Quantum vs. Classical

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1 Classical and Quantum Hamiltonians

In this section, we will discuss the classical and quantum notions of Hamiltonians, and we will demonstrate under what circumstances these notions of Hamiltonian are equivalent.

1.1 Classical mechanics

Classical mechanics is concerned with the dynamics of macroscopic objects. That is, we are interested in a *deterministic* system where we have complete information. The system is defined by a configuration space M of possible configurations that the system can be in. We denote an individual configuration by $\xi \in M$. We can define a (classical) Hamiltonian H for our system as a function $H : M \to \mathbb{R}$ that maps each configuration ξ onto the energy $H(\xi)$ of that particular state. In this classical setup, the goal is simply to find the configuration $\xi \in M$ with the minimum energy. (This energy minimization can be done efficiently with a variety of different techniques, including annealing.)

1.2 Quantum mechanics

Given a classical configuration space M, we can make it quantum-mechanical by allowing for the system to be in probabilistic superpositions of different configurations. The space of all such quantum states is the Hilbert space $\mathcal{H}$, and we denote the states in it by $|\psi\rangle \in \mathcal{H}$.

A natural way to think about defining the Hilbert space is to define the basis states

$$\{|\xi_0\rangle, |\xi_1\rangle, \ldots\} \tag{1.1}$$

where each state $|\xi_n\rangle$ in this basis is the quantum state that corresponds exactly to one classical configuration $\xi_n \in M$. Then, the most general quantum state possible is given by

$$|\psi\rangle = \alpha_0 |\xi_0\rangle + \alpha_1 |\xi_1\rangle + \ldots \ , \tag{1.2}$$

for some complex numbers $\alpha_0, \alpha_1, \ldots \in \mathbb{C}$. Equivalently, we can define an operator $\hat{\xi} : \mathcal{H} \to \mathcal{H}$ whose eigenstates are simply these basis states $\{|\xi_n\rangle\}$, i.e.

$$\hat{\xi} |\xi_n\rangle = \xi_n |\xi_n\rangle \ . \tag{1.3}$$

That is, $\hat{\xi}$ is a diagonalizable operator on our Hilbert space whose eigenvalues comprise all configurations $\xi \in M$ and whose eigenvectors form a complete orthonormal basis for the entire Hilbert space.

Once we have specified our Hilbert space, we can encode the *dynamics* of the system (by which I mean how the system evolves over time) in the Hamiltonian $\hat{H} : \mathcal{H} \to \mathcal{H}$. Importantly, the Hamiltonian must be Hermitian:

$$\hat{H}^\dagger = \hat{H} \ . \tag{1.4}$$

This guarantees that the eigenvalues of the $\hat{H}$ are real and also that the eigenvectors of the $\hat{H}$ can be chosen such that they form a complete, orthonormal basis for $\mathcal{H}$. We will denote the eigenvalues of the Hamiltonian by $\{E_0, E_1, \ldots\}$, and the eigenvectors by

$$\{|E_0\rangle, |E_1\rangle, \ldots\} \ , \tag{1.5}$$

such that $\hat{H}\,|E_n\rangle = E_n\,|E_n\rangle$. These eigenvectors form a complete basis, and so we can represent the most general quantum state by

$$|\psi\rangle = \beta_0\,|E_0\rangle + \beta_1\,|E_1\rangle + \ldots \ , \tag{1.6}$$

for some complex numbers $\beta_0, \beta_1, \ldots \in \mathbb{C}$.

The Hamiltonian generates the time-evolution of the states in our quantum system according to the Schrödinger equation:

$$i\hbar \frac{d}{dt}\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle \ . \tag{1.7}$$

Another way of phrasing this is that, if we prepare an initial state $|\psi(0)\rangle$ at time $t = 0$, then the state at a time t in the future is given by

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle \ , \quad \hat{U}(t) = \exp\left(-i\hat{H}t/\hbar\right) \ . \tag{1.8}$$

The operator $\hat{U}(t)$ is usually referred to as the time-evolution operator. If our initial state is chosen to be one of the eigenstates of the Hamiltonian, then the time-evolution operator simply amounts to a phase factor:

$$|\psi(0)\rangle = |E_n\rangle \quad \Longrightarrow \quad |\psi(t)\rangle = \hat{U}(t)\,|E_n\rangle = \exp\left(-iE_nt/\hbar\right)|E_n\rangle \ . \tag{1.9}$$

We therefore find that the eigenstates of the Hamiltonian remain eigenstates of the Hamiltonian, with precisely the same eigenvalue, at all times. Thus, the Hamiltonian eigenvalues are naturally interpreted as *energy levels* that are stationary under time evolution.

1.3 When can you treat a quantum mechanics problem classically?

The key point is this: if the configuration operator $\hat{\xi}$ and the Hamiltonian $\hat{H}$ commute, then you can treat the quantum-mechanical system classically.

To see this, we first recall from equations (1.1) and (1.5) that the eigenstates of $\hat{\xi}$ form a complete basis of $\mathcal{H}$, as do the eigenstates of $\hat{H}$. If these two operators commute, then the operators are simultaneously diagonalizeable. This means that we can judiciously choose a new basis $\{|\psi_n\rangle\}$ of states for $\mathcal{H}$ that are eigenstates of both $\hat{\xi}$ and $\hat{H}$:

$$\begin{aligned} \hat{\xi}\,|\psi_n\rangle &= \xi_n\,|\psi_n\rangle \ , \\ \hat{H}\,|\psi_n\rangle &= E_n\,|\psi_n\rangle \ . \end{aligned} \tag{1.10}$$

That is, the states $\{|\psi_n\rangle\}$ are such that they each have a definite energy E_n as well as a definite configuration ξ_n associated with them. Thus, if our goal is to find the state with the lowest associated energy, we don't have to worry about probabilistic superpositions of configurations; there is a suitable basis of states for which each energy level (including the ground state energy level) corresponds to exactly one classical configuration $\xi \in M$.

Therefore, for the purposes of finding the ground state, we do not have to solve the Schrödinger equation. From our quantum Hamiltonian $\hat{H}$, we can simply define a classical Hamiltonian $H(\xi)$ as follows: given a classical configuration ξ, first find the basis state $|\psi\rangle$ such that $\hat{\xi}\,|\psi\rangle = \xi\,|\psi\rangle$. Then, define $H(\xi)$ to be the eigenvalue of $\hat{H}$ when acting on $|\psi\rangle$.

1.4 Examples

In this section, we will detail some examples that might help to demonstrate things more explicitly.

1.4.1 Single-spin systems

Let's consider a system where we have a single spin that can point up or down. The configuration space can be represented as $M = \{-1, +1\}$, where $\xi = +1$ represents the spin up state and $\xi = -1$ represents the spin down state.

In a quantum-mechanical description of this single spin, we can represent the spin up and spin down states by $|\uparrow\rangle$ and $|\downarrow\rangle$, respectively, which in matrix form are written as

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ , \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ . \tag{1.11}$$

The most general quantum state can be written as a superposition of the up and down spin states:

$$|\psi\rangle = a\,|\uparrow\rangle + b\,|\downarrow\rangle \ , \tag{1.12}$$

for $a, b \in \mathbb{C}$. Thus, we can think of the Hilbert space of all states as simply $\mathcal{H} = \mathbb{C}^2$.

The configuration operator $\hat{\xi}$ is defined by its action on the configuration basis states as follows:

$$\hat{\xi}\,|\uparrow\rangle = |\uparrow\rangle \ , \quad \hat{\xi}\,|\downarrow\rangle = -\,|\downarrow\rangle \ . \tag{1.13}$$

Equivalently, in matrix form, we can write this configuration operator as

$$\hat{\xi} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \hat{\sigma}_z \ , \tag{1.14}$$

where $\hat{\sigma}_z$ is the usual Pauli matrix associated with the z-direction.

A commuting Hamiltonian:

If we apply a magnetic field in the z-direction, the associated Hamiltonian is written as

$$\hat{H} = h\hat{\sigma}_z \ , \tag{1.15}$$

where h is a constant that represents the magnetic field strength. In this case, both $\hat{\xi}$ and $\hat{H}$ are proportional to $\hat{\sigma}_z$, and thus the two operators commute. Accordingly, the states $|\uparrow\rangle$ and $|\downarrow\rangle$ are also eigenstates of the Hamiltonian:

$$\hat{H}\,|\uparrow\rangle = h\,|\uparrow\rangle \ , \quad \hat{H}\,|\downarrow\rangle = -h\,|\downarrow\rangle \ . \tag{1.16}$$

Thus, the classical up and down configurations also have definite energies under the action of $\hat{H}$. We can thus define a classical Hamiltonian $H(\xi)$ simply by

$$H(\xi) = h\xi \ , \tag{1.17}$$

such that $\hat{H}\,|\uparrow\rangle = H(\xi = +1)\,|\uparrow\rangle$ and $\hat{H}\,|\downarrow\rangle = H(\xi = -1)\,|\downarrow\rangle$. Therefore the spectrum of quantum mechanical energies and classical energies are exactly the same, and a classical picture of our system is sufficient to find the ground state.

A non-commuting Hamiltonian:

Another possible Hamiltonian for our system arises if we were to apply a magnetic field in the x-direction. In that case, we would have

$$\hat{H} = h\hat{\sigma}_x \ , \tag{1.18}$$

where h is constant and $\hat{\sigma}_x$ is the x-direction Pauli matrix. Since $\hat{\sigma}_x$ and $\hat{\sigma}_z$ do not commute, this means that $\hat{\xi}$ and $\hat{H}$ do not commute and are thus not simultaneously diagonalizeable. In fact, the eigenspectrum of $\hat{H}$ is as follows:

$$\begin{aligned} \hat{H} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} &= h \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \ , \\ \hat{H} \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} &= -h \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \ . \end{aligned} \tag{1.19}$$

These eigenstates are linear superpositions of the configuration basis states $|\uparrow\rangle$ and $|\downarrow\rangle$, which means that the states in our system with definite energies do not have definite configurations, and vice-versa. In fact, the ground state of the system will necessarily be in a superposition of up and down spins, rather than being in one or the other, which is clearly not an allowable state in the classical

system. Therefore we cannot treat this system classically when the classical configuration space comprises up and down spins.

However, if we were to change our classical configuration space such that it comprises spin-left and spin-right states, rather than spin-up and spin-down states, then we would have $\hat{\xi} = \hat{\sigma}_x$ and thus we would be able to have a classical description of our quantum mechanical system. So, in some cases there could be a classical description, but it requires having the right choice of classical configuration space.

1.4.2 Quantum annealing

Let's now consider a system where we have a chain of N spins, subject to the following time-dependent Hamiltonian:

$$\hat{H} = A(t) \left[\sum_i \hat{\sigma}_x^{(i)} \right] + B(t) \left[\sum_{i,j} J_{ij} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} + \sum_i h_i \hat{\sigma}_z^{(i)} \right] , \tag{1.20}$$

where at the initial time $t = t_i$ we have $A(t_i) = 1$ and $B(t_i) = 0$ and at the final time $t = t_f$ we have $A(t_f) = 0$ and $B(t_f) = 1$. Here, $\hat{\sigma}_{x,z}^{(i)}$ represents the x, z-direction Pauli matrices acting on the i^{th} spin on our chain.

The final time Hamiltonian can therefore be written as

$$\hat{H}_f = \sum_{i,j} J_{ij} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} + \sum_i h_i \hat{\sigma}_z^{(i)} . \tag{1.21}$$

Since this only depends on the operators $\hat{\sigma}_z^{(i)}$, we can choose the classical configuration space $M^{(i)}$ for each spin to simply be the up-spin state $\xi^{(i)} = +1$ and the down-spin state $\xi^{(i)} = -1$. The corresponding configuration operators $\hat{\xi}^{(i)}$ can thus be taken as

$$\hat{\xi}^{(i)} = \hat{\sigma}_z^{(i)} , \tag{1.22}$$

which will guarantee that $\hat{H}_f$ commutes with each of these configuration operators $\hat{\xi}^{(i)}$. Additionally, the configuration operators all commute with one another, since they act independently on different sites on the spin chain. Thus the Hamiltonian and all configuration operators are all simultaneously diagonalizable, and so we can choose a basis of Hilbert space states that are eigenvectors under the action of $\hat{H}_f$ as well as all $\hat{\xi}^{(i)}$. We can therefore map the quantum mechanical problem onto a classical one and define the corresponding classical Hamiltonian simply as

$$H_f(\xi) = \sum_{i,j} J_{ij} \xi^{(i)} \xi^{(j)} + \sum_i h_i \xi^{(i)} , \tag{1.23}$$

with precisely the same spectrum as $\hat{H}_f$.

Similarly, we now consider the initial time Hamiltonian

$$\hat{H}_i = \sum_i \hat{\sigma}_x^{(i)} . \tag{1.24}$$

By taking the configuration space $M^{(i)}$ for each spin to comprise the spin-left and spin-right states, we can define the configuration operators $\hat{\xi}^{(i)} = \hat{\sigma}_x^{(i)}$, and we will automatically have $\hat{H}_i$ commute with all such $\hat{\xi}^{(i)}$. So, we can describe this initial time Hamiltonian classically as well, albeit *with a different classical configuration space*!

At any intermediate time $t_i < t < t_f$, we cannot describe the system classically. The Hamiltonian has non-trivial $\hat{\sigma}_x^{(i)}$ as well as $\hat{\sigma}_z^{(i)}$ dependence, and there are no configuration operators $\hat{\xi}^{(i)}$ we can define at these intermediate times that will commute with the Hamiltonian. Moreover, the Hamiltonian does not commute with itself at different instances in time. So, the states with definite energy under the action of $\hat{H}$ will necessarily be probabilistic superpositions of classical configurations, and thus we cannot hope to describe our system classically at these intermediate times.

We therefore have a quantum mechanical system where there is an initial classical description and a final classical description, but at all intermediate times no such classical description exists. To evolve the system fully in time, then, we must truly study the Schrödinger evolution of the actual quantum system.