfect matchings)

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Examples:

Permanent of a {0,1} matrix (counts perfect matchings) Output probability of a randomized classical circuit (counts computational paths)

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A related class gapP captures certain "signed" counting problems...

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gapP is the class of functions that can be expressed as the difference of two functions in #*P*.

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gapP is the class of functions that can be expressed as the difference of two functions in #*P*. (Example: output probability of quantum circuit)



Computing a #P function is just as hard as computing a gapP function. Both tasks are as powerful as the polynomial hierarchy [Toda's theorem]. So why do we care about the difference between #P and gapP?



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Math perspective: #P functions have combinatorial interpretations, while gapP functions may not.



WHAT IS A COMBINATORIAL INTERPRETATION?

IGOR PAK*

ABSTRACT. In this survey we discuss the notion of *combinatorial interpretation* in the context of Algebraic Combinatorics and related areas. We approach the subject from the Computational Complexity perspective. We review many examples, state a workable definition, discuss many open problems, and present recent results on the subject.



Computing a #P function is just as hard as computing a gapP function. Both tasks are as powerful as the polynomial hierarchy [Toda's theorem]. So why do we care about the difference between #P and gapP?

Computer Science perspective: There is a vast difference in the complexity of relative-error approximation...





Larry Stockmeyer

Michael Sipser

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Proof idea:

 $S \subseteq \{0,1\}^n$ Membership can be verified efficiently

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If $2^k < |S|$ then there is a collision.

Conversely if $2^k \gg |S|$ then there is no collision w.h.p.

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You can find a collision by asking the NP oracle.

	Function contained in	Approximation task upper bound
Classical counting	# <i>P</i>	FBPP ^{NP}
Signed counting	gapP	#P-hard

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Easy special case: If circuit implements a projective measurement. Then we can count the rank of the projector associated with "accept" outcome.

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More generally: Look at measurement operator A corresponding to accept outcome.

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Does it make sense to count the number of accepting witnesses?

More generally: Look at measurement operator *A* corresponding to accept outcome. Count the dimension of the vector space spanned by its eigenvectors with eigenvalues close to 1.

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Issue: A witness may be accepted with probability $p \in (0,1)$. How do we decide which ones to count?

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Let N_y be the number of eigenvalues of A with eigenvalue at least y.



Consider a quantum (QMA) verifier circuit



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#BQP is the class of problems of the form

Input: verifier circuit, two thresholds $0 < b < a \le 1$ **Output:** A number *M* such that $N_a \le M \le N_b$

$$p = 0 \qquad b \qquad a \qquad p = 1$$

Theorem[Brown Flammia Schuch 2010][Shi Zhang 2009] #BQP functions are polynomial-time equivalent to #P functions.

Quantum approximate counting

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QXC is the class of problems of the form **Input:** verifier circuit, $\delta \in (0,1)$, two thresholds $0 < b < a \le 1$ **Output:** A number *M* such that $(1 - \delta)N_a \le M \le N_b(1 + \delta)$

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Possibly controversial statement: QXC is the reason to care about #BQP!
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There is no known quantum version of Stockmeyer approximate counting and so complexity of QXC is poorly understood (cf. lack of quantum Valiant Vazirani theorem [Aharonov Ben-Or Brandao Sattath 2008])

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Theorem [Bravyi Chowdhury QPF is QXC-complete.	DG Wocjan 2022]	

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Theorem [Bravyi Chowdhury Do QPF is QXC-complete.	G Wocjan 2022] Marriott-Watro 2-local Circuit-te	reduce QXC to 2-local QPF): us error reduction for QMA [Marriott Watrous 2005 o-Hamiltonian mapping [Kempe Kitaev Regev 2004]	

Number of QMA witnesses ~number of low energy states

	Exact	Approximate
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imaginary temperature

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Challenging question: how does QXC relate to other known complexity classes?

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Challenging question: how does QXC relate to other known complexity classes? Easier: can we find other interesting problems in QXC?...

imaginary temperature

Kronecker coefficients = Clebsch-Gordan coefficients for the symmetric group

Recall that irreps of S_n are labeled by partitions of n or equivalently Young diagrams. For any three partitions $\mu, \nu, \lambda \vdash n$, there is a Kronecker coefficient $g_{\mu\nu\lambda}$ defined as:

$$\rho_{\mu} \otimes \rho_{\nu} \simeq \bigoplus_{\lambda} g_{\mu\nu\lambda}\rho_{\lambda}$$
Tensor product of two
irreps
$$f_{\text{Multiplicities}}$$

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Modern rephrasing: Do the Kronecker coefficients admit a #*P* formula?

e.g. [Burgisser Ikenmeyer 2008] [Pak Panova 2014] [Ikenmeyer Mulmuley Walter 2017]...

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Modern rephrasing: Do the Kronecker coefficients admit a #*P* formula?

e.g. [Burgisser Ikenmeyer 2008] They admit a gapP formula [Pak Panova 2014] [Ikenmeyer Mulmuley Walter 2017] They are #P-hard to compute

Claim [Bravyi, Anirban Chowdhury, DG, Vojtech Havlicek, Guanyu Zhu 2022]

 $d_{\mu}d_{\nu}d_{\lambda}g_{\mu\nu\lambda}$

Efficiently computable prefactor

Claim [Bravyi, Anirban Chowdhury, DG, Vojtech Havlicek, Guanyu Zhu 2022]

For any $\mu, \nu, \lambda \vdash n$, there is a quantum circuit of size poly(n) that measures a projector with rank $d_{\mu}d_{\nu}d_{\lambda}g_{\mu\nu\lambda}$

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In other words: $g_{\mu\nu\lambda}$ is proportional to a #BQP function [Christandl, Harrow, Walter] [Kuperberg, Pak, Panova]

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Corollary

The problem of approximating $g_{\mu\nu\lambda}$ to within a given relative error is in QXC.

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Proof sketch

For any representation ρ of S_n we can define a projective quantum measurement with outcomes labeled by partitions $\lambda \vdash n$:

$$\Pi_{\lambda} = \frac{d_{\lambda}}{n!} \sum_{g \in S_n} \chi_{\lambda}(g) \rho(g) \qquad \text{Projector for outcome } \lambda$$

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This projective measurement can be implemented in time poly(n) on a quantum computer using Beals' quantum Fourier transform over the symmetric group.

[Beals 1997] via generalized phase estimation [Harrow 2005]

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It is not hard to show that

$$d_{\mu}d_{\nu}d_{\lambda}g_{\mu\nu\lambda} = Tr(\Pi_{\mu}\otimes\Pi_{\nu}\otimes\Pi_{\lambda}P)$$

Defined as on previous slide with ρ = left regular representation

$$P = \frac{1}{n!} \sum_{g \in S_n} g \otimes g \otimes g$$

This projector can also be measured efficiently on a quantum computer

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The quantum circuit first measures $\Pi_{\mu} \otimes \Pi_{\nu} \otimes \Pi_{\lambda}$ and then measures *P*, and accepts iff both outcomes are +1.

Row sums of the character table

[Bravyi, Anirban Chowdhury, DG, Vojtech Havlicek, Guanyu Zhu 2022]

There is a similar story for the row sums of the character table of the symmetric group, for which a combinatorial representation is also an open question [Stanley 1999]

$$R_{\lambda} = \sum_{\mu \vdash n} \chi_{\lambda}(\mu)$$

These can also be expressed as multiplicities and can be shown to be proportional to a #BQP function, and therefore approximable in QXC.

Summary so far

The computational complexity of relative-error approximation of quantum partition functions or equivalently quantum approximate counting is a fascinating mystery.

Some mathematical quantities that are not known to admit combinatorial interpretations may in fact be quantum counting problems. In that case the related approximation tasks are no harder than approximating the partition function of 2-local Hamiltonians.

Can we find efficient algorithms for QPF in special cases?

Mean field theory via convex optimization (but worse approximation guarantee) Dense Hamiltonians, ground energy problems [Brandao Harrow 2013] Dense classical Ising partition functions [Risteski 2016] Dense quantum partition functions [Sergey Bravyi, Anirban Chowdhury, DG, Pawel Wocjan 2022]

Rigorous Monte Carlo methods

Classical ferromagnetic Ising model [Jerrum Sinclair 1993] Quantum transverse Ising ferromagnet [Bravyi 2014] Broader class of quantum ferromagnets (e.g. XY model) [Bravyi DG 2017]

High temperature expansion

General local Hamiltonians above a critical temperature [Harrow Mehraban Soleimanifar 2020]

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High temperature expansion General local Hamiltonians above a critical temperature [Harrow Mehraban Soleimanifar 2020] **Quantum Monte Carlo:** a powerful suite of probabilistic classical simulation algorithms for quantum many-body systems.

Can simulate systems orders of magnitude larger than with exact diagonalization...

What's the catch?

Quantum Monte Carlo can only be used to study stoquastic Hamiltonians

 $\langle x|H|x\rangle \in \mathbb{R}$ $\langle y|H|x\rangle \leq 0$ $x \neq y$

Stoquastic i.e., "sign-problem free"

Examples:

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Particle in a potential



$$H = \frac{p^2}{2m} + V(\vec{x})$$

Hopping and interacting bosons



 $H = -(1-s)\sum_{i} X_{i} + sV\left(\vec{Z}\right)$

 $H = -\sum_{\langle ij\rangle} (a_i^{\dagger} a_j + a_j^{\dagger} a_i) + V(\vec{n})$

How does it work?

Quantum Monte Carlo is based on a probabilistic representation of the Gibbs state

$$\rho = \frac{e^{-\beta H}}{Z(\beta)} \qquad \qquad Z(\beta) = \operatorname{Tr}(e^{-\beta H})$$

A collection of samples from a certain probability distribution associated with ρ are sufficient to evaluate expectation values of observables.

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Clever choice of probabilistic representation and sampling method is key.

Can we identify cases where Quantum Monte Carlo is provably efficient?

$$H = \sum_{1 \le i < j \le n} h(i, j)$$

Approximate	Approximate
Ground energy	Partition Function

Ferromagnetic Ising model	$h(i,j) = - \alpha_{ij} Z_iZ_j$	Trivial	In BPP [Jerrum ,Sinclair 1989]
Ferromagnetic Transverse-field Ising model	$h(i,j) = - \alpha_{ij} X_iX_j - \gamma_iZ_i - \gamma_jZ_j$	In BPP [Bravyi 2015]	In BPP [Bravyi 2015]
Ferromagnetic XY model	$h(i,j) = - \alpha_{ij} (X_iX_j + Y_iY_j)$	In BPP [Bravyi DG 2017]	In BPP [Bravyi DG 2017]

$$H = \sum_{i < j} -b_{ij} X_i X_j + c_{ij} Y_i Y_j + \sum_{i=1}^n d_i (I + Z_i)$$

Coefficients must satisfy

 $|b_{ij}|, |c_{ij}|, |d_i| \le 1$ (sets energy scale)

$$|c_{ij}| \le b_{ij}$$
 (ensures stoquasticity)

$$H = \sum_{i < j} -b_{ij} X_i X_j + c_{ij} Y_i Y_j + \sum_{i=1}^n d_i (I + Z_i)$$

$$\begin{pmatrix} 0 & 0 & 0 & -b_{ij} - c_{ij} \\ 0 & 0 & c_{ij} - b_{ij} & 0 \\ 0 & c_{ij} - b_{ij} & 0 & 0 \\ -b_{ij} - c_{ij} & 0 & 0 & 0 \end{pmatrix}$$

 $|c_{ij}| \le b_{ij}$ (ensures stoquasticity)

$$H = \sum_{i < j} -b_{ij} X_i X_j + c_{ij} Y_i Y_j + \sum_{i=1}^n d_i (I + Z_i)$$
$$p_{ij} (Y_i Y_j - X_i X_j) + q_{ij} (-Y_i Y_j - X_i X_j) \qquad p_{ij}, q_{ij} \ge 0$$

$$H = \sum_{i < j} -b_{ij} X_i X_j + c_{ij} Y_i Y_j + \sum_{i=1}^n d_i (I + Z_i)$$

Special cases:

- $d_i = 0$ $c_{ij} = 0$ Classical Ferromagnetic Ising model
 - $c_{ij} = 0$ Ferromagnetic transverse-field Ising model
- $b_{ij} = 1$ $c_{ij} = -1$ Ferromagnetic XY model
- $b_{ij} = 1$ $c_{ij} = 1$ (name?)

Efficient algorithm for the partition function

Theorem [Bravyi DG 2017]

There exists a classical randomized algorithm which, given H, β , and a precision parameter $\epsilon \in (0,1)$ outputs an estimate satisfying $Z \approx^{\epsilon} Z(\beta)$ with high probability.

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The proof is based on a reduction to counting perfect matchings...

A **perfect matching** of a graph G = (V, E) is a subset of edges $M \subseteq E$ such that every vertex is incident to exactly one edge in M



Now suppose the graph has edge weights $\{w_e\}_{e \in E}$. Each perfect matching *M* is assigned weight



Perfect matching sum:

$$PerfMatch(G) = \sum_{Perfect matchings M} \prod_{e \in M} w_e$$

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A nearly perfect matching of a graph G = (V, E) is a subset of edges $M \subseteq E$ such that every vertex is incident to exactly one edge in M, except for 2 vertices which are untouched.

Nearly perfect matching sum:



Suppose *G* is a graph with nonnegative edge weights.

	Exactly compute PerfMatch(<i>G</i>)	<pre> ϵ-approximation to PerfMatch(G) </pre>
Planar graphs:	In P Fisher, Kasteleyn, Temperley algorithm	In P
Bipartite graphs: (permanent of nonnegative matrix)	#P-hard [Valiant 1979]	In BPP [Jerrum, Sinclair, Vigoda 2004]
General graphs:	# P-hard	[Jerrum Sinclair 1989] Algorithm with runtime $poly(V , \epsilon, {}^{-1} R)$
		$R = \frac{\text{NearPerfMatch}(G)}{\text{PerfMatch}(G)}$

These partition functions reduce to perfect matchings

Theorem [Bravyi DG 2017] There is an (efficiently computable) graph *G* with positive edge weights, such that

 $Z(\beta) \approx^{\epsilon} \operatorname{PerfMatch}(G)$

and

 $\frac{\text{NearPerfMatch}(G)}{\text{PerfMatch}(G)} = O(\text{poly}(\beta, n, \epsilon^{-1}))$

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We then use [Jerrum, Sinclair 1989] which gives an efficient algorithm for approximating the perfect matching sum.

The spin model can be defined on any graph! The graph G obtained from the reduction always has the desired feature that makes [Jerrum Sinclair 1989] efficient.

Start with a Trotter-Suzuki style approximation

$$\operatorname{Tr}(e^{-\beta H}) \approx^{\epsilon} \operatorname{Tr}(G_J \dots G_2 G_1) \qquad J = \operatorname{poly}(n, \beta, \epsilon^{-1})$$

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The resulting G_i are very special gates...

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Each *G_I* is from the gate set containing 1-qubit gates

and two qubit gates
$$\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\begin{pmatrix}
t & 0 \\
0 & 1
\end{pmatrix}
t > 0$$
"Matchgates"
$$\begin{pmatrix}
1 + t^2 & 0 & 0 & t \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
t & 0 & 0 & 1
\end{pmatrix}
t > 0$$

Let Γ be a a weighted graph with special input and output edges (*k* of each, say) We say Γ implements a *k*-qubit operator *G* if

$$\langle y|G|x\rangle = \text{PerfMatch}(\Gamma_{xy})$$

 Γ_{xy} = remove input edges with $x_i = 0$ and output edges with $y_i = 0$. Require that a perfect matching includes the remaining external edges.



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Matchgates compose nicely



Implements a 2 qubit gate G





Matchgates compose nicely



Implements a 2 qubit gate G



Implements G₁₂G₂₃

Matchgates compose nicely



Implements a 2 qubit gate G



Implements Tr(G)

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Each G_J is a matchgate.

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Matchgate implementable with n input edges and n output edges

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This gives first part of theorem:

 $Z(\beta) \approx^{\epsilon} \operatorname{PerfMatch}(G)$

We need to show:

$$\frac{\text{NearPerfMatch}(G)}{\text{PerfMatch}(G)} = O(\text{poly}(\beta, n, \epsilon^{-1}))$$

Recall that a nearly perfect matching is like a perfect matching but with 2 vertices unmatched.

We need to show:

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$$\sum_{u,v\in G} \Omega_{u,v}$$
 $\Omega_{u,v} =$ sum of nearly perfect matchings with u, v unmatched.

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To complete the proof we show that

$$\frac{\Omega_{u,v}}{\operatorname{PerfMatch}(G)} \approx \frac{\operatorname{Tr}(G_J G_{J-1} \dots G_j O G_{j-1} G_{j-2} \dots G_i P G_{i-1} G_{i-2} \dots G_2 G_1)}{\operatorname{Tr}(G_J \dots G_2 G_1)} = O(1)$$

Imaginary time spin-spin correlation function

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Some mathematical quantities that are not known to admit combinatorial interpretations may in fact be quantum counting problems. In that case the related approximation tasks are no harder than approximating the partition function of 2-local Hamiltonians.

Efficient algorithms reveal exploitable structure and more should be found...