Quantum Marginal Consistency

The k-local Hamiltonian problem is QMA-complete. By the variational principle, the complexity of the problem is unchanged if we ask for a solution over the space of density matrices:

$$E_0 = \min_{\rho} \mathrm{tr}\,(H\rho)$$

By linearity, this minimum can be expressed in terms of the local reduced density matrices:

$$H = \sum_{a=1}^{m} H_a \qquad \Longrightarrow \quad E_0 = \sum_{a=1}^{m} \mathrm{tr}\,(\rho H_a) = \sum_{a=1}^{m} \mathrm{tr}\,(\rho_a H_a)$$

Where ρ_a is the RDM of the k-qubits on which H_a acts on nontrivially. How many independent parameters can there be in $\rho_1, \ldots, \rho_m$, as compared to ρ? Can we minimize over the $\rho_1, \ldots, \rho_m$?

Quantum Marginal Consistency

The problem with minimizing over the RDMs $\rho_1, \ldots, \rho_m$ is that we would also need to check that these local RDMs are consistent, that they could legitimately arise from some global state ρ.

We touched on this issue briefly in the context of monogamy of entanglement. If A shares a Bell state with B, then B cannot also share a Bell state with C,

$$\rho_{AB} = |\Phi^+\rangle\langle\Phi^+| \qquad \rho_{BC} = |\Phi^+\rangle\langle\Phi^+|$$

$$\neg\exists\rho_{ABC} : [\rho_{AB} = \mathrm{tr}_C\,(\rho_{ABC}) \wedge \rho_{BC} = \mathrm{tr}_A\,(\rho_{ABC})]$$

This example implies that not every choice for the local RDMs will be consistent with a global state.

Quantum Marginal Consistency

Given 3 qubits, A,B,C, and marginal states ρ_{AB} and ρ_{BC} , we ask when there is a ρ_{ABC} with

$$\rho_{AB} = \mathrm{tr}_C\left(\rho_{ABC}\right) \wedge \rho_{BC} = \mathrm{tr}_A\left(\rho_{ABC}\right)$$

It turns out that even for this case there is no analytic solution. But if assume symmetry between B and C,

$$\rho_{AB} = \rho_{AC}$$

Then ρ_{ABC} is called a symmetric extension of ρ_{AB} . For this special case there is an elegant solution, the two-qubit state ρ_{AB} has a symmetric extension if and only if

$$\mathrm{tr}\left(\rho_B^2\right) \geq \mathrm{tr}\left(\rho_{AB}^2\right) - 4\sqrt{\det\left(\rho_{AB}\right)}$$

Note that $\mathrm{tr}\left(\rho^2\right) \leq 1$ is sometimes called the *purity* of the state ρ since it is equal to 1 for pure states, and less than 1 for impure states.

Quantum Marginal Consistency

Active learning: assume that $\rho_{ABC} = |\psi_{ABC}\rangle\langle\psi_{ABC}|$ is a symmetric extension of ρ_{AB} which happens to be pure (a pure symmetric extension), show that

$$\mathrm{tr}\left(\rho_B^2\right) \geq \mathrm{tr}\left(\rho_{AB}^2\right) - 4\sqrt{\det\left(\rho_{AB}\right)}$$

Necessarily holds.

Quantum Marginal Consistency

Returning to the general case, we've recast the local Hamiltonian problem in terms of reduced density matrices, reducing from exp(n) to poly(n) parameters (matrix entries) used to describe the state:

$$H = \sum_{a=1}^{m} H_a \quad \Longrightarrow \quad E_0 = \sum_{a=1}^{m} \mathrm{tr}\left(\rho H_a\right) = \sum_{a=1}^{m} \mathrm{tr}\left(\rho_a H_a\right)$$

In the context of NP (or MA), Merlin could give us a classical witness that describes these RDMs $\rho_1, \ldots, \rho_m$

However we believe that $NP \neq QMA$. So the problem with such a witness must be our inability to check for consistency of the RDMs. This suggests a reduction from LH to marginal consistency.

Theorem: the marginal consistency problem is as hard as the local Hamiltonian problem. "Consistency of local density matrices is QMA-complete", Liu 2006.

Yi-Kai Liu

Quantum Marginal Consistency

Liu's theorem generalizes an analogous statement in classical complexity theory: deciding whether marginal probability distributions are consistent with some global distribution is NP-hard.

In the classical case, the reduction is based on graph coloring (3-COLORING). For each vertex u, we have a random variable that takes values in $\{r, g, b\}$. For each edge there is a marginal which is uniform over

$$\{r, g, b\}^2 / \{rr, gg, bb\}$$

And these marginals are consistent if and only if the graph is 3-colorable.

Liu's proof is based on a different kind of reduction. Rather than mapping a specific instance of consistency to a specific instance of LH, it uses the ability to repeatedly solve the consistency problem (for different inputs) to solve any local Hamiltonian problem.

In complexity theory, this ability to solve any problem in a class "on-demand" is called an *oracle*. If A, B are classes then A^B is "A with an oracle for problems in B", e.g. P^{NP}.

Quantum Marginal Consistency

Definition (CONSISTENCY):

Consider a system of n qubits. We are given a collection of local density matrices $\rho_1, \ldots, \rho_m$, where each ρ_i acts on a subset of qubits $C_i \subseteq \{1, \ldots, n\}$. Each matrix entry is specified with $\text{poly}(n)$ bits of precision. Also, $m \leq \text{poly}(n)$, and each subset C_i has size $|C_i| \leq k$, for some constant k.

In addition, we are given a real number β (specified with $\text{poly}(n)$ bits of precision) such that $\beta \geq 1/\text{poly}(n)$.

The problem is to distinguish between the following two cases:

- There exists an n-qubit state σ such that, for all i, $\|\text{tr}_{\{1,\ldots,n\}-C_i}(\sigma) - \rho_i\|_1 = 0$. In this case, output "YES."
- For all n-qubit states σ, there exists some i such that $\|\text{tr}_{\{1,\ldots,n\}-C_i}(\sigma) - \rho_i\|_1 \geq \beta$. In this case, output "NO."

Quantum Marginal Consistency

How would you show CONSISTENCY is in QMA? (assume you can trust the prover to send many copies)

Therefore showing CONSISTENCY is in QMA is the "easy direction", and the interesting direction is to show that CONSISTENCY is QMA-hard by a reduction to the local Hamiltonian problem.

Liu's proof is based on a different kind of reduction then we have seen so far.

Rather than mapping a specific instance of consistency to a specific instance of LH, it uses the ability to repeatedly solve the consistency problem (for different inputs) to solve any local Hamiltonian problem.

In complexity theory, this ability to solve any problem in a class "on-demand" is called an *oracle*. If A, B are classes then A^B is "A with an oracle for problems in B", e.g. P^{NP}.

Quantum Marginal Consistency

Liu's reduction is based on a connection between the local Hamiltonian problem, and an important field of optimization known as convex programming.

Definition (CONVEX PROGRAMMING):

Let $K \subseteq \mathbb{R}^n$ be a convex set, specified by a membership oracle O_K.
Let $f : K \to \mathbb{R}$ be a convex function, which is efficiently computable.
Find some $x \in K$ that minimizes $f(x)$.

The membership oracle O_K takes as input a point $x \in \mathbb{R}^n$ and returns 1 if x is in K, and 0 if x is not in K.

Note that while convex programming problems always have the form of optimizing a function over a convex set, there can be differences in the way the set is specified. Instead of a membership oracle, the set could (for example) be defined implicitly by equations and inequalities.

Quantum Marginal Consistency

Definition (CONVEX PROGRAMMING):

Let $K \subseteq \mathbb{R}^n$ be a convex set, specified by a membership oracle O_K.
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Find some $x \in K$ that minimizes $f(x)$.

In 2004, Bertsimas and Vempala gave a rigorous poly-time algorithm for a version of this problem. Their algorithm is based on random walks. Liu uses their result as a black box.

Theorem 1 *(Bertsimas and Vempala) Consider the convex program described above. Suppose K is contained in a ball of radius R centered at the origin. Also, suppose we are given a point y, such that the ball of radius r around y is contained in K. Then this problem can be solved in time* $\mathrm{poly}(n, L)$*, where* $L = \log(R/r)$.

Quantum Marginal Consistency

The local Hamiltonian can be cast in the form of a convex program:

Let ρ be any $2^n \times 2^n$ complex matrix.
Find some ρ that minimizes $\mathrm{tr}(H\rho)$,
such that $\rho \succeq 0$ and $\mathrm{tr}(\rho) = 1$.

This version of the problem has a solution that involves exponentially many variables (matrix entries), so we recast it in a form with polynomially many variables,

Let $\rho_1, \ldots, \rho_m$ be complex matrices, where ρ_i has size $2^{|C_i|} \times 2^{|C_i|}$.
(We interpret each ρ_i as the reduced density matrix for the subset C_i.)
Find some $\rho_1, \ldots, \rho_m$ that minimize $\mathrm{tr}(H_1\rho_1) + \cdots + \mathrm{tr}(H_m\rho_m)$,
such that each ρ_i satisfies $\rho_i \succeq 0$ and $\mathrm{tr}(\rho_i) = 1$,
and $\rho_1, \ldots, \rho_m$ are consistent.

Therefore if one has a membership oracle for the set $K = \{(\rho_1, \ldots, \rho_m) \text{ which are consistent}\}$ then its possible to apply the Bertismas and Vempala algorithm to solve the LH problem in poly-time!

Quantum Marginal Consistency

Prior to being considered by quantum information theorists, the marginal consistency problem had a long history in quantum chemistry, where it is called the N-representability problem.

In the context of electronic structure, the molecular Hamiltonian only depends on interactions involving at most two electrons at a time (2-RDMs). The question of whether these (fermionic) 2-RDMs are consistent with some global fermionic wave function is the N-representability problem.

The N-representability problem was shown to be QMA-complete in 2006 by Liu, Christandl, and Verstraete.

The main thing that needs to be done is to recast spin Hamiltonians in terms of fermions (which is the opposite direction from the Jordan Wigner transformation…). Each qubit i is a fermion with two modes a,b,

$$|z_1\rangle \otimes \cdots \otimes |z_N\rangle \mapsto (a_1^\dagger)^{1-z_1}(b_1^\dagger)^{z_1} \cdots (a_N^\dagger)^{1-z_N}(b_N^\dagger)^{z_N}|\Omega\rangle$$

$$\sigma_i^x \leftrightarrow a_i^\dagger b_i + b_i^\dagger a_i,\ \sigma_i^y \leftrightarrow i\left(b_i^\dagger a_i - a_i^\dagger b_i\right),\ \sigma_i^z \leftrightarrow \mathbb{1} - 2b_i^\dagger b_i$$

$$P_i = (2a_i^\dagger a_i - \mathbb{1})(2b_i^\dagger b_i - \mathbb{1})$$

(Additional term enforcing 1 fermion per site)