Establishing Fundamental Lower Bounds for Variational Quantum Algorithms

Based on: arXiv:2303.13478

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Thank you to my collaborators

Connor Mooney

Jacob Bringewatt

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potentially repeatedly, with some easy-to-prepare ϕ_k and evolve it by some Hamiltonian $H(s)$ hoping $\psi_f(T_f) \approx \phi(t)$ where $\phi(T)$ is somehow the solution to a problem we care about.

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  potentially repeatedly, with some easy-to-prepare ϕ_k and evolve it by some Hamiltonian $H(s)$ hoping $\psi_f(T_f) \approx \phi(t)$ where $\phi(T)$ is somehow the solution to a problem we care about.
- Solutions to Schrödinger's equation can be expressed in terms of unitary transformations U such that $\psi(t) = U(t, 0)\psi(0)$

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- Few rigorous results outside the adiabatic ($T \to \infty$) regime, but various numerics results and different protocols
  - QAOA
  - Counterdiabatic driving
  - Optimal Control
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  - Many/most of these approaches have been motivated in loose analogy to adiabatic quantum computing
- Recent work on rigorous performance guarantees:
  - Guaranteed approximation ratios for certain optimization problems on bounded degree graphs via Lieb-Robinson bounds.
    [Quantum Sci. Technol. (2022) 045030]
  - Lower bounds on annealing times via quantum speed limits.
    [PRL 130, 140601]

Goals

- Establish performance guarantees for relevant problem classes
- Establish **lower bound** no-gos classes of problems
- Explain the gap between numerical experiments and relevant theory

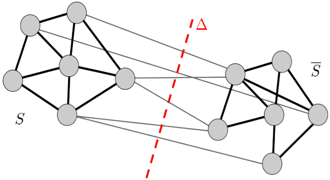
Intuition

- Hamiltonians have off-diagonal elements $|i\rangle\langle j|$ and these define a notion of computational locality.

Theorem

Consider a Hamiltonian $H + \Delta \equiv H_S \oplus H_{\overline{S}} + \Delta$ *with* $\dot{H} = \dot{\Delta} = 0$. *Then, for* $|\mu\rangle$, *an eigenstate of* H, *there exists an* $h = \Omega(\gamma)$ *such that,*

$$\left\| (e^{-i(H+\Delta)T} - e^{-i\mu T}) |\mu\rangle \right\| \leq 2\sqrt{hT}.$$

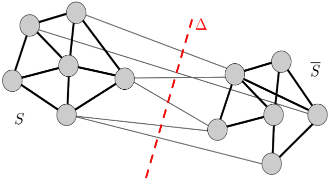


Notions from Spectral Graph Theory

- We can quantitatively understand tunneling in low energy states using the **Cheeger constant**

$$h := \frac{-\langle\lambda|\,\Delta\,|\lambda\rangle}{\min\{\langle\lambda|\,H_S\,|\lambda\rangle\,,\langle\lambda|\,H_{\overline{S}}\,|\lambda\rangle\}}$$

  - ▶ Inspired by Cheeger constant from graph theory [arXiv:1804.06857]



  - ▶ Bounds the spectral gap of H:

$$\Omega(h^p) \underset{*}{=} \Gamma \leq 2h.$$

* $p \in [1, 2]$, holds if H is stoquastic.

Partial Proof

Decompose $|\mu\rangle = \sum_i \alpha_i |\lambda_i\rangle$

$$\sum_i |\alpha_i|^2 \lambda_i = \mu. \tag{1}$$

and $\mu - \lambda_0 < 2h$.

$$\begin{aligned}
\left\| \left(e^{-i((H+\Delta)-\mu)t} - I \right) \vec{\mu} \right\|^2 &= \sum_i |\alpha_i|^2 |e^{-i(\lambda_i - \mu)t} - 1|^2 \\
&= 4 \sum_i |\alpha_i|^2 \sin^2 \left(\frac{\lambda_i - \mu}{2} \right) t \\
&\leq 2 \sum_i |\alpha_i|^2 |\lambda_i - \mu| t \leq 4ht,
\end{aligned}$$

- As minor as it is, this is already a fairly strong constraint on a number of quantum algorithms
- Still need to adapt this to time-dependent Hamiltonians

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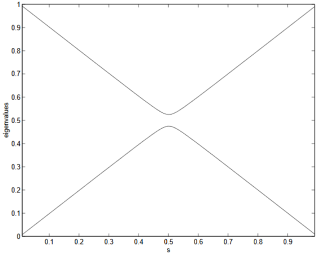

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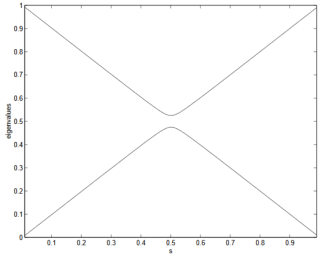

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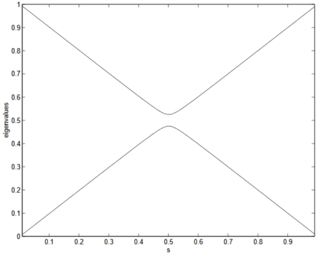

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- However, this condition is insufficient [PRL 93, 160408, PRL 95, 110407]
- How can we make this rigorous?

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- "Beweis des Adiabatensatzes"
- Showed that, if a time dependent Hamiltonian has lowest eigenvalue, eigenvector pair $\lambda(t), \phi(t)$ and $\lambda(t)$ is separated from the rest of the spectrum by a gap $\Gamma(t)$, then solutions to Schrodinger's equation $\psi(t)$ with initial condition $\psi(0) = \phi(0)$ satisfy $\langle \phi(t), \psi(t) \rangle = 1 + \mathcal{O}(T^{-1})$.

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$$i\dot{U}_{\mathrm{ad}} = TH + [\dot{P}, P]$$

where $P = |\lambda\rangle\langle\lambda|$, (the rank 1 orthogonal projector corresponding to $\phi(t) \equiv |\lambda(t)\rangle$) which has the intertwining property:

$$U_{\mathrm{ad}}(s)P(0) = P(s)U_{\mathrm{ad}}(s).$$

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- Showed that

$$\|U(s) - U_{\mathrm{ad}}(s)\| = \mathcal{O}(T^{-1})$$

  if λ is separated from rest of spectrum by a gap for all s.

The Adiabatic Theorem: History

- Jansen, Ruskai, and Seiler gave us a coefficient on the $\mathcal{O}(T^{-1})$ term.
- "Bounds for the adiabatic approximation with applications to quantum computation"
- Showed that

$$\|U(s) - U_{\mathrm{ad}}(s)\| \leq \frac{A}{T}$$

where

$$A = \frac{\|\dot{H}(0)\|}{\Gamma^2(0)} + \frac{\|\dot{H}(1)\|}{\Gamma^2(1)} + \int_0^1 \mathrm{d}s \left(\frac{\|\ddot{H}\|}{\Gamma^2} + 7\frac{\|\dot{H}\|^2}{\Gamma^3} \right),$$

where $\Gamma(s)$ is the gap separating $\lambda(s)$ from the rest of the spectrum of $H(s)$.

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  3. Local Adiabatic Evolution

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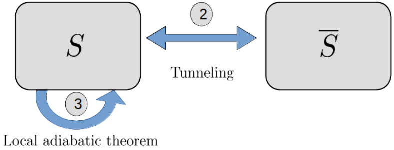


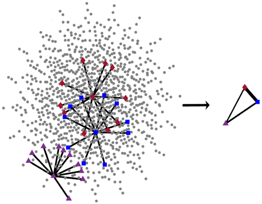
Motivation

- AQC fails for random NP-hard problems due to a similar phenomenon to Anderson Localization

[arXiv:0908.2782v2]

- Other systems have been studied that also show localization/validity of the tight binding approximation

[PRA 100, 032336]



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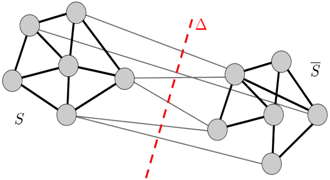
  - Inspired by Cheeger constant from graph theory [arXiv:1804.06857]



  - Bounds the spectral gap of H:

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Tight Binding

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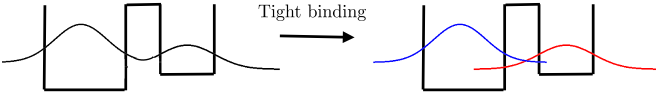

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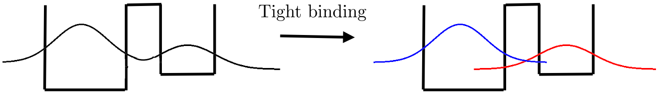

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Theorem

Let $|\lambda\rangle$ be the lowest eigenvector of H, and h, H_S be as above. Further, let $|\mu\rangle$ be the lowest eigenvector of H_S, and Γ_S H_S's gap. Then,

$$\frac{P_S\,|\lambda\rangle}{\|P_S\,|\lambda\rangle\,\|} = |\mu\rangle + \mathcal{O}\left(\sqrt{\frac{h}{\Gamma_S}}\right)$$

Tunneling

- What if our Hamiltonian is approximately block-diagonal, i.e.,

$$H = \begin{pmatrix} H_S & \Delta \\ \Delta^\dagger & H_{\overline{S}} \end{pmatrix},$$

where $\|\Delta\| \ll \|H_S \oplus H_{\overline{S}}\|$?

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- But we can't just assume $\|\Delta\|$ is small! Tight binding is valid outside of that regime!
- If $\dot{H} = 0$, we can bound tunneling by $2\sqrt{hT}$.
- **General Strategy:** Bound low-energy tunneling contributions and treat rest of tunneling (called $\Delta^\perp$) as a perturbation to local adiabatic evolution.

Local Adiabatic Evolution

- Apply the adiabatic theorem to $H_\perp := \begin{pmatrix} H_S & \Delta^\perp \\ (\Delta^\perp)^\dagger & H_{\overline{S}} \end{pmatrix}$, expand out in terms of $H_{b.d.} := \begin{pmatrix} H_S & 0 \\ 0 & H_{\overline{S}} \end{pmatrix}$.

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assuming z is in neither's spectrum.

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- We slot the perturbative expression for $R_{H_\perp}(z)$ into the adiabatic theorem and turn the crank.

Our Result

Theorem

Let $H(s) = H_S + H_{\overline{S}}$. Let $\Delta(s)$ be a block-antidiagonal perturbation, $U(s)$ the unitary generated by the Hamiltonian $H(s) + \Delta(s)$ acting for time T, and let $|\mu\rangle$ be the ground state of H_S. Then

$$\| U(1) \,|\mu(0)\rangle - |\mu(1)\rangle \| \leq \underbrace{\sqrt{hBT} + \sqrt{\epsilon_T \|H - \lambda\| \sqrt{h} T}}_{①} + \underbrace{\frac{C}{\eta T}}_{②} .$$

① Tunneling term

② Local adiabatic term

- B, C and η are independent of T, Γ.
- $\epsilon_T \in O(T^{-1}) \cap [0, 1]$.

Bounding Annealing With Our Result

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- For appropriate T, we thus have $U(1) |\phi(0)\rangle \approx c_1 |\mu(1)\rangle + c_2 |\overline{\mu}(1)\rangle$. If $c_1 |\mu(1)\rangle + c_2 |\overline{\mu}(1)\rangle$ is far from the target state, you have a lower bound by the reverse triangle inequality.

Rough Example: Grover's Algorithm

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- Tunneling error is $\sqrt{2T|\langle\psi_0|m\rangle|} = \sqrt{\frac{2T}{\sqrt{N}}}$.
- To drive $|m\rangle$ to $|\psi_0\rangle$ we need $\sqrt{\frac{2T}{\sqrt{N}}} \geq \|\,|\psi_0\rangle - |m\rangle\,\|$, or

$$T \geq \frac{\|\,|\psi_0\rangle - |m\rangle\,\|^2}{2|\langle\psi_0|m\rangle|} = \sqrt{N}\left(1 - \frac{1}{\sqrt{N}}\right) = \Omega(\sqrt{N}).$$

Further Work and Open Questions

- Can we use our theorem to get similar lower bounds for more complicated annealing routines?
  - Reverse annealing?
  - Variational Algorithms?
- How can we “clean up” our bounds?
- Could we use k-local Hamiltonians to implement complicated gates as a submatrix?

Thank you for listening! Any questions?

Proof Outline: Tunneling

- Define an auxiliary unitary $U'_\perp$ generated by $H + \Delta^\perp + (\overline{\mu} - \mu)P_{\overline{S}}$.
- Then,

$$\|(U(1) - U'_\perp(1))\,|\mu(0)\rangle\,\|^2 \leq 2|\,\langle\mu(0)|\,U^\dagger(1)U'_\perp(1)\,|\mu(0)\rangle - 1|$$
$$= T\left|\int_0^1 \mathrm{d}s\,\langle\mu(0)|\,U^\dagger(s)(\Delta - \Delta^\perp - (\mu - \overline{\mu})P_{\overline{S}})U'_\perp(s)\,|\mu(0)\rangle\right|$$

- We can then bound this via some analysis tricks.

Proof Outline: Local Adiabatic Evolution

- We can apply the adiabatic theorem onto $H + \Delta^{\perp} + (\mu - \overline{\mu})P_{\overline{S}}$ and get a bound on the deviation from local adiabatic evolution.
- Use the second resolvent identity

$$R_A(z) - R_B(z) = R_A(z)(A - B)R_B(z)$$

  to write the resolvent of $H + \Delta^{\perp} + (\mu - \overline{\mu})P_{\overline{S}}$ as a perturbation of H's.
- Run through proof of adiabatic theorem, slotting in the perturbed expression for the resolvent.

The Tunneling term

We have that B is

$$B := 2 + \mathcal{O}\left(\sqrt{\frac{\|H - \lambda\|}{\min\{\Gamma_S, \Gamma_{\overline{S}}\}}}\right)$$

The Local Adiabatic Term

Letting $\Delta^{\perp} := (I - |\mu\rangle\langle\mu| - |\overline{\mu}\rangle\langle\overline{\mu}|)\Delta(I - |\mu\rangle\langle\mu| - |\overline{\mu}\rangle\langle\overline{\mu}|)$, and $\eta := 1 - \|\Delta^{\perp}\| / \min\{\Gamma_S, \Gamma_{\overline{S}}\}$, We have that C is

$$
\begin{aligned}
C &:= D(0) + D(1) + \int_0^1 \mathrm{d}s F \\
D &:= \frac{\|\dot{H}_S\|}{\Gamma_S^2} \\
F &:= D\left(1 + \frac{1}{\eta}\mathcal{O}\left(\max\left\{\frac{\|\dot{\Delta}^{\perp}\|}{\min\{\Gamma_S, \Gamma_{\overline{S}}\}}, D, \frac{2\|\dot{H}_S\| + \|\dot{H}_{\overline{S}}\|}{\Gamma_{\overline{S}}^2}, \eta\frac{\|\dot{H}_S\|}{\Gamma_S}\right\}\right)\right) \\
&\quad + \frac{\|\ddot{H}_S\|}{\Gamma_S^2}.
\end{aligned}
$$