Bosonic N-representability problem is also QMA-complete

Tzu-Chieh Wei

Michele Mosca & Ashwin Nayak

Institute for Quantum Computing

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Motivations

- Fermion problems seem intractable:
  e.g. "fermion sign problem" in Quantum Monte Carlo

- Solving ground-state energy of interacting electrons (fermion) is QMA-hard

  [Schuch & Verstraete, arXiv '07]

  [Liu, Christandl & Verstraete, PRL '07]

- (fermionic) N-representability problem is QMA-complete

- Boson problems seem tractable: no "sign problem"

- Interesting phenomena and models assoc. with bosons:
  BEC, superfluidity/supersoilidity, Bose-Hubbard models, etc

- Can bosonic problems be hard?

Main results

- Solving ground-state energy of interacting bosons
  ➔ QMA-hard (actually QMA-complete)

- Bosonic *N*-representability problem is QMA-complete

Complexity class: QMA

- QMA = Quantum Merlin-Arthur
  an analog of NP in quantum setting

[Kitaev]

  - *L* ϵ QMA: ∃ quantum poly-time verifier *V* and poly *p*

- Problems easy to check YES with a quantum computer

$$\forall\ x \in L,\ \exists\ |\xi\rangle \in \boldsymbol{B}^{p(|x|)},\ \Pr[(V(|x\rangle|\xi\rangle)=1] \geq 2/3$$

- For No instance, not likely to be convinced otherwise

$$\forall\ x \notin L,\ \forall\ |\xi\rangle \in \boldsymbol{B}^{p(|x|)},\ \Pr[(V(|x\ |\xi\rangle)=1] \leq 1/3$$

[To show containment in QMA, suffice to have gap ~1/poly(N)]

Fermions vs Bosons

N-particle state: $|\psi\rangle = \sum_{n_1+..+n_m=N} c_{n_1,\ldots,n_m} (a_1^\dagger)^{n_1} \ldots (a_m^\dagger)^{n_m} |\Omega\rangle$

$$\{a_i, a_j^\dagger\} \equiv a_i\, a_j^\dagger + a_j^\dagger\, a_i = \delta_{ij}$$

$$\{a_i, a_j\} = 0$$

- No two fermions occupy same state

$$|n_i\rangle, \quad n_i = 0 \text{ or } 1$$

$$[a_i, a_j^\dagger] \equiv a_i\, a_j^\dagger - a_j^\dagger\, a_i = \delta_{ij}$$

$$[a_i, a_j] = 0$$

- Many bosons can occupy same state

$$|n_i\rangle, \quad n_i = 0, 1, 2, \ldots, N$$

➔
- Particle-hole duality for fermions ➔ used to show N-rep convex region is big enough
- No such duality for bosons ➔ need other approach to show N-rep convex region is big enough

First Result:

- Solving ground-state energy of interacting bosons is QMA-hard

QMA-hardness of interacting bosons:
reduction from Local Hamiltonian problem

- Our strategy: construct a bosonic Hamiltonian whose GS energy = answer to a hard problem

- [Oliveira & Terhal '05]:
  Solving ground-state energy of spin-1/2 *H* is QMA-hard:

$$\mathcal{H} = \sum_{\langle i,j \rangle} \sum_{\mu,\nu=0}^{3} c_{ij}^{\mu\nu} \sigma_i^{(\mu)} \otimes \sigma_j^{(\nu)} \qquad \begin{array}{l} \sigma^{(0)} = \mathbb{1},\ \sigma^{(1)} = \sigma^x, \\ \sigma^{(2)} = \sigma^y,\ \sigma^{(3)} = \sigma^z \end{array}$$

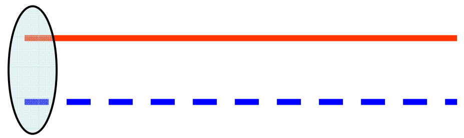
  - can also use the real Hamiltonian by [Biamonte and Love '08] see next talk

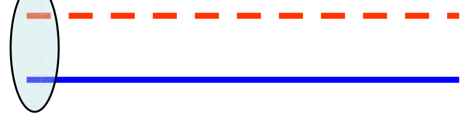
QMA-hardness--- from Local Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} \sum_{\mu,\nu=0}^{3} c_{ij}^{\mu\nu} \sigma_i^{(\mu)} \otimes \sigma_j^{(\nu)}$$

- Spin↔ Bosons mapping: use KLM linear-optics dual-rail encoding, a.k.a. Schwinger representation

$$|1\rangle_i \leftrightarrow |n_a = 1, n_b = 0\rangle_i \qquad |0\rangle_i \leftrightarrow |n_a = 0, n_b = 1\rangle_i$$





$$\sigma_i^x \leftrightarrow a_i^\dagger b_i + b_i^\dagger a_i, \;\; \sigma_i^y \leftrightarrow i(b_i^\dagger a_i - a_i^\dagger b_i), \;\; \sigma_i^z \leftrightarrow a_i^\dagger a_i - b_i^\dagger b_i$$

$$\mathcal{H} \leftrightarrow \widetilde{\mathcal{H}} = \text{quartic} + \text{quadratic terms in } a^\dagger, b^\dagger, a, b,$$

Two-body One-body

QMA-hardness--- from Local Hamiltonian

- Constrain one boson per site (total *N* bosons)
  ---penalty in Hamiltonian:

$$\mathcal{H}_B = \widetilde{\mathcal{H}} + c\sum_i (a_i^\dagger a_i + b_i^\dagger b_i - 1)^2, \quad c \sim \mathrm{poly}(N)$$

- Solve GS energy of H_B ➔ GS energy of the spin *H*
  ➔ solve QMA-hard problem

- Actually QMA-complete for *k*-body interacting Hamiltonian

Second result:

- Bosonic N-representability problem is QMA-complete

Bosonic N-representability

- Inspired by the paper : [Liu, Christandl & Verstraete, PRL '07] on fermions

- N-representability problem:

Given a two-particle density matrix $\rho^{(2)}$, determine whether there is an *N*-particle state $\sigma^{(N)}$ such that

$$\rho^{(2)} = \mathrm{Tr}_{N-2}(\sigma^{(N)})$$ (tracing out N-2 bosons)

- in terms of matrix elements of $\rho^{(2)} := \sum_{ijkl} \rho^{(2)}_{ij;kl} \, |1_i 1_j\rangle\langle 1_k 1_l|$

$$\rho^{(2)}_{ij;kl} = \frac{1}{N(N-1)} \mathrm{Tr}(a_k^\dagger a_l^\dagger a_i a_j \, \sigma^{(N)})$$

(Normalization st Tr(ρ)=1)

N-representability: examples

- 2 bosons at two sites/modes, p and q

- Example 1:

$$\rho^{(2)} = |2_p 0_q\rangle\langle 2_p 0_q| \quad \longleftarrow \quad |\psi^{(3)}\rangle = |3_p 0_q\rangle$$

✓ 3-representable

tracing out 1 particle

- Example 2:

$$\rho^{(2)} = \frac{2}{3}|1_p 1_q\rangle\langle 1_p 1_q| + \frac{1}{3}|2_p 0_q\rangle\langle 2_p 0_q| \quad \longleftarrow \quad |\psi^{(3)}\rangle = |2_p 1_q\rangle$$

- Example 3:

$$|\psi^{(2)}\rangle = \frac{1}{\sqrt{2}}(|2_p 0_q\rangle + |0_p 2_q\rangle)$$

Q: 3-representable?

Bosonic N-rep: QMA-hard

- *N*-representability algorithm enables determination of ground-state energy of (2-body) interacting bosons

$$\mathcal{H} = \sum_{ijkl} f_{ijkl}\, a_k^\dagger a_l^\dagger a_i a_j$$

Recall:

$$\rho^{(2)}_{ij;kl} = \frac{1}{N(N-1)} \mathrm{Tr}(a_k^\dagger a_l^\dagger a_i a_j\, \sigma^{(N)})$$

GS energy: $E_0^{(N)} = \min_{\sigma^{(N)}} \mathrm{Tr}\big(\sigma^{(N)}\mathcal{H}\big)$

$$= N(N-1) \min_{\rho^{(2)}} \sum_{ijkl} f_{ijkl}\, \rho^{(2)}_{ij;kl} \sim \vec{f} \cdot \vec{\rho}$$

Linear function

Convex constraint: $\rho^{(2)} = \mathrm{Tr}_{N-2}\big(\sigma^{(N)}\big)$

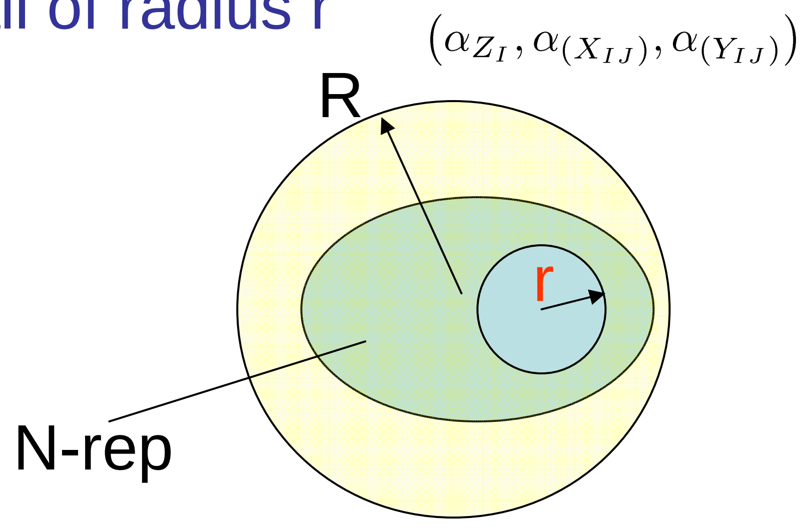
- Convex optimization: can be solved efficiently if given algorithm for *N*-representability (membership)

Convex optimization ➔ membership

- Need to make sure that

$$\rho^{(2)} = Z_L + \sum_{I \prec L} \alpha_{Z_I}(Z_I - Z_L) + \frac{1}{2}\sum_{I \prec J} \alpha_{(X_{IJ})} X_{IJ} + \alpha_{(Y_{IJ})} Y_{IJ}$$

  - Convex N-rep region is contained in a ball of radius R centered at origin
  - Convex region contains a ball of radius r
  - Require: R/r = poly(N)
    - Run time ~ poly(log(R/r)) but precision ~ 1/poly(R/r)



Convex N-rep region

- A complete set *P* of two-particle observables (P's)

$$a_I \equiv a_{i_2} a_{i_1}, \text{ for all pairs } I = (i_1, i_2),\ i_1 \leq i_2$$

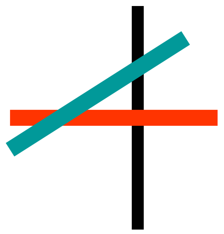
an ordering

$$P \begin{cases} X_{IJ} \equiv \dfrac{1}{(n_I n_J)^{1/2}} (a_I^\dagger a_J + a_J^\dagger a_I), & \text{for } I \prec J, \\ Y_{IJ} \equiv \dfrac{-i}{(n_I n_J)^{1/2}} (a_I^\dagger a_J - a_J^\dagger a_I), & \text{for } I \prec J, \\ Z_I \equiv \dfrac{1}{n_I} a_I^\dagger a_I, & \text{for } I \prec L, \end{cases}$$

$$n_I = 1 \text{ if } i_1 \neq i_2$$
$$n_I = 2 \text{ if } i_1 = i_2$$

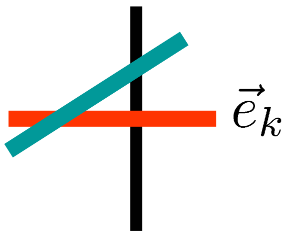
L is last pair

- N-rep region contains a ball with radius ≧ 1/poly(N)



- Via constructing N-boson states to make <*P*> as large and as small as possible
- Convex region defined by orthogonal "sticks"

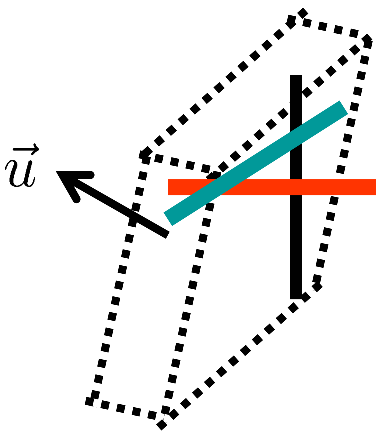
Convex N-rep region (details)



- Sufficient to show that center of mass X_{cm} has distance to every outer face $\geqq$ 1/poly(N)

$$\vec{X}_{cm} = \frac{1}{2\mathcal{N}} \sum_{k=1}^{2\mathcal{N}} \vec{X}_k$$

extremal points



- If otherwise, all extremal points lie in an exponentially small thin slab ➔ contradicting construction by “sticks”

$$\vec{u} = \sum_{k=1}^{\mathcal{N}} (\vec{u} \cdot \hat{e}_k)\hat{e}_k \longrightarrow \sum_{k=1}^{\mathcal{N}} |\hat{e}_k \cdot \hat{u}|^2 = 1$$

$$\longrightarrow \exists k \ s.t. \ |\hat{e}_k \cdot \hat{u}| \geq 1/\sqrt{\mathcal{N}}$$

Bosonic N-rep: inside QMA

- First need a mapping from bosons to spins (a la Holstein-Primakoff)

$$a_i \leftrightarrow \frac{1}{\sqrt{s+S_i^z}} S_i^+, \quad a_i^\dagger \leftrightarrow \frac{1}{\sqrt{s+S_i^z+1}} S_i^-$$

$$|n\rangle \in \{|0\rangle, |1\rangle, ..., |2s\rangle\} \leftrightarrow |s_n\rangle \in \{|s\rangle, |s-1\rangle, ..., |-s\rangle\}, \quad \text{with } 2s \geq N$$

- Answer representable or not by measuring two-spin observables on given certificate state and comparing with results from given $\rho^{(2)}$

If consistent within error ➔ output representable, otherwise ➔ not representable

Bosonic N-rep: QMA-complete

- If N-representable (YES instance), prover gives the correct N-particle state ➔ verifier always answers yes

- If not N-representable (No instance), can show that (using Markov argument) prover cannot cheat even if he hands in an entangled state (among different blocks)

  ➔ With probability ≥ 1/poly(N), verifier answers No

- Thus inside QMA (not harder than QMA)
  ➔ QMA-complete

Bosonic rep: given only diagonals?

- Full N-rep is QMA complete, but what about a simplified version? ---given only diagonal elements in $\rho^{(2)}$

$$\rho^{(2)} = Z_L + \sum_{I \prec L} \alpha_{Z_I} (Z_I - Z_L) + \underbrace{\tfrac{1}{2} \sum_{I \prec J} \alpha_{(X_{IJ})} X_{IJ} + \alpha_{(Y_{IJ})} Y_{IJ}}_{\text{We don't fix off-diagonals}}$$

- Using same argument of mapping spin-1/2 to bosons via Schwinger representation

➔ The restricted N-rep can solve the ground state energy of H_{Ising}, which is NP-hard

$$\mathcal{H}_{Ising} = \sum_{\langle i,j \rangle} c_{ij}\, \sigma_i^z \otimes \sigma_j^z$$

[Barahona '82]

Interacting Bosons: QMA-complete

- Holstein-Primakoff mapping from bosons to spins
  (plus penalty to constrain total number of bosons)

  - maps k-body interacting boson H to
    a k-local spin-(N/2) H

  - at most $O(k \log(N))$-local spin-1/2 H

  ➔ Inside QMA [Kitaev; Aharonov]

- We showed this is QMA-hard

  ➔ Thus k-body interacting bosons are QMA-complete

Summary

Main results:

- Solving ground-state energy of interacting bosons
  ➔ QMA-hard (complete for *k*-body interaction)

- Bosonic N-representability problem is QMA-complete
  ➔ as hard as fermionic problem

(Bosonic N-representability problem given only diagonal elements is NP-hard)