13.6. *Find the entanglement of formation for the state in Exercise 13.5.*

13.7. *Find the entropy of the state*

$$\rho = \begin{pmatrix} \frac{5}{6} & 0 \\ 0 & \frac{1}{6} \end{pmatrix}$$

13.8. *Find the entropy of the state*

$$|\psi\rangle = \frac{2}{3}|0\rangle + \frac{\sqrt{5}}{3}|1\rangle$$

13.9. *Consider the product state $|A\rangle|B\rangle$ used in Example 5.11 where*

$$|A\rangle = \frac{|0\rangle - i|1\rangle}{\sqrt{2}}, \quad |B\rangle = \sqrt{\frac{2}{3}}|0\rangle + \frac{1}{\sqrt{3}}|1\rangle$$

The density matrix is

$$\rho = \begin{pmatrix} \frac{1}{3} & \frac{1}{\sqrt{18}} & \frac{i}{3} & \frac{i}{\sqrt{18}} \\ \frac{1}{\sqrt{18}} & \frac{1}{6} & \frac{i}{\sqrt{18}} & \frac{i}{6} \\ \frac{-i}{3} & \frac{-i}{\sqrt{18}} & \frac{1}{3} & \frac{1}{\sqrt{18}} \\ \frac{-i}{\sqrt{18}} & \frac{-i}{6} & \frac{1}{\sqrt{18}} & \frac{1}{6} \end{pmatrix}$$

(A) Show that the entropy of the density operator for $|A\rangle|B\rangle$ is zero.
(B) Find the entropy for the density operator seen only by Alice, ρ_A.

13.10. *Consider the density operators for the state*

$$|\psi\rangle = \sqrt{\frac{3}{7}}|0\rangle + \frac{2}{\sqrt{7}}|1\rangle$$

and the state

$$|\phi\rangle = \sqrt{\frac{2}{3}}|0\rangle + \frac{1}{\sqrt{3}}|1\rangle$$

Which state has a higher entropy?

14

ADIABATIC QUANTUM COMPUTATION

Adiabatic quantum computation is an alternative approach to quantum computation based on the time evolution of a quantum system. Before describing adiabatic processes, let's quickly review the dynamics of a quantum system. The time evolution of a quantum state $|\psi(t)\rangle$ is described by the Schrödinger equation

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle \tag{14.1}$$

where H is the Hamiltonian operator. This operator is the total energy of the system and can be expressed in terms of kinetic and potential energies

$$H = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V \tag{14.2}$$

where ∇^2 is the *Laplacian* operator and V is the potential energy function. In one dimension (14.2) becomes

$$H = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \tag{14.3}$$

Quantum Computing Explained, by David McMahon

In many cases of interest, the potential V is time-independent. Where this is the case, then solutions of (14.1) are products of a function that depends only on the spatial coordinates and a function that depends only on time. In one dimension the solution can be written in the form

$$\Psi(x,t) = \psi(x)f(t) \tag{14.4}$$

By inserting (14.4) into (14.1) and using (14.3), its not too hard to show that the solution can be written as

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \tag{14.5}$$

Solutions of Schrödingers equation are known as *wave functions*. Using (14.5) in (14.1), we also arrive at a *time-independent* Schrodinger's equation that gives a solution for the spatial part of the wave function:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{14.6}$$

where E is the energy of the system. The modulus squared of the wave function is a probability density, where $|\Psi(x,t)|^2dx$ is the probability of finding the particle in a volume dx. The total probability over all space must be equal to one, so the normalization condition for a wave function is

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx = 1 \tag{14.7}$$

Solutions of the type (14.5) are called *stationary*. This is because when we calculate the modulus squared of (14.5), we see that the probability density does not change with time:

$$|\Psi(x,t)|^2 = |\psi(x)e^{-iEt/\hbar}|^2 = (\psi^*(x)e^{iEt/\hbar})(\psi(x)e^{-iEt/\hbar}) = |\psi(x)|^2 \tag{14.8}$$

The eigenstates of the Hamiltonian $\Phi_n(x,t) = \phi_n(x)f_n(t)$ have eigenvalues that are the energies E_n that the system can assume. Bound states have discrete energy levels; that is, the system can only take on specific energy values like the rungs on a ladder. Unbound systems have continuous energy spectra (they can assume any energy value). The general solution to the time-dependent Schrödinger equation is a superposition of energy eigenstates

$$\Psi(x,t) = \sum_n c_n\phi_n(x)\exp\left(-i\frac{E_nt}{\hbar}\right) \tag{14.9}$$

The lowest energy that the system can assume is called the *ground state*.

Example 14.1

Find the energy eignstates and most general solution to the Schrödinger equation for an infinite unsymmetric square well:

$$V(x) = \begin{cases} +\infty & x<0 \\ 0 & 0 \le x \le a \\ +\infty & x>a \end{cases}$$

Solution

A particle confined to an infinite square well is a bound system. Hence it will have a discrete energy spectrum. At the boundaries of the well, the potential is infinite. The wave function must vanish outside this region as well as at the boundaries for continuity. Inside the well, the time-independent Schrödinger equation (14.6) can be written as

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \tag{14.10}$$

where we define k^2 as

$$k^2 = \frac{2mE}{\hbar^2} \tag{14.11}$$

The solutions of (14.10) are

$$\psi(x) = A\sin kx + B\cos kx \tag{14.12}$$

The constants A and B are determined by the boundary conditions. The first of these is the vanishing of the wave function at the left boundary—that is, $\psi(0)=0$. This tells us that $B=0$. The other boundary condition is $\psi(a)=0$, from which we conclude that

$$k_na = n\pi \tag{14.13}$$

where $n = 1,2,3,\ldots$. Using this together with (14.11) allows us to determine the energies that the system can assume, which are

$$E_n = \frac{\hbar^2}{2m}k_n^2 = \frac{\hbar^2\pi^2}{2ma^2}n^2, \quad n = 1,2,3,\ldots \tag{14.14}$$

Therefore the wave functions are of the form

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right), \quad n = 1,2,3,\ldots \tag{14.15}$$

The constant $\sqrt{2/a}$ is called the normalization constant. It is determined from

$$I = \int_{-\infty}^{\infty} \psi_n^*(x)\,\psi_n(x)\,dx \tag{14.16}$$

The most general solution to (14.10) is a superposition of all possible solutions:

$$\Psi(x,t) = \sum_{n=1}^{\infty} \psi_n(x) e^{-iE_n t/\hbar} = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{a}\right) \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right) \tag{14.17}$$

ADIABATIC PROCESSES

An *adiabatic process* is one for which the rate of change of the Hamiltonian is slow with respect to the characteristic time of the system (i.e., the time scale over which changes to the system occur). If we denote the characteristic time scale for changes in the system by T_c and the time change over which the Hamiltonian changes as T_H, then we denote the condition for an adiabatic process as

$$T_H \gg T_c \tag{14.18}$$

In quantum mechanics, an adiabatic process is one for which the initial Hamiltonian H_{init} slowly changes to some different, final Hamiltonian H_{final}:

$$H_{init} \underset{slowly}{\rightarrow} H_{final} \tag{14.19}$$

with the time scale over which this occurs being T_H. The *adiabatic theorem* tells us that if a system is in the nth energy eigenstate of H_{init}, it will also be in the nth energy eigenstate of H_{final} if the change is adiabatic. For a change to be adiabatic, the time scale of the change must be proportional to the energy gap between the ground state and the lowest excited state:

$$T \propto \frac{1}{\Delta E} \tag{14.20}$$

Example 14.2

A particle is in an infinite unsymmetric square well of width a; the potential is

$$V(x) = \begin{cases} +\infty & x<0 \\ 0 & 0 \le x \le a \\ +\infty & x>a \end{cases}$$

It is known that the particle is in the ground state. What is the state of the system if the width of the well is very slowly widened to $3a$?

Solution

In this case H_{init} is just the Hamiltonian for Example 14.1. The system starts off in the ground state for which we set $n=1$ in (14.15), giving

$$\psi_{init}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right) \tag{14.21}$$

The energy of the particle is found using (14.14), which is

$$E_{init} = \frac{\hbar^2\pi^2}{2ma^2}$$

For H_{final}, the energy eigenstates are found by letting $a \rightarrow 3a$ in (14.15). These are

$$\psi_n(x) = \sqrt{\frac{2}{3a}} \sin\left(\frac{n\pi}{3a}x\right), \quad n = 1, 2, 3, \ldots \tag{14.22}$$

with energies

$$E_n = \frac{\hbar^2\pi^2}{18ma^2}n^2, \quad n = 1, 2, 3, \ldots \tag{14.23}$$

We see that widening the well lowers the energies. The adiabatic theorem tells us that if the well is widened slowly, that a system in the nth energy eigenstate of H_{init} will go to the nth energy eigenstate of H_{final}. Since we started in the ground state, we end up in the ground state of the new Hamiltonian, which is found from (14.22). We obtain

$$\psi_{final}(x) = \sqrt{\frac{2}{3a}} \sin\left(\frac{\pi}{3a}x\right)$$

The final energy of the particle is

$$E_{final} = \frac{\hbar^2\pi^2}{18ma^2}$$

What sort of time scale should be used to implement the change? We can give the time required by looking at (14.5) where we have an expression of the form $e^{-iEt/\hbar}$. The characteristic time can be estimated from

$$t_c = \frac{\hbar}{\Delta E} = \frac{\hbar}{(4\hbar^2\pi^2/2ma^2) - (\hbar^2\pi^2/2ma^2)} = \frac{2ma^2}{3\hbar\pi^2} \tag{14.24}$$

where we took the energy gap to be between the ground state and the first excited state, which is found by setting $n=2$ in (14.14) giving $E_2 = 4\hbar^2\pi^2/2ma^2$. So, if the time over which the walls of the potential well are expanded satisfies

$$T \gg \frac{2ma^2}{3\hbar\pi^2}$$

the process will be adiabatic.

ADIABATIC QUANTUM COMPUTING

Adiabatic quantum computation uses adiabatic processes to do a computation using the following steps:

- Create an initial state of qubits that will be used to calculate the result of a computation.
- Start with an initial Hamiltonian, and very it slowly (adiabatically) so that it transforms into a final Hamiltonian whose eigenstates encode the solution.

Let's look at the process more formally. The adiabatic process starts with a known easy to prepare Hamiltonian. This Hamiltonian should have a ground state that is easy to create. The quintessential example is a Hamiltonian consisting of Pauli operators

$$H_{init} = -\sum_j X^{(j)} \tag{14.25}$$

Next let's select a *problem Hamiltonian*. The ground state of the problem Hamiltonian encodes the solution to the problem we are trying to solve:

$$H_{final} = \sum_x c_x |x\rangle\langle x| \tag{14.26}$$

An interpolation Hamiltonian is used to connect H_{init} and H_{final}. If T is the total time over which the computation is completed, and we let $s = t/T$ and $0 \le s \le 1$, then

$$\tilde{H} = (1-s)H_{init} + sH_{final} \tag{14.27}$$

Example 14.3

Describe how the Hadamard gate can be implemented using adiabatic quantum computation.

Solution

First we recall the action of the Hadamard gate. This gate creates superposition states out of the computational basis in the following way:

$$H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \quad H|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

In the computational basis the Hadamard gate has the representation

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

In order to implement the Hadamard gate using adiabatic quantum computation, we need to find a Hamiltonian that will create superposition states out of the computational basis, and we need to find an initial Hamiltonian with a ground state that is easy to prepare. One such Hamiltonian is

$$H_{init} = -|0\rangle\langle 0| + |1\rangle\langle 1|$$

The matrix representation of this Hamiltonian is

$$H_{init} \doteq \begin{pmatrix} \langle 0|H_{init}|0\rangle & \langle 0|H_{init}|1\rangle \\ \langle 1|H_{init}|0\rangle & \langle 1|H_{init}|1\rangle \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

The characteristic equation is

$$0 = \det|H_{init} - I| = \det\left|\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}\right| = \det\begin{vmatrix} -1-\lambda & 0 \\ 0 & 1-\lambda \end{vmatrix} = -1 + \lambda^2$$

Therefore the eigenvalues of the matrix (the Hamiltonian H_{init}) are

$$\lambda_{0,1} = \pm 1$$

The eigenvalues of the Hamiltonian are the energy levels that the system can assume. The ground state has the lowest energy, so the ground state in this case corresponds to $\lambda_0 = -1$. The eigenvector corresponding to this eigenvalue is found from

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = -\begin{pmatrix} a \\ b \end{pmatrix}$$

We obtain the equations

$$-a = -a, \quad \Rightarrow a = 1$$
$$b = -b, \quad \Rightarrow b = 0$$

We chose $a = 1$so that the eigenvector is normalized (has unit norm). The eigenvector corresponding to $\lambda_0 = -1$ is the ground state of H_{init}:

$$|u_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle$$

A similar procedure taking $\lambda_1 = 1$ gives the second eigenvector of H_{init}:

$$|u_1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$

Now let's look at the final Hamiltonian. We can create a superposition state with

$$H_{final} = -|0\rangle\langle 1| - |1\rangle\langle 0| = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} = -X$$

Let's explicitly calculate the eigenvectors even though some readers may know what they are. First we have the characteristic equation

$$0 = \det|H_{final} - I| = \det\left|\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} - \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}\right| = \det\begin{vmatrix} -\lambda & -1 \\ -1 & -\lambda \end{vmatrix} = \lambda^2 - 1$$

$$\Rightarrow \lambda_{0,1} = \pm 1$$

The ground state is found by taking the lowest energy, which is the smallest eigenvalue. So choosing $\lambda_0 = -1$, we have

$$H_{final}|v_0\rangle = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = -\begin{pmatrix} a \\ b \end{pmatrix}$$

This yields the equations

$$-b = -a$$
$$-a = -b$$
$$\Rightarrow a = b$$

We can compute the value of the coefficients by "normalizing" the vector

$$1 = \begin{pmatrix} a^* & a^* \end{pmatrix}\begin{pmatrix} a \\ a \end{pmatrix} = 2|a|^2$$

$$\Rightarrow a = \frac{1}{\sqrt{2}}$$

Hence the eigenvector is

$$|v_0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

A similar procedure applied to $\lambda_1 = 1$ give the eigenvector corresponding to the excited state of H_{final}

$$|v_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

So we have our initial and final states that correspond to the output of the Hadamard gate.

To implement a Hadamard gate $H|0\rangle = (1/\sqrt{2})(|0\rangle + |1\rangle)$ using adiabatic quantum computation, we proceed as follows:

- We prepare the system in the ground state of H_{init}, which is $|\psi_0\rangle = |0\rangle$.
- We evolve the Hamiltonian using $H(s) = (1-s)H_{init} + sH_{final}$ by which the process evolves slowly.

- By the adiabatic theorem, when $t = T(s = 1)$, the system is in the ground state of the final Hamiltonian:

$$|v_0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

So we have implemented a Hadamard gate.

EXERCISES

14.1. *Derive (14.5) by solving the differential equation that results from (14.1). Assume that (14.5) is a separable solution of the form (14.4), and the constant of integration is the energy E.*

14.2. *Verify that the unit of time in (14.24) is seconds by taking a to be in meters and doing dimensional analysis. The units of $\hbar$ are joule-seconds.*

14.3. *A square well is gradually decreased from width a to $\frac{1}{2}a$. If the change is adiabatic and the system starts off with the particle in the first excited state, what is the energy of the particle when the width is $\frac{1}{2}a$?*

14.4. *Consider the implementation of a CNOT gate using adiabatic computation. Take*

$$H_0 = 3|00\rangle\langle 00| + 2|01\rangle\langle 01| + |10\rangle\langle 10|$$
$$H_1 = 3|00\rangle\langle 00| + 2|01\rangle\langle 01| + |11\rangle\langle 11|$$
$$H_{01} = |10\rangle\langle 11| + |11\rangle\langle 10|$$

and let

$$H(s) = (1-s)H_0 + sH_1 + s(1-s)H_{01}$$

Follow the procedure used in Example 14.3 and show this system can be used to implement a CNOT gate.