# Quantum algorithms for Nuclear Physics IV

Dean Lee Facility for Rare Isotope Beams Michigan State University

Co-ordinated Mini-Lecture Series on Quantum Computing and Quantum Information Science for Nuclear Physics

> Jefferson Laboratory March 17, 2020





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# <u>Outline</u>

Combinatorial optimization

Adiabatic theorem and adiabatic evolution

Quantum annealing

Quantum approximate optimization algorithm

Projected cooling algorithm

Transverse Ising model

Combinatorial optimization

Minimum spanning tree



# Maximum Cut



wikipedia.org

Ising spin glass





# Adiabatic theorem



# Adiabatic theorem



### Adiabatic evolution

Initial Hamiltonian  $H_I$  (simple), final Hamiltonian  $H_F$  (target)

$$H(0) = H_I, \ H(t_F) = H_F$$
$$H(t) = \frac{t_F - t}{t_F} H_I + \frac{t}{t_F} H_F$$

The unitary time evolution operator is

$$U(t + dt, t) = e^{-iH(t)dt}$$
$$|\psi(t + dt)\rangle = U(t + dt, t) |\psi(t)\rangle$$
$$|\psi(t_2)\rangle = U(t_2, t_1) |\psi(t_1)\rangle$$

Start from an eigenstate of the initial Hamiltonian

$$H_I \left| \psi_I \right\rangle = E_I \left| \psi_I \right\rangle$$

In the limit of slow time evolution we remain in an eigenstate of H(t)throughout

$$|\psi(t)\rangle = U(t,0) |\psi_I\rangle$$
  
 $H(t) |\psi(t)\rangle = E(t) |\psi(t)\rangle$ 

And so at the end of the evolution we have

$$H_F |\psi(t_F)\rangle = E_F |\psi(t_F)\rangle$$

### Quantum annealing

Quantum annealing is the application of adiabatic evolution to a combinatorial optimization problem. Consider, for example, the Ising spin glass

$$H_F = -\sum_{\langle ij\rangle} J_{ij} \sigma_i^z \sigma_j^z$$

For the initial Hamiltonian we can take the simple operator

$$H_I = -\sum_i \sigma_i^x$$

with ground state

$$|\psi_I\rangle = |\sigma^x = 1\rangle \otimes |\sigma^x = 1\rangle \otimes \cdots$$

We then apply adiabatic evolution

$$H(0) = H_I, \ H(t_F) = H_F$$
$$H(t) = \frac{t_F - t}{t_F} H_I + \frac{t}{t_F} H_F$$
$$|\psi(t)\rangle = U(t,0) |\psi_I\rangle$$

At the end of the evolution we have

$$H_F |\psi(t_F)\rangle = E_F |\psi(t_F)\rangle$$

### Trotter approximation

The Hamiltonian usually contains terms that do not commute. For the time evolution we have

$$U(t+dt,t) = e^{-iH(t)dt}$$

for

$$H(t) = \frac{t_F - t}{t_F} H_I + \frac{t}{t_F} H_F$$

We can use the Trotter approximation

$$e^{-iH(t)dt} \approx e^{-i\frac{t_F - t}{t_F}H_I dt} e^{-i\frac{t}{t_F}H_F dt}$$

And so we have

$$U(t_F,0) \approx \cdots e^{-i\frac{t_F - t_k}{t_F}H_I dt} e^{-i\frac{t_k}{t_F}H_F dt} \cdots e^{-i\frac{t_F - 0}{t_F}H_I dt} e^{-i\frac{0}{t_F}H_F dt}$$

This is very difficult to implement on current quantum devices due to the large number of gates required per qubit.

### Quantum approximate optimization algorithm

Farhi, Goldstone, Gutmann, arXiv:1411.4028 (2014) [quant-ph]

The quantum approximate optimization algorithm (QAOA) is a cheap approximation to adiabatic evolution. We make the variational ansatz

$$|\psi(\vec{\beta},\vec{\gamma})\rangle = U(\vec{\beta},\vec{\gamma}) |\psi_I\rangle$$
$$U(\vec{\beta},\vec{\gamma}) \approx e^{-i\beta_k H_I} e^{-i\gamma_k H_F} \cdots e^{-i\beta_1 H_I} e^{-i\gamma_1 H_F}$$

We then use the variational principle

$$E_F^{\text{ground}} \leq \langle \psi(\vec{\beta}, \vec{\gamma}) | H_F | \psi(\vec{\beta}, \vec{\gamma}) \rangle$$

and minimize the value of  $E(\vec{\beta}, \vec{\gamma}) = \langle \psi(\vec{\beta}, \vec{\gamma}) | H_F | \psi(\vec{\beta}, \vec{\gamma}) \rangle$ 

#### arXiv:1910.07708

#### **Projected Cooling Algorithm for Quantum Computation**

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In the current era of noisy quantum devices, there is a need for quantum algorithms that are efficient and robust against noise. Towards this end, we introduce the projected cooling algorithm for quantum computation. The projected cooling algorithm is able to construct the localized ground state of any Hamiltonian with a translationally-invariant kinetic energy. The method can be viewed as the quantum analog of evaporative cooling. We start with an initial state with support over a compact region of a large volume. We then drive the excited quantum states to disperse and measure the remaining portion of the wave function left behind. The method can be used in concert with other techniques such as variational methods and adiabatic evolution to achieve better performance than existing approaches for the same number of quantum gates per qubit. For the nontrivial examples we consider here, the improvement is substantial. The only additional resource required is performing the operations in a volume significantly larger than the size of the localized state.

### Projected cooling algorithm

Consider a Hamiltonian H with a translationally-invariant kinetic energy and a localized ground state

$$H \left| \psi_0 \right\rangle = E_0 \left| \psi_0 \right\rangle$$

We first consider the case where there is exactly one bound state. We take the system volume to be infinite (or large enough to avoid rebounding reflections from the boundary). Let P be a projection operator onto a compact region  $\rho$ . In the limit of large time t, the projected time evolution has a stable fixed point

$$Pe^{-iHt}P |\psi_I\rangle \rightarrow e^{-iE_0t}P |\psi_0\rangle \langle \psi_0|P|\psi_I\rangle$$

Overlap with  $P \ket{\psi_0}$ 



### Convergence rate



# Reflection rebound



# Limit cycle

 $PU(t)P|\psi_I\rangle \to e^{-iE_0t} \langle \psi_0|P|\psi_I\rangle P|\psi_0\rangle + \dots + e^{-iE_{n_B-1}t} \langle \psi_{n_B-1}|P|\psi_I\rangle P|\psi_{n_B-1}\rangle$ 



For the case where there are more than one bound state and want extract only the ground state, we need a time-dependent Hamiltonian. We first evolve to the ground state of another Hamiltonian that has only one bound state

$$H' \left| \psi_0' \right\rangle = E_0' \left| \psi_0' \right\rangle$$

We then use adiabatic evolution to flow to the ground state of the desired Hamiltonian H.

One-particle system on an L = 51 chain



Two-particle system on two linked L = 51 chains



# Comparison of wave functions





### **JavaFXpert** @JavaFXpert · Oct 19

Congrats to Jacob Watkins, Ilaria Siloi and @Joey\_Bonitati for winning first place in the #qcbq #QuantumComputing Bootcamp with @qiskit hackathon at @michiganstateu #IBMQ





#### arXiv:2002.06222

#### Projective cooling for the transverse Ising model

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We demonstrate the feasibility of ground state preparation for the transverse Ising model using projective cooling, and show that the algorithm can effectively construct the ground state in the disordered (paramagnetic) phase. On the other hand, significant temperature effects are encountered in the ordered (ferromagnetic) phase requiring larger lattices to accurately simulate.



Figure 1: Depiction of the regions  $R_b$  and  $R_s$  for a lattice with  $N_b = 10$  total sites and an  $N_s = 4$  sites contained within  $R_s$ . In this case  $N_1 = 4$  and  $N_2 = 7$ 



Figure 3: Energy per site of the state using projective cooling as a function of time in the ordered phase; J = 1.4,  $n_s = 6$ .



Figure 6: Re-scaled magnetic susceptibility as a function of the re-scaled nearest neighbor coupling for various ratios of  $N_s/N_b$ . Black (online) curve: is an interpolation for the exact magnetic susceptibility for 14 sites; green (online) points and blue (online) crosses: the calculated susceptibilities using projective cooling.

# Recap of lecture

Combinatorial optimization

Adiabatic theorem and adiabatic evolution

Quantum annealing

Quantum approximate optimization algorithm

Projected cooling algorithm

Transverse Ising model