# Turning Quantum Hamiltonians into Images: A Framework for Noise-Resilient Representations

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# Acknowledgements


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# Outline

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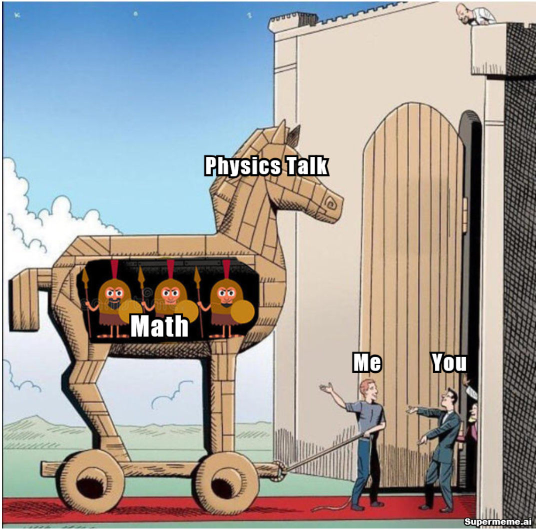

# Revisiting a few definitions

- **Hermitian Matrix:** $H = H^\dagger$
- **Unitary Matrix:** $U^\dagger U = UU^\dagger = I$
- **Orthogonal Matrix:** $O^T O = OO^T = I$

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$$A^{100} = \begin{pmatrix} 2^{100} & 0 \\ 0 & 4^{100} \end{pmatrix} \qquad B^{100} = ????$$

## A Hidden Connection

Are the matrices $A$ and $B$ in the previous slides completely unrelated?

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$$B^{100} = (S^{-1}AS)^{100} = S^{-1}A^{100}S = \begin{pmatrix} 2^{99} + 4^{99}2 & 2^{99} - 4^{99}2 \\ 2^{99} - 4^{99}2 & 2^{99} + 4^{99}2 \end{pmatrix}$$

## Similar Matrices

- $A, B \in \mathbb{C}^{n\times n}$ are similar if $\exists S \in \mathbb{C}^{n\times n}$ invertible such that $B = S^{-1}AS$
- The transformation is called a similarity transformation.
- If $A$ and $B$ are similar, they represent the same linear operator under different bases.
- Similar matrices share many properties, including eigenvalues, determinant, trace, and rank.

# Is the Diagonal Representation Always the Best?

$$H_{\text{diag}} = \begin{pmatrix} -4.488 & 0 & 0 & 0 & 0 & 0 \\ 0 & -3.225 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1.850 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1.000 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.775 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.663 \end{pmatrix}$$

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$$H = \begin{pmatrix} -2 & -1 & -0.5 & 0 & 0 & 0 \\ -1 & -2 & -1 & -0.5 & 0 & 0 \\ -0.5 & -1 & -2 & -1 & -0.5 & 0 \\ 0 & -0.5 & -1 & -2 & -1 & -0.5 \\ 0 & 0 & -0.5 & -1 & -2 & -1 \\ 0 & 0 & 0 & -0.5 & -1 & -2 \end{pmatrix}$$

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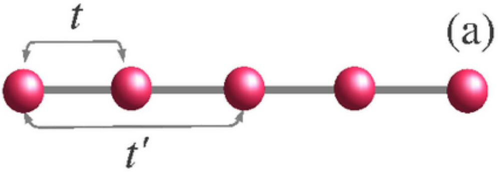

## Turning Hamiltonians into Images

- We can represent a Hamiltonian as a grayscale image where each matrix element corresponds to a pixel intensity.

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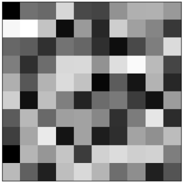

Figure 1: A random $10 \times 10$ matrix represented as a grayscale image.

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- We can represent a Hamiltonian as a grayscale image where each matrix element corresponds to a pixel intensity.

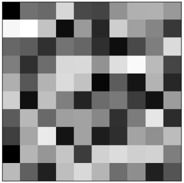


Figure 1: A random $10 \times 10$ matrix represented as a grayscale image.

- Most often, this image will lack any discernible structure and will have a lot of rough variations.

## Problem Statement

- Can we find a good orthonormal basis, equivalently a unitary transformation, such that the Hamiltonian represented in that basis yields a "smooth" image?
- Does this image have some underlying structure that can be exploited?

## Roughness of an Image

- **Roughness** of an image $H \in \mathbb{R}^{n\times n}$ is defined as:

$$\mathcal{R}(H) = \sum_{i=1}^{n-1}\sum_{j=1}^{n}(H_{i,j} - H_{i+1,j})^2 + \sum_{i=1}^{n}\sum_{j=1}^{n-1}(H_{i,j} - H_{i,j+1})^2$$
$$= ||RH||_F^2 + ||HR^T||_F^2 = 2||RH||_F^2$$

where $R \in \mathbb{R}^{n\times n}$ is the first-order forward difference matrix and $||.||_F$ is the Frobenius norm.

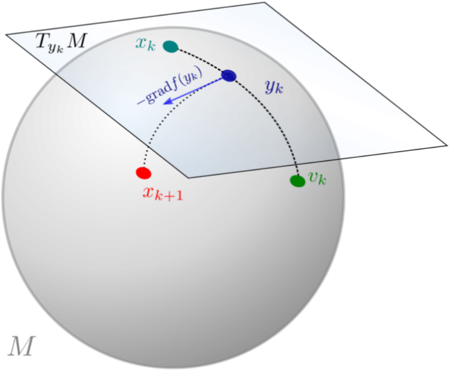
# Formal Problem Statement

## Problem

Given a Hermitian matrix (Hamiltonian) $H \in \mathbb{C}^{n\times n}$, find a unitary matrix $U \in \mathbb{C}^{n\times n}$ such that the roughness $\mathcal{R}(U^\dagger HU)$ is minimized:

$$U^* = \arg \min_{U\in\mathbb{C}^{n\times n},\, U^\dagger U=I} \mathcal{R}(U^\dagger HU)$$

# Initial Attempt: RGD



1. Introduction
2. Problem Statement
3. Exact Solution
   - Supporting Theorems
   - Exact Solution using Lagrange Multipliers
   - Examples
4. Structural Properties
5. Noisy Hamiltonians
6. Summary

# Spectral Theorem

## Theorem

Let $H \in \mathbb{C}^{n \times n}$ be a Hermitian matrix. Then there exists a unitary transformation $V \in \mathbb{C}^{n \times n}$ such that:

$$H = V \Lambda V^{\dagger}$$

where $\Lambda$ is a diagonal matrix containing the real eigenvalues of $H$ and the columns of $V$ are the orthonormal eigenvectors of $H$.

## Simultaneous Diagonalization

### Theorem

Let $A, B \in \mathbb{C}^{n\times n}$ be two Hermitian matrices that commute, i.e., $[A, B] = AB - BA = 0$. Then there exists a unitary transformation $U \in \mathbb{C}^{n\times n}$ such that both $A$ and $B$ are simultaneously diagonalized:

$$U^\dagger AU = D_A, \quad U^\dagger BU = D_B$$

where $D_A$ and $D_B$ are diagonal matrices containing the eigenvalues of $A$ and $B$, respectively.

## Exact Solution using Lagrange Multipliers

Inspired by the generalized orthogonal Procrustes solution of Schönemann (1966), we define the Lagrangian as:

$$\begin{aligned}\mathcal{L}(U,\Lambda) &= \mathcal{R}(U^\dagger H U) + \mathrm{Tr}(\Lambda(U^\dagger U - I)) \\ &= 2||RU^\dagger H U||_F^2 + \mathrm{Tr}(\Lambda(U^\dagger U - I)) \\ &= 2\mathrm{Tr}(U^\dagger A U B) + \mathrm{Tr}(\Lambda(U^\dagger U - I))\end{aligned}$$

where $A = H^2$ and $B = R^T R$.

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where $A = H^2$ and $B = R^T R$.
Imposing the stationarity condition, one obtains the equation:

$$[U^{*\dagger} AU^*, B] = 0$$

## Exact Solution using Lagrange Multipliers (Contd.)

Further analysis shows that the optimal $U^*$ can be constructed from the eigenvectors of $A$ and $B$ as:

$$U^* = E_A^\dagger E_B$$

where $E_A$ and $E_B$ are the unitary matrices constructed out of the eigenvectors of $A$ and $B$, respectively. The optimal ordering pairs the smallest eigenvalues of $A$ with the largest of $B$, minimizing the sum of their products.

# Example 1: Quantum Harmonic Oscillator

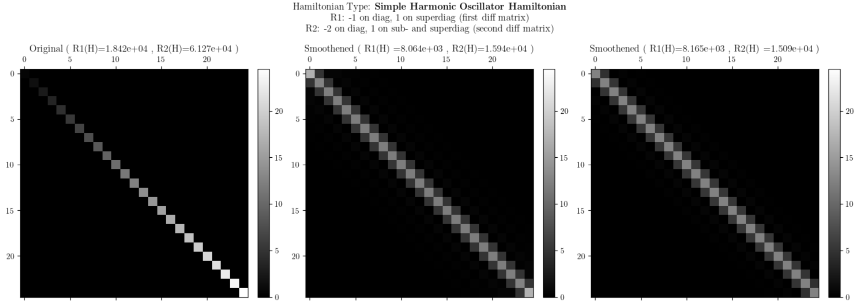


Figure 2: Smooth Image Representation of the Hamiltonian of a Quantum Harmonic Oscillator.

# Example 2: Tight Binding Hamiltonian (Open Boundary Conditions)

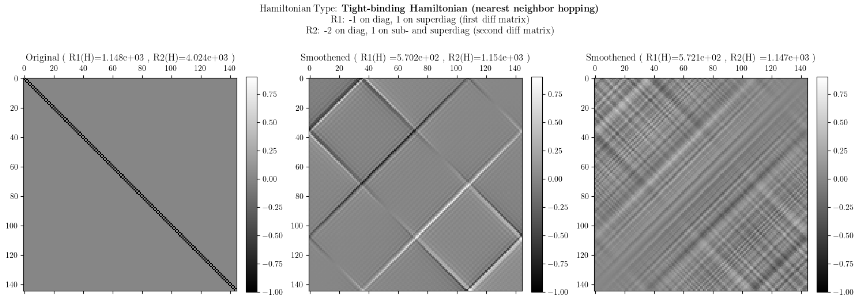


Figure 3: Smooth Image Representation of a 1D Tight-Binding Hamiltonian with Nearest-Neighbor Hopping and Open Boundary Conditions.

# Example3: Tight Binding Hamiltonian (Periodic Boundary Conditions)

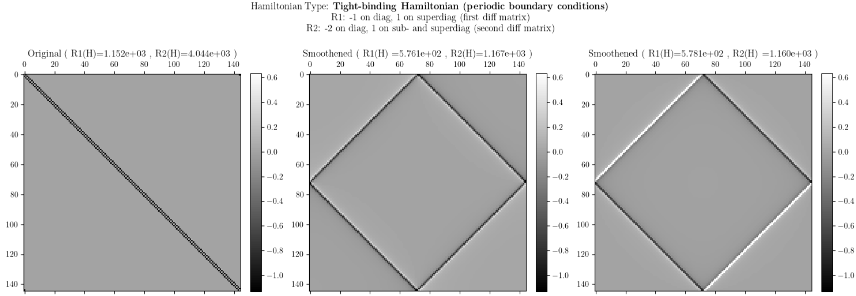


Figure 4: Smooth Image Representation of a 1D Tight-Binding Hamiltonian with Nearest-Neighbor Hopping and Periodic Boundary Conditions.

# Digression: JPEG Compression


Figure 5: JPEG Compression Example.

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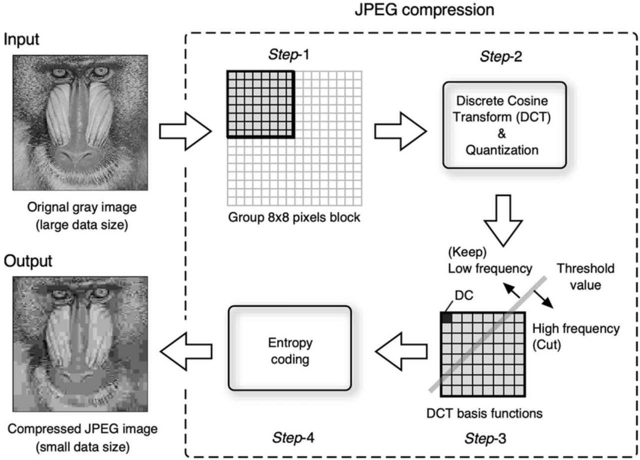


Figure 6: JPEG Compression Process.

## Discrete Cosine Transform

- $B = R^T R =$ Discrete Laplacian with Neumann Boundary Conditions.
- $B$ is diagonalized by the 2D Discrete Cosine Transform (DCT) matrix.
- Therefore, the smooth image of the Hamiltonian is the inverse DCT of the diagonal representation with absolute values of the eigenvalues sorted in descending order.

## Symmetries of the Smooth Image

- Main Diagonal Symmetry
- Anti-Diagonal Symmetry
- Centro-Symmetry
- Toeplitz-Hankel Decomposition

# Reduced Smooth Representations

$$\begin{pmatrix} \lambda_1 & \lambda_2 & \lambda_4 & \cdots & 0 & 0 \\ \lambda_3 & \lambda_5 & \cdots & \cdots & 0 & 0 \\ \lambda_6 & \cdots & \cdots & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \cdots & 0 & 0 \end{pmatrix}_{m\times m} \xrightarrow{\text{Inverse DCT}} \text{Reduced Smooth Image}$$

where $m \geq \lfloor\sqrt{n}\rfloor$ and $|\lambda_1| \geq |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_n|$.

# Reduced Smooth Representations(Contd.)

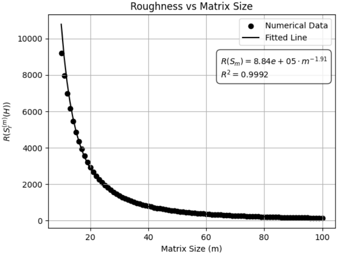


Figure 7: Variation of Roughness as a function of $m$ for a random Hamiltonian of size $n = 100$.

# Reduced Smooth Representations: Examples

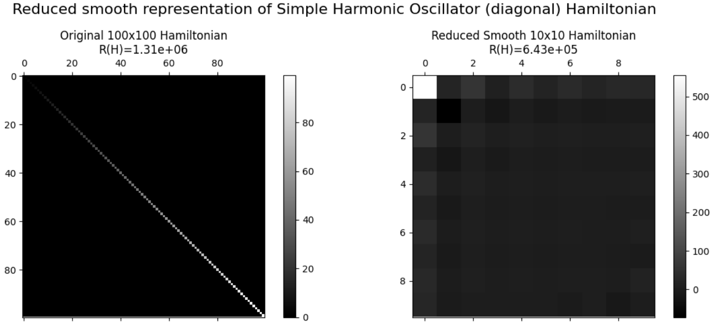


Figure 8: Reduced Smooth Image Representation of the Hamiltonian of a Quantum Harmonic Oscillator.

# Reduced Smooth Representations: Examples

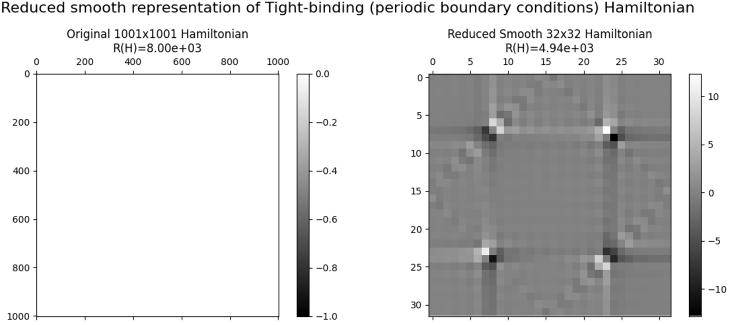


Figure 9: Reduced Smooth Image Representation of a 1D Tight-Binding Hamiltonian with Nearest-Neighbor Hopping and Periodic Boundary Conditions.

## Noisy Images

**How do you remove noise from an image?**

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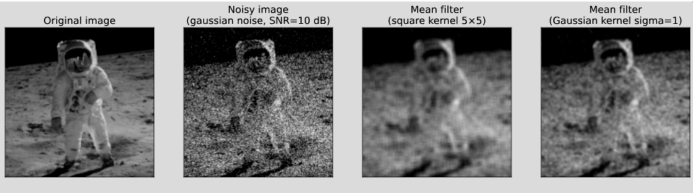


Figure 10: Blurring technique to remove noise from an image.

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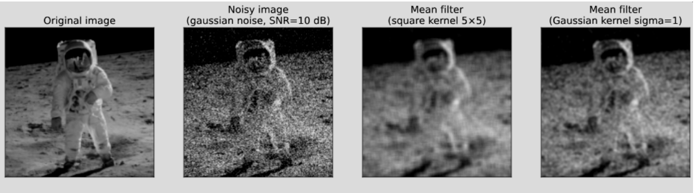


Figure 10: Blurring technique to remove noise from an image.

**Can we apply a similar technique to Hamiltonians?**

## Definition

Blurred version of a matrix $A \in \mathbb{R}^{n\times n}$ of order $m$ :

$$(A_b^{(m)})_{i,j} = \frac{1}{4m+1}\left(A_{i,j} + \sum_{k=1}^{m}(A_{i-k,j} + A_{i+k,j} + A_{i,j-k} + A_{i,j+k})\right)$$

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**But how badly does the blurring affect the Hamiltonian's properties, in particular, its spectrum?**

## Transformation of Eigenvectors

### Theorem 1

Let $H$ be a $n \times n$ Hamiltonian and $S(H)$ be its smoothest representation. Then the eigenvectors of $S(H)$ remain unchanged under blurring of any order $m$.

## Transformation of Spectrum

### Theorem 2

Let $H$ be a $n \times n$ Hamiltonian and $S(H)$ be its smoothest representation. Then the eigenvalues of $S(H)$ change under blurring of order $m$ as follows:

$$\tilde{\lambda}_k = \frac{1}{4m+1}\left(2sin\left(\frac{k\pi}{2n}(2m+1)\right)csc\left(\frac{k\pi}{2n}\right) - 1\right)\lambda_k \tag{1}$$

where $\tilde{\lambda}_k$ are the eigenvalues of the blurred matrix $S_b^{(m)}(H)$.

# Large $n$ limit

## Corollary

Let $H$ be a $n \times n$ Hamiltonian and $S(H)$ be its smoothest representation. Then for any $k \in \mathbb{N}$, the $k^{th}$ eigenvalue and eigenvector of $S(H)$ remain unchanged under blurring of any order $m$ as $n \to \infty$.

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- **Remark:** If we let $k$ increase with $n$, such that $lim_{n\to\infty}\frac{k}{n} = t$ where $t$ is a finite constant, then the eigenvalues of the blurred matrix $S_b^{(m)}(H)$ converge to:

$$\lim_{n\to\infty} \tilde{\lambda}_k = \frac{2\frac{\sin\left(\frac{\pi}{2}(2m+1)t\right)}{\sin\left(\frac{\pi}{2}t\right)} - 1}{4m+1}\lambda_k \tag{2}$$

## Summary

- We proposed a mathematical framework to map Hamiltonians to smooth images using unitary transformations.
- This notion of image agrees with the understanding of a "natural image" in image processing.
- The image representation has several interesting structural properties and symmetries.
- The eigensystem of the Hamiltonian remains robust under blurring of the image.

# Future Directions

- Developing a denoising algorithm for Hamiltonians based on image processing techniques.
- Extending discrete images on a grid to continuous images using Chebyshev polynomials.
- Deducing physical properties of the quantum system directly from the image representation.

[1] N. Boumal, *An introduction to optimization on smooth manifolds*.
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[4] P. H. Schönemann, "A generalized solution of the orthogonal procrustes problem," *Psychometrika*, vol. 31, no. 1, pp. 1–10, 1966.

*Thanks For Your Attention!*

Any questions?