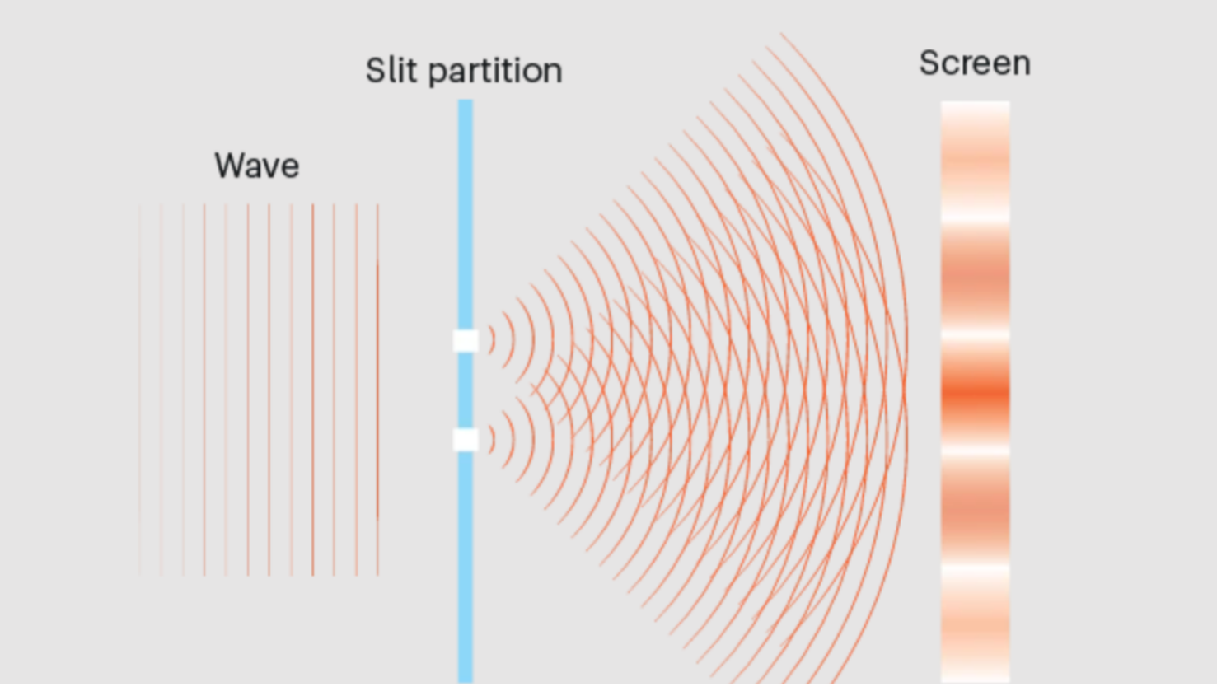
Out of Potential, Into Possibility: Algebraic Reduction of Quantum Hamiltonians

Samuel Liu

Advisor: Dr. Elodie Pozzi
Department of Mathematics, Saint Louis University

From Observation to Abstraction



When electrons are sent toward a barrier with two slits, the resulting pattern on the screen suggests an interference effect—not from the electrons behaving as classical waves, but from the probabilistic nature encoded in their quantum description. **This experiment illustrates a core principle of quantum mechanics: particles are governed not by definite trajectories, but by probability amplitudes defined by the wavefunction $\psi(x)$.**

Wavefunction: The Core Descriptor

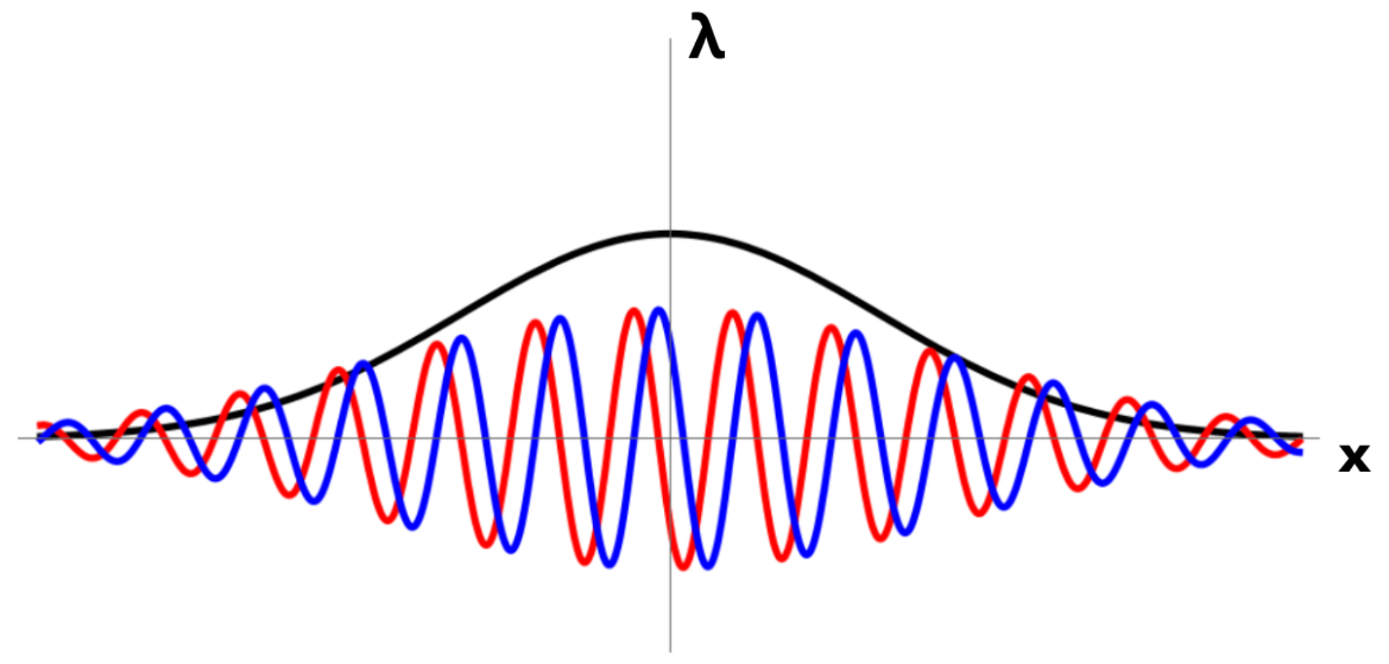


Figure 1. Visual representation of a wavefunction showing its real component (red), imaginary component (blue), and the probability density function (black).

A wavefunction $\psi(x)$ is a mathematical representation of a particle, holding all the information about a quantum system.

Mathematical Properties:

A wavefunction is a complex-valued function:

$$\psi(x) = \text{Re}(\psi(x)) + i\ \text{Im}(\psi(x))$$

whose squared magnitude $|\psi(x)|^2$ gives the probability density of finding the particle at position x . For normalization:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1.$$

This probabilistic framework underpins all quantum models.

Time-Dependent Schrödinger Equation (TDSE)

The Schrödinger equation governs how the wavefunction evolves in time. The TDSE represents a fundamental eigenvalue problem:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x)$$

where: $\psi(x)$ is an eigenfunction and $\hat{H}$ is the Hamiltonian operator.

Example: The Centrifugal Potential

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{x^2}\right]\psi(x,t)$$

Green's Function Method and Motivation

The Green's function $G(x,x';t)$ is a powerful tool for solving the time-dependent Schrödinger equation:

$$\psi(x,t) = \int_{-\infty}^{\infty} G(x,x';t)\,\psi(x',0)\,dx'$$

It evolves the wavefunction in time via the equation:

$$i\hbar\frac{\partial}{\partial t}G(x,x';t) = \hat{H}G(x,x';t), \quad G(x,x';0) = \delta(x-x')$$

Alternatively, $G(x,x';t)$ can be expressed in terms of eigenfunctions and eigenvalues:

$$\begin{aligned} G(x,x';t) &= \sum_n \phi_n(x)\,\phi_n^*(x')\,e^{-iE_nt/\hbar} \\ &= \langle x|e^{-i\hat{H}t/\hbar}|x'\rangle \end{aligned}$$

However, this form depends critically on knowing exact eigenfunctions $\phi_n(x)$ and eigenvalues E_n.

The Challenge

For $V(x) = \frac{1}{x^2}$: Even though the formalism is elegant, computing $G(x,x';t)$ becomes intractable when eigenfunctions are difficult or impossible to obtain.

$\Rightarrow$ **What if we could eliminate the potential instead?**

Rather than solving the Schrödinger equation directly, we ask: Can we transform the Hamiltonian in a way that removes the potential term, making it easier to track eigenfunctions and construct Green's functions analytically?

What if We Transform Instead of Solve?

$$\hat{H} = \frac{p^2}{2} + V(x) \to P, \quad \text{where P is a simplified, solvable operator}$$

By reducing the Hamiltonian to an elementary operator without a potential, we shift the problem from solving to transforming—then build the Green's function from the simplified form.

Research Question

Can these transformations be generalized?

Furthermore, can they be extended into a unified, systematic framework for solving a wider range of quantum systems?

Introducing Elementary Transformations

In 2006, Tsaur and Wang proposed a set of transformations—called *elementary transformations*—that serve as algebraic manipulations on the Hamiltonian while preserving the fundamental operator structure of quantum mechanics.

- **Interchange Transformation** $(\mathcal{I})$: Swaps position (x) and momentum (p), useful in problems with symmetric roles.
- **Similarity Transformation** $(\mathcal{S})$: Applies a unitary operator U to change the basis, resulting in $\hat{H}' = U^\dagger\hat{H}U$.
- **Point Canonical Transformation** $(\mathcal{P})$: Rewrites variables $x \to f(x)$ to simplify the potential function $V(x)$.
- **x-Linear Transformation** $(\mathcal{L}_x)$: Adjusts the position operator algebraically via linear combinations of x and p.

These transformations are not just formal tricks, they allow us to analytically reduce unsolvable Hamiltonians while maintaining key physical relationships like commutation relations.

Elementary Transformations in Action

To reduce complex quantum systems into elementary ones, we apply a structured sequence of algebraic transformations that preserve the Hamiltonian's operator structure while eliminating the potential term.

Step 1: Point Transformation $\mathcal{P}$

Change of variables: $(p,x) = \left(2\sqrt{x_1}\,p_1, \sqrt{x_1}\right)$

$$\begin{aligned} H &= \frac{p^2}{2} + \frac{1}{x^2} \\ &= 2\left(\sqrt{x_1}\,p_1\right)^2 + \frac{1}{x_1} = H_1 \end{aligned}$$

Step 2: Similarity Transformation $\mathcal{S}$

Change of variables: $(p_1,x_1) = \left(p_2 + \frac{i\beta}{x_2}, x_2\right)$, where $\beta = \frac{-1\pm\sqrt{1+8}}{4}$

- Use identity: $[p_2, \frac{1}{x_2}] = \dfrac{i}{x_2^2}$

$$H_1 \to 2(\sqrt{x_2}\,p_2)^2 + 4i\,\beta\,p_2 - \left(\frac{2\beta^2+\beta}{x_2}\right) = H_2$$

Step 3: x-Linear Transformation $\mathcal{L}_x$

Key identity: $[p_2, \sqrt{x_2}] = \frac{-i}{2\sqrt{x_2}}$

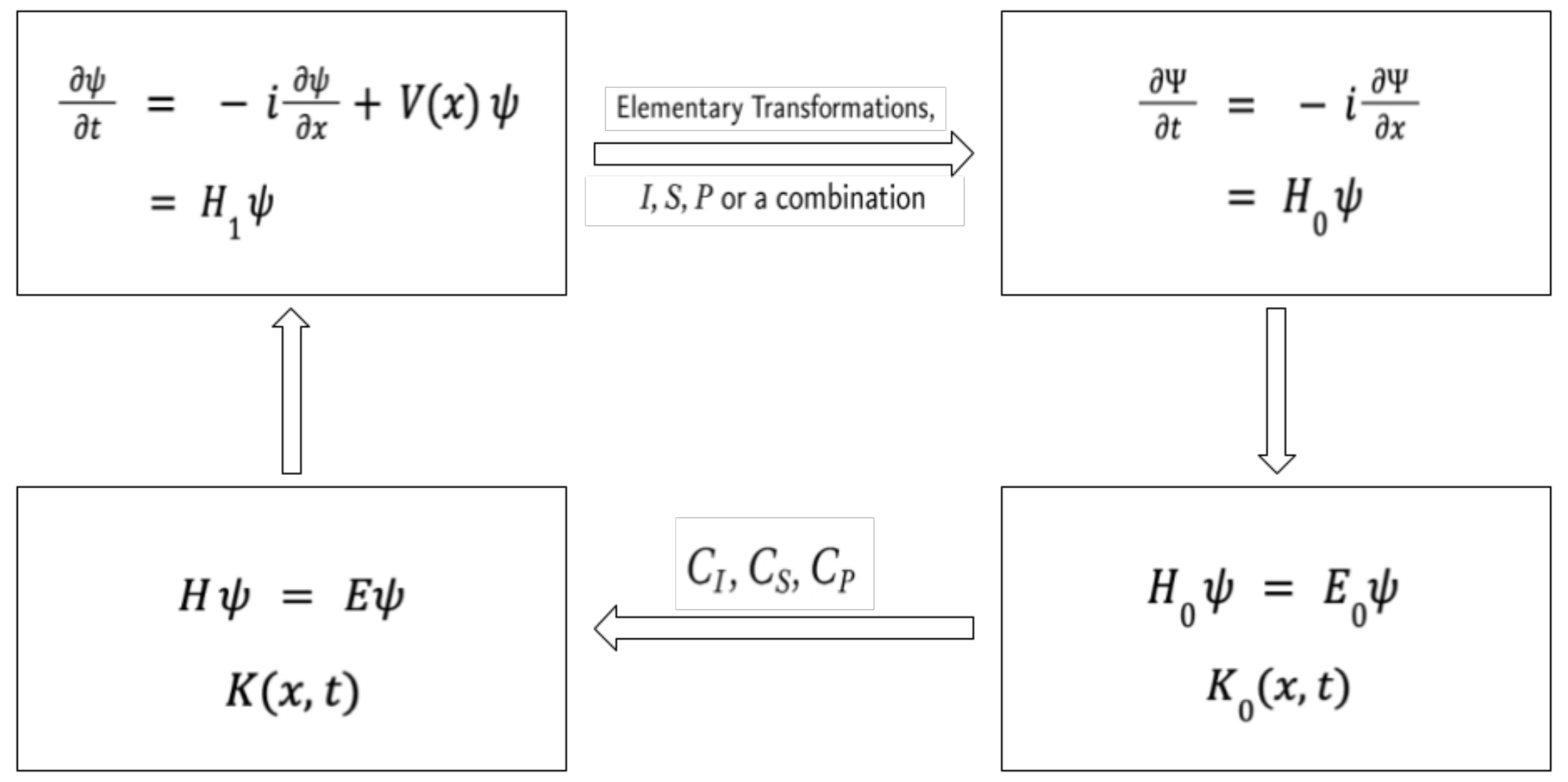
$$\begin{aligned} \left(\sqrt{x_2}\,p_2\right)^2 &= \sqrt{x_2}\left(\sqrt{x_2}\,p_2 + [p_2,\sqrt{x_2}]\right)p_2 \\ &= p_2^2\,x_2 + \frac{3\,i\,p_2}{2} \\ \Rightarrow H_3 &= 2\,p_2^2\,x_2 + i\,(4\beta+3)\,p_2 \end{aligned}$$

Final Simplified Hamiltonian

$$H_3 = 2L_z + i\gamma p_2, \quad \text{where } L_z = p_2^2x_2, \quad \gamma = 4\beta + 3$$

This transformed Hamiltonian is now elementary and solvable, enabling construction of the Green's function from a simplified form.

An 'Elementary' Framework



The Commutator and Canonical Structure Verification

The commutator $[\hat{p},\hat{x}] = -i\hbar$ is a foundational concept in quantum mechanics. Transformations such as $\mathcal{P}$ and $\mathcal{S}$ preserve this structure:

Lemma: Let $(P,X) = \mathcal{T}(p,x)$ where $\mathcal{T} \in \{\mathcal{S},\mathcal{P}\}$. Then:

$$[P,X] = [p,x]$$

This ensures the uncertainty principle and quantum behavior are preserved throughout transformations.

Supporting identities:

- $[p_2, x_2] = -i$ — canonical form preserved
- $\left[p_2, \frac{1}{x_2}\right] = \frac{i}{x_2^2}$ — used in $\mathcal{S}$
- $\left[p_2, \sqrt{x_2}\right] = \frac{-i}{2\sqrt{x_2}}$ — used in $\mathcal{L}_x$

Future Direction

We are expanding this method to handle more complex systems:

- Anharmonic Oscillators: $V(x) = ax^2 + bx^4 + cx^6$
- Morse Potential: $V(x) = D_e(1 - e^{-a(x-x_e)})^2$
- Double-Well: $V(x) = a(x^2 - b^2)^2$

Our goal is to construct exact Green's functions even when the potential is nonlinear or nontrivial.

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