The story so far:

- Intro to Python: Lectures, tutorials and problem set
- Project 1: Solving ODE's and applications in Classical Mechanics : Harmonic oscillator and Kepler's laws
- Project 2: Diagonalization of Matrices and applications in Quantum Mechanics: Anharmonic oscillator

Quantum Mechanics: a brief review

- A primary question in mechanics is: "How do objects move under the influence of forces acting on them?"
- In classical mechanics, one way to formulate this is: Given an initial configuration and a Hamiltonian, what is the time evolution, i.e., the configuration at any further time?"
- When we study quantum mechanics, this question has to be posed differently. We could ask, given an initial state at $t = 0$, (with all that that implies), what is the state at some future instant, t?

Quantum Mechanics: a brief review

- The answer is provided by Schrodinger's Equation:
- $i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$.

Asides:

- What does a state mean?
- Why don't we encounter the effects of Quantum Mechanics in our day to day life?

Stationary States:

- These states that have a special significance: Probability distribution stays constant unless there is a transition caused by an external perturbation
- The eigenstates of the Hamiltonian are the stationary states.
- A significant skill in being a quantum mechanic therefore is being able to diagonalize Hamiltonians.

Many can be diagonalized analytically. Examples:

- H atom
- Quantum Harmonic Oscillator

Quantum Harmonic Oscillator

- Ubiquitous: Why?
- A theorists delight: amenable to a particularly elegant theoretical treatment
- Historically important: B
- Many interesting features:
  - Eigenstates are coherent states
  - Model quite well the motion of atoms that leads to the transmission of sound waves in solids (what are they called?)
  - The theory of the quantum Harmonic Oscillator is quite similar to the quantum field theory of bosons

Ok, then, lets get on with it!

- Write down the Hamiltonian:
  -
    $$H_0 = \frac{1}{2m}p^2 + V(x) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2$$
- where ω is a constant that measures the strength of the potential. For the remainder of this treatment, we work in units where $m = 1$ and $\omega = 1$. This means that the Hamiltonian can be written as

$$H_0 = \frac{1}{2}(p^2 + x^2)$$

`- Solve it!`

Quantum Harmonic Oscillator

- Can work in "theorist units", where $\hbar = 1$.
- $$\hat{H}_0 = \frac{1}{2}(\hat{p}^2 + \hat{x}^2), \qquad [\hat{x}, \hat{p}] = i$$

How do we solve the Quantum Harmonic Oscillator?

- We start by defining two operators:
-

$$\hat{a}_+ = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{p}) \tag{1}$$
$$\hat{a}_- = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}) \tag{2}$$

Solving the QHO

- Then there is a basis of vectors for the Hilbert space of the system commonly denoted $|n\rangle$ with $n = 0, 1, 2, \ldots$ such that

$$\hat{a}_{+}|n\rangle = \sqrt{n+1}|n+1\rangle \tag{3}$$
$$\hat{a}_{-}|n\rangle = \sqrt{n}|n-1\rangle \tag{4}$$

- The Hamiltonian can be written as follows using these operators:

$$\hat{H}_0 = \hat{a}_{+}\hat{a}_{-} + \frac{1}{2}\hat{I}$$

Solving the QHO contd

– Now one simply notices that

$$\hat{H}_0|n\rangle = (\hat{a}_+\hat{a}_- + \frac{1}{2}\hat{I})|n\rangle \tag{5}$$

$$= \hat{a}_+\sqrt{n}|n-1\rangle + \frac{1}{2}|n\rangle = \sqrt{n}\sqrt{n}|n\rangle + \frac{1}{2}|n\rangle \quad = (n + \frac{1}{2})|n\rangle. \tag{6}$$

In other words, the set $B = \{|0\rangle, |1\rangle, \dots\}$ is a basis for the Hilbert space consisting of eigenvectors of $\hat{H}_0$

Solving the QHO contd

– Matrix representations of $\hat{a}_+$, $\hat{a}_-$, and $\hat{H}_0$ in the basis B:

We compute

$$\langle m|\hat{a}_+|n\rangle = \langle m|\sqrt{n+1}|n+1\rangle = \sqrt{n+1}\delta_{m,n+1} \tag{7}$$
$$\langle m|\hat{a}_-|n\rangle = \langle m|\sqrt{n}|n-1\rangle = \sqrt{n}\delta_{m,n-1} \tag{8}$$

In matrix form, this looks as follows:

$$[\hat{a}_+]_B = \begin{pmatrix} 0 & & & \\ \sqrt{1} & 0 & & \\ & \sqrt{2} & 0 & \\ & & \ddots & \ddots \end{pmatrix}$$

Solving the QHO contd

$$[\hat{a}_-]_B = \begin{pmatrix} 0 & \sqrt{1} & & \\ & 0 & \sqrt{2} & \\ & & 0 & \ddots \\ & & & \ddots \end{pmatrix}$$

and of course

$$[\hat{H}_0]_B = \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & \ddots \end{pmatrix}$$

QHO Wavefunctions

The function that corresponds to $|n\rangle$ is the function ψ_n defined by

$$\psi_n(x) = (2^n n! \sqrt{\pi})^{-1/2} e^{-x^2/2} H_n(x)$$

where H_n is the **Hermite polynomial** of order n which can be computed in a number of ways, one of which is the following recursion relations:

$$H_0(x) = 1 \tag{9}$$
$$H_1(x) = 2x \tag{10}$$
$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{11}$$

The Anharmonic Oscillator

– We can perturb the Harmonic oscillator and obtain the following hamiltonian (really a family of hamiltonians) depending on a parameter λ:

$$\hat{H}(\lambda) = \hat{H} + \lambda \hat{x}^4$$

– Notice that if a classical particle were moving in the now quartic potential, it would not feel much of a difference if it were near $x = 0$ since the potential looks close to quadratic there. In other words, if a classical particle has low energy, the classical motion will pretty much look harmonic.

The Anharmonic Oscillator

- But if it has high energy, then it's motion will go to large values of x, and it will "feel" the anharmonicness more. Moreover, notice that the extent to which this is true depends on the size of λ. Smaller λ means less of a deviation from harmonic.
- From this classical intuition, we might speculate that the eigenvalues and eigenvectors for the anharmonic oscillator hamiltonian are close to those of the harmonic oscillator hamiltonian for small energy eigenvalues and small λ, but we can't be sure until we do the diagonilization and compute them!

Solving the Anharmonic Oscillator

- How do we find the eigenvalues and eigenvectors of the anharmonic hamiltonian?
  - No exact methods, as far as I am aware
  - Perturbation theory
  - Numerics
- If someone gave you a linear operator to compute eigenvalues and eigenvectors for, how might you try to do this in practice?
  - We can do this by determining a matrix representation of the Hamiltonian and then using built-in Python eigensolvers to compute its eigenvectors and eigenvalues.

Solving the anharmonic Oscillator

- Notice however that there is a bit of a problem here: the harmonic oscillator vector space is infinite-dimensional, so the hamiltonian cannot be written as some $N \times N$ matrix that we can feed into the Python interpreter.
- The best we can do is to approximate the problem as a finite-dimensional problem, and natural way to do this is to find the matrix representation of the hamiltonian only using, say, the vectors $B_N = \{|0\rangle, |1\rangle, \ldots, |N\rangle\}$ spanning a finite-dimensional subspace of the whole vector space and diagonalize the finite matrix. We expect that as $N \to \infty$, the eigenvalues and eigenvectors we obtain will converge to the exact result.

Solving the anharmonic Oscillator

– In mathematical terms, let $|n, \lambda\rangle$ and $E_n(\lambda)$ denote the eigenvectors and corresponding eigenvalues of the anharmonic oscillator hamiltonian, and let $|n, \lambda, N\rangle$ and $E_n(\lambda, N)$ denote the eigenvectors and eigenvalues of the Hamiltonian restricted to only the subspace spanned by B_N, then we expect that as $N \to \infty$,

$$|n, \lambda, N\rangle \to |n, \lambda\rangle, \qquad E_n(\lambda, N) \to E_n(\lambda).$$

Numerical Matrix Diagonalization

- Now, lets focus our attention on numerical methods to diagonalize matrices.
- There are pre-existing modules in numpy, scipy which allow one to diagonalize matrice, but we want to understand the algorithms behind matrix diagonalization, so we will build our own solvers.

Reviewing some basic Linear Algebra

Suppose that S is an $n \times n$ real, symmetric matrix which means that its entries are real numbers, and its transpose equals itself;

$$S^T = S. \tag{12}$$

The Spectral Theorem of linear algebra guarantees that there is an orthogonal matrix O that diagonalizes S which means that there is a diagonal matrix D such that

$$O^{-1} S O = D. \tag{13}$$

The diagonal entries of D are the eigenvalues of S, which are guaranteed to be real since S is symmetric, and the columns of O are corresponding eigenvectors of S. Since O is orthogonal, its transpose equals its inverse;

$$O^{-1} = O^T, \tag{14}$$

This means that we can also write

$$O^T S O = D. \tag{15}$$

Hermitian Matrices

Consider instead an $n \times n$ Hermitian matrix H which means that the entries of H can be complex numbers, and H equals its adjoint;

$$H^\dagger = H, \tag{16}$$

where the adjoint operation $\dagger$ is simply defined as taking the transpose followed by complex conjugation of all entries of the matrix;

$$H^\dagger = (H^T)^*. \tag{17}$$

In this case, the Spectral Theorem guarantees that there is a unitary matrix U that diagonalizes H which means that there is a diagonal matrix D such that

$$U^{-1}HU = D. \tag{18}$$

The diagonal entries of D are the eigenvalues of S, which are guaranteed to be real since S is hermitian, and the columns of U are corresponding eigenvectors of S.

Since U is unitary, its adjoint equals its inverse;

$$U^{\dagger} = U^{-1}, \tag{19}$$

and this means that we can also write

$$U^{\dagger}HU = D. \tag{20}$$

Measures for approximate diagonalization

Define:

$$\mathrm{off}(M) = \sqrt{\sum_{i \neq j} |M_{ij}|^2}. \tag{21}$$

If M is diagonal, off M is equal to 0, so one way of saying that M is "approximately" diagonal is to say that $\mathrm{off}(M)$ is close to 0.

For any complex or real $n \times n$ matrix M, we define the **Frobenius norm** of the matrix as follows:

$$|M| = \sqrt{\sum_{i,j=1}^{n} |M_{ij}|^2}. \tag{22}$$