Week 6

Quantum Oscillators

1 Why do we care about Hamiltonians?

In the dynamics project, we leveraged the fact that for classical Hamiltonian systems, the the time evolution of the system is generated entirely by knowledge of the system's Hamiltonian through Hamiltoni's equations, a coupled system or first-order ODEs on phase space;

$$\dot{q}^k(t) = \frac{\partial H}{\partial p_k}(t, q(t), p(t)) \tag{1}$$

$$\dot{p}_k(t) = -\frac{\partial H}{\partial q^k}(t, q(t), p(t)). \tag{2}$$

If we use our general dynamical systems notation and write the phase space state of the system as

$$s = (q^1, q^2, \ldots, q^d, p_1, p_2, \ldots, p_d), \tag{3}$$

and if we define

$$f = \left(\frac{\partial H}{\partial p_1}, \ldots, \frac{\partial H}{\partial p_d}, -\frac{\partial H}{\partial q^1}, \ldots, -\frac{\partial H}{\partial q^d}\right). \tag{4}$$

then we can write

$$\dot{s}(t) = f(t, s(t)). \tag{5}$$

What about for quantum systems? How does the time-evolution of such systems work? At every moment in time, the state[1] of a

[1] There is actually a more general notion of the state of a quantum system for systems that are more properly modeled as occupying statistical mixtures of vectors in Hilbert space. For such systems, the state of the system is modeled as an operator $\hat{\rho}$ called the **density operator**. This is particularly important (in fact necessary) for quantum mechanical systems in statistical mechanics.

quantum system is a vector in a Hilbert space (a special kind of complex vector space with an inner product). How do we determine how the state evolves over time? As in classical mechanics, for isolated systems the state evolves deterministically according to a first-order differential equation, the **Shrodinger equation**:

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}\hat{H}|\psi(t)\rangle \tag{6}$$

where $\hat{H}$ is a hermitian linear operator on the Hilbert space of the system. So how does one solve this equation? There are at least two ways of doing things, and they end up being equivalent in the end.

1.1 Method 1 - Time evolution operator

We might be tempted to write the following as the solution to the Shrodinger equation:

$$|\psi(t)\rangle = e^{-i\hat{H}(t-t_0)/\hbar}|\psi(t_0)\rangle \tag{7}$$

which formally seems to solve the equation if we are allowed to somehow define the exponential of an operator in such a way that its derivative with respect to time behaves much like if $\hat{H}$ were just a number. In fact, the operator exponential is defined in a way that makes this the correct solution. In fact, for any operator $\hat{O}$, the operator exponential is defined by the same power series expansion that can be used to define the exponential of a number;[2]

$$e^{\hat{O}} = \hat{I} + \hat{O} + \frac{\hat{O}^2}{2!} + \cdots + \frac{\hat{O}^n}{n!} + \cdots \tag{8}$$

Given this definition, (7) is the solution to the Shrodinger equation, so it remains to compute the operator $e^{-i\hat{H}(t-t_0)/\hbar}$. This operator has a special name: it is the **time evolution operator** and is often writen as $U(t-t_0)$;

$$U(t-t_0) = e^{-i\hat{H}(t-t_0)/\hbar}. \tag{9}$$

[2]Special care must be taken for some examples where this reasoning is being applied to infinite-dimensional vector spaces, but for finite dimensional vector spaces, everything we write here is correct without qualification.

There is a clever way to compute this operator. Let's go back, for a moment, to the general case of computing $e^{\hat{O}}$ for an operator $\hat{O}$. Let O be the matrix representation of $\hat{O}$ in some basis. If the operator $\hat{O}$ is diagonalizable, then there exists an invertible matrix A and a diagonal matrix D such that

$$O = A^{-1}DA. \tag{10}$$

It follows that

$$e^{O} = e^{A^{-1}DA} = A^{-1}e^{D}A, \tag{11}$$

but the exponential of a diagonal matrix is just a diagonal matrix consisting of the exponentials of its entries:

$$e^{D} = \begin{pmatrix} e^{D_{11}} & & \\ & e^{D_{22}} & \\ & & \ddots \end{pmatrix} \tag{12}$$

So we've reduced the task of computing the exponential of some arbitrary diagonalizable operator to diagonalization of that operator. In other words, if you can diagonalize the Hamiltonian of a quantum system, then computing the time evolution operator isn't so hard.

1.2 Method 2 - Expanding in basis of eigenvectors

Since the hamiltonian is hermitian, the spectral theorem guarantees that there exists an orthonormal basis $|n\rangle$ for the Hilbert space consisting of eigenvectors of the hamiltonian. This means that at every time t, there exist complex numbers $c_n(t)$ such that

$$|\psi(t)\rangle = \sum_n c_n(t)|n\rangle. \tag{13}$$

Moreover, if ϵ_n is the energy eigenvalue for state $|n\rangle$, then by definition we have

$$H|n\rangle = \epsilon_n|n\rangle. \tag{14}$$

Combining all of these facts and using linear independence of the basis elements gives

$$\dot{c}_n(t) = -\frac{i\epsilon_n}{\hbar}c_n(t) \tag{15}$$

for *all* n. Each of these differential equations is easy to solve, and the results are:

$$c_n(t) = c_n(t_0)e^{-i\epsilon_n(t-t_0)/\hbar}. \tag{16}$$

This implies that the state of the system as a function of time is

$$|\psi(t)\rangle = \sum_n e^{-i\epsilon_n(t-t_0)/\hbar} c_n(t_0)|n\rangle. \tag{17}$$

All of this shows that in order to determine the state of a system as a function of time, we need only do the following:

1. Diagonalize the hamiltonian: find it's eigenvectors $|n\rangle$ and corresponding eigenvalues ϵ_n.

2. Determine $c_n(t_0)$.

Diagonalizing the Hamiltonian is thus the holy grail of time evolution for quantum systems. Since as far as we know, quantum mechanics is a fundamental description of nature down to the smallest length scales we have probed, diagonalization of hermitian operators is one of the most important mathematical operations one could want to do in physics.

2 The quantum harmonic oscillator

The **quantum harmonic oscillator** is defined by the following Hamiltonian given in non-dimensionalized form:

$$\hat{H}_0 = \frac{1}{2}(\hat{p}^2 + \hat{x}^2) \tag{18}$$

where $\hat{x}$ and $\hat{p}$ satisfy the **canonical commutation relation**

$$[\hat{x}, \hat{p}] = i\hat{I}. \tag{19}$$

Here we work in units where $\hbar = 1$. It is possible to diagonalize the Hamiltonian by purely algebraic means by introducing the **raising operator** $\hat{a}_+$ and **lowering operator** $\hat{a}_-$, defined by

$$\hat{a}_+ = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{p}) \tag{20}$$

$$\hat{a}_- = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}). \tag{21}$$

In particular, by some clever argumentation, one can show that there exists an orthonormal basis

$$B_0 = \{|0\rangle, |1\rangle, \dots\} \tag{22}$$

for the Hilbert space of this system satisfying

$$\hat{a}_+|n\rangle = \sqrt{n+1}|n+1\rangle \tag{23}$$

$$\hat{a}_-|n\rangle = \sqrt{n}|n-1\rangle \tag{24}$$

and moreover that the hamiltonian can be written in terms of the raising and lowering operators as

$$\hat{H}_0 = \hat{a}_+\hat{a}_- + \frac{1}{2}\hat{I}, \tag{25}$$

from which it follows that

$$\hat{H}_0|n\rangle = (n + \tfrac{1}{2})|n\rangle. \tag{26}$$

In other words, the Hamiltonian is diagonal in the basis B_0, and the eigenvalue E_n corresponding to eigenvector $|n\rangle$ is

$$E_n = n + \tfrac{1}{2} \tag{27}$$

In fact, the matrix elements of $\hat{H}_0$ in the basis B_0 are

$$\langle m|\hat{H}_0|n\rangle = (n + \tfrac{1}{2})\delta_{mn} \tag{28}$$

$$\langle m|\hat{a}_+|n\rangle = \sqrt{n+1}\delta_{m,n+1} \tag{29}$$

$$\langle m|\hat{a}_-|n\rangle = \sqrt{n}\delta_{m,n-1} \tag{30}$$

These expressions give the matrix representations of these three operators in the basis B_0, and if one restricts attention to the subspace spanned by the basis vectors $|0\rangle, |1\rangle, \dots, |N\rangle$, then one can write $(N+1) \times (N+1)$ matrix representations of these operators restricted to that subspace. These matrix representations can then be put on computer, e.g. as numpy arrays in Python, and one can use them to numerically compute eigenvectors and eigenvalues.

2.1 Wavefunctions

Note that it is also possible to think of the vectors $|n\rangle$ in the basis B_0 as **wavefunctions** instead of in the abstract, and in factor the wavefunction ψ_n that corresponds to $|n\rangle$ is

$$\psi_n(x) = (2^n n!\sqrt{pi})^{-1/2} e^{-x^2/2} h_n(x) \tag{31}$$

where h_n is the n^{th} Hermite polynomial which can be determine according to the following definitions of the first two:

$$h_0(x) = 1 \tag{32}$$
$$h_1(x) = 2x \tag{33}$$
$$\tag{34}$$

and the recursion relation

$$h_{n+1}(x) = 2xh_n(x) - 2nh_{n-1}(x). \tag{35}$$

3 The quantum anharmonic oscillator

Let $\lambda > 0$, and consider the **quantum anharmonic oscillator** defined by

$$\hat{H}_\lambda = \hat{H}_0 + \lambda \hat{x}^4. \tag{36}$$

Unfortunately, the elegant algebraic method used to diagonalize the quantum harmonic oscillator hamiltonian does not work for this modified hamiltonian. Instead, we can find approximate numerical eigenvectors and eigenvalues according to the following scheme.

1. Determine the matrix elements of $\hat{H}_\lambda$ in the harmonic oscillator basis B_0 using raising and lowering operators.

2. Restrict attention to the subspace spanned by the basis

$$B_{0,N} = \{|0\rangle, |1\rangle, \ldots, |N\rangle\} \tag{37}$$

   and find the matrix representation of $\hat{H}$ in this bases – an $(N + 1) \times (N + 1)$ matrix.

3. Using Python to numerically diagonalize this matrix representation.

4. Find N large enough that the eigenvalues and eigenvectors begin to converge to stable values which are approximations to the true eigenvalues and eigenvectors.