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Quantum Approximate Optimization

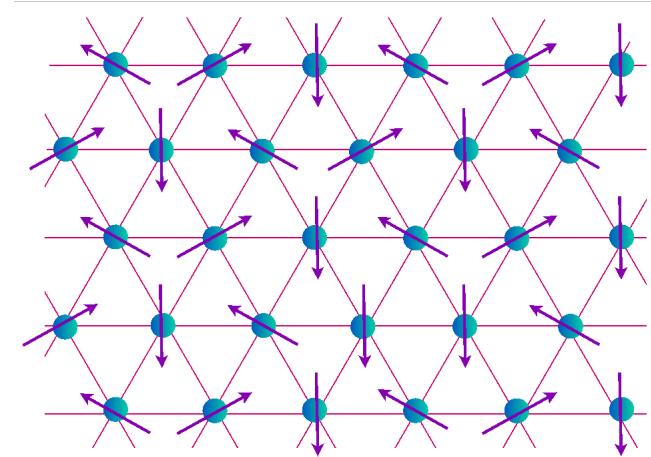
Kevin Thompson (1464)



Controlled by:

LOCAL HAMILTONIAN PROBLEM

- **Hamiltonian** – energy function for quantum system
 - Exponentially large matrix $H \in 2^{\#DoF} \times \#DoF$
 - eigenvalues \leftrightarrow energy levels,
 - Eigenvectors \leftrightarrow fixed points
- Low energy states important for understanding exotic physics, i.e. solid state physics (superconductivity, quantum sensing, etc.)
- Direct diagonalization intractable, **Hamiltonian complexity theory** implies difficulty of physically relevant models:
 - Chemistry (Electronic Structure problem)
 - Heisenberg model
 - Translation invariant Hamiltonians
 - ...

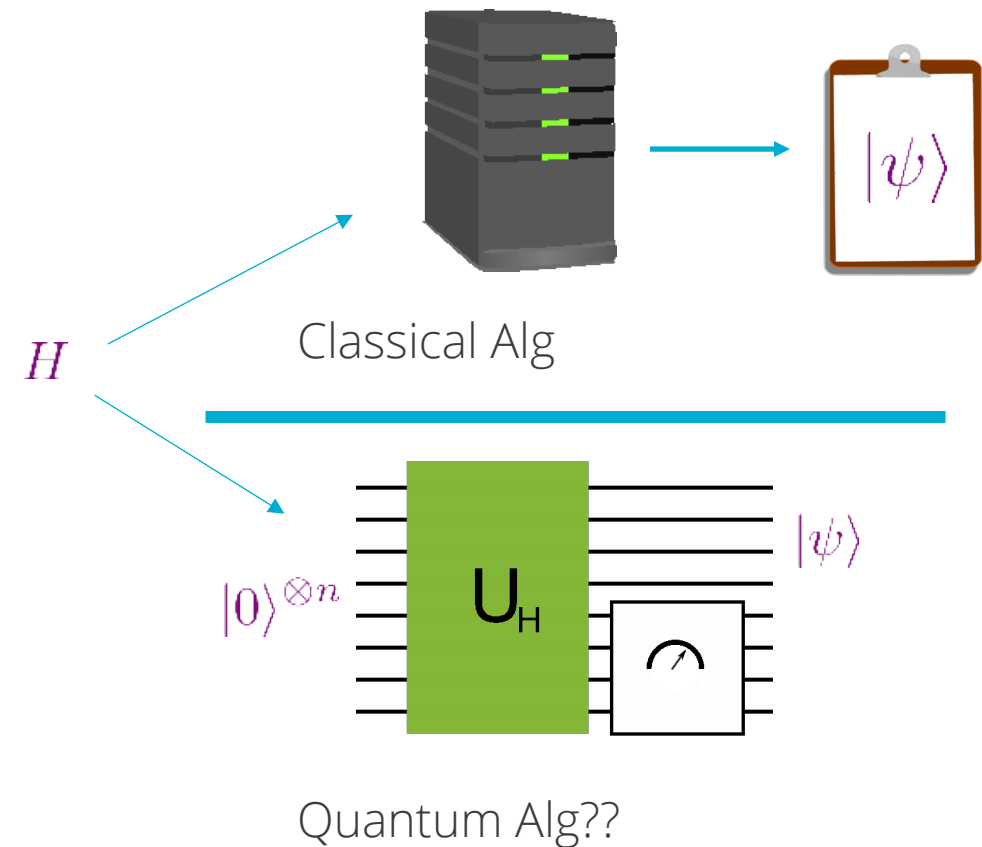


Anti-ferromagnetic Heisenberg model: roughly neighboring quantum particles aim to align in opposite directions. This kind of Hamiltonian appears, for example, as an effective Hamiltonian for so-called Mott insulators.

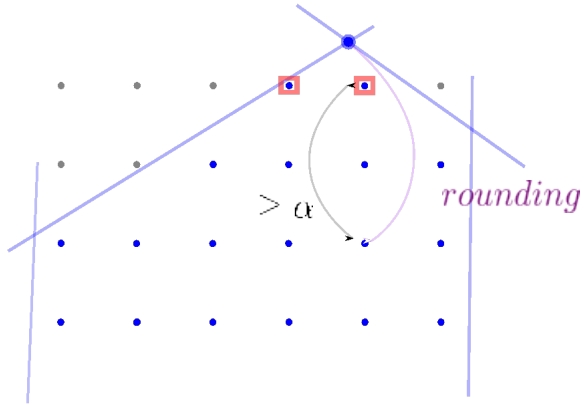
[Image: Sachdev, arXiv:1203.4565]

EIGENVALUE APPROXIMATION

- Exact solution hard, can we find approximate solution? How well “should we expect” to be able to approximate? What do we mean by approximate?
- Optimize using classical or quantum computer? Must settle for description if using classical computer
- Find $|\psi\rangle$ with good energy as well as **proof** that energy is close to optimal
 - Heuristics work well in practice, but until recently not many known rigorous bounds on performance
- How? Bridge quantum and classical techniques.



CLASSICAL TECHNIQUES



[Goemans and Williamson, 1995]

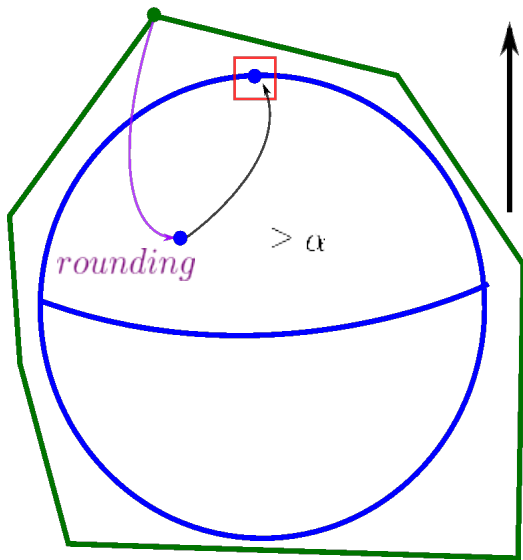
[Nesterov, 1998]

[Charikar, Wirth 2004]

[Williamson, Shmoys, 2011]

[Vazarani, 2001]

...



- Sandia pioneering use of classical techniques for quantum problems

[Bravyi, Gosset, Konig, Temme, 2018]

[Parekh, T., 2022]

[Gharibian, Parekh 2019]

[Lee, 2022]

[Hallgren, Lee, Parekh, 2020]

[King, 2022]

[Parekh, T. 2020]

[Hothem, Parekh, T. 2023]

[Parekh, T. 2021]

[Hwang, Neeman, Parekh, T., Wright, 2021]

- Developed lower and upper i.e. we can approximate the Hamiltonian this well and we should not expect to approximate the Hamiltonian better than this (up to conjectures)

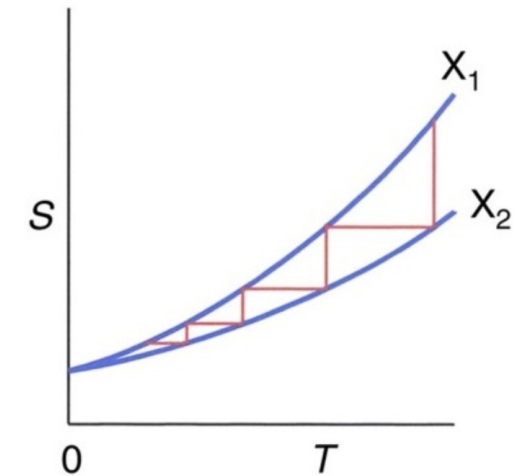
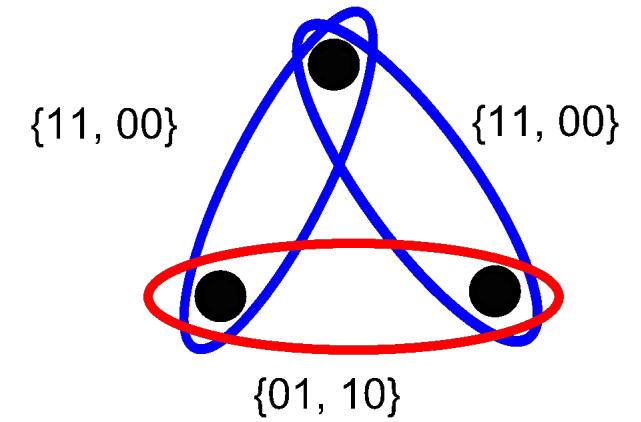
KEY DIFFERENCES BETWEEN CLASSICAL/QUANTUM

- Can't describe generic quantum state with classical resources
 - **Important design choice: ansatz** - kind of quantum state used
 - We use simple locally entangled ansatz.
 - More sophisticated ansatz known (MPS, tensor network states, etc.) but are difficult to work with
- Richness present in quantum optimization
 - “Most natural” alg. is optimal for many classical problems, not the case for quantum
 - Optimal algorithm for particular ansatz known [Parekh, T., 2022], but unknown in general
 - Optimal algorithm for simple ansatz is **not** the “most natural” one
 - **Even unclear what the optimal ansatz is/if there exists an optimal ansatz**



APPLICATIONS (REALIZED)

- Approximability is important from CS perspective: Provides provable limits on classical and quantum computers for optimizing
 - Anti-ferromagnetic Heisenberg
 - Arbitrary PSD local Hamiltonians
 - Sparse Fermionic Hamiltonians
- Limits on approximability correspond to “computational 3rd law of thermodynamics”, i.e. **for this Hamiltonian should not expect to cool to T_{min} in subexponential time under complexity theory**
- New perspectives for modelling quantum states
 - Pseudo-states – “mimicking” entanglement in classical models
 - C*/representation theoretic ways for certifying extremal energy **for some Hamiltonians**
- **Complete** understanding of approximability of anti-ferromagnetic Heisenberg model by product states, does this have implications for low temperature Gibbs states?



[Masanes, Oppenheim '14]

APPLICATIONS (POTENTIAL)

- Driving force is understanding what “kind” of states achieve low energy
- By complexity theory (and 3rd law) should not expect to find quantum states in the ground state ($T = 0$), nature “must be” approximating.
- **Study of approximate ground states is practically relevant**
- Deepening knowledge of exotic physics useful for
 - Lossless power grids (strange metals)
 - Quantum chemistry simulations
 - Quantum sensing
 - ...

MOVING FORWARD

- Current research directions centered on removing the need for an ansatz
 - Prove the **existence** of a state **with good objective** without explicitly defining it?
- Leverage known techniques for more exotic Hamiltonians, i.e. quantum Chemistry
- Prove more limitations on approximation algorithms?
 - [Hwang, Neeman, Parekh, T., Wright, 2021] likely not tight
- Exploring other physical quantities of interest with our techniques? E.g. correlation functions
- Quantum quantum approximation algorithms?
- Thank You!

