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A Concise Introduction to Quantum Computing

Lectures given for the Course of Topics in Physics

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3 Physical Realizations of Quantum Computers

The properties of a real Quantum Computer have been listed by DiVincenzo in his 2000 papers (**DiVinc1DiVinc2**):

- a scalable physical system with well characterized qubits,
- the ability to initialise the state of the qubits to a simple fiducial state,
- long relevant decoherence times, much longer than the gate operation time,
- the ability to interconvert stationary and flying qubits,
- the ability to faithfully transmit flying qbits between specified locations.

3.1 Particle in a Box as a Quantum Computer

In chapter .... we have solved Schrödinger equation for the particular case of a particle of mass m in a potential well of length L with walls of infinite height. We have seen that the presence of the walls originated a quantization of the possible energy values of the particle, corresponding to different wave functions. Using the Dirac formalism, we can write again the time-independent Schrödinger equation, now considering the Hamiltonian of the system as an operator, with quantized energy values $E_n = \hbar^2\pi^2 n^2/2mL^2$ which are the eigenvalues of the eigenstates $|\psi(x)_n\rangle$:

$$\hat{H}\,|\psi(x)_n\rangle = E_n\,|\psi(x)_n\rangle \tag{3.1}$$

The normalised form of $|\psi(x)_n\rangle$ is:

$$|\psi_n\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{n}{\pi}Lx\right) \tag{3.2}$$

The $\hat{H}$ operator is Hermitian and hence its eigenfunctions are an orthonormal base for a generic state $|\phi\rangle$ of the system:

$$|\phi\rangle = \sum_n \alpha_n\,|\psi_n\rangle \tag{3.3}$$

Moreover, as discussed in chapter ..., the time evolution of $|\phi(t)\rangle$ can be written in terms of the eigenvalues of $\hat{H}$:

$$|\phi(t)\rangle = \sum_n \alpha_n(t)\,|\psi_n\rangle = \sum_n \alpha_n(0)e^{-\frac{i}{\hbar}E_n t}\,|\psi_n\rangle \tag{3.4}$$

In order to use this system as a quantum computer, let us arrange things in such a way that we consider only the two lowest energy levels. In this case, we can write a generic state of interest as:

$$|\phi(t)\rangle = \alpha_1(t)\,|\psi_1\rangle + \alpha_2(t)\,|\psi_2\rangle = \alpha_1(0)e^{-\frac{i}{\hbar}E_1 t}\,|\psi_1\rangle + a_2(t)e^{-\frac{i}{\hbar}E_2 t}\,|\psi_2\rangle \tag{3.5}$$

where, being only E_1 and E_2 different from zero, we have:

$$\hat{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \tag{3.6}$$

Now, let us assume $\hbar\omega = \frac{E_1 - E_2}{2}$. With this position, we can write:

$$\begin{aligned} E_1 &= E_1 + \hbar\omega - \hbar\omega = \\ &= E_1 + E_1/2 - E_2/2 - E_1/2 + E_2/2 = \\ &= E_1/2 + E_2/2 + E_1 - E_1/2 - E_2/2 = \\ &= E_1/2 + E_2/2 + E_1/2 - E_2/2 = \\ &= \frac{E_1 + E_2}{2} + \hbar\omega \end{aligned}$$

and:

$$\begin{aligned} E_2 &= E_2 + \hbar\omega - \hbar\omega = \\ &= E_2 + E_1/2 - E_2/2 - E_1/2 + E_2/2 = \\ &= E_1/2 + E_2/2 + E_2 - E_1/2 - E_2/2 = \\ &= E_1/2 + E_2/2 - E_1/2 + E_2/2 = \\ &= \frac{E_1 + E_2}{2} - \hbar\omega \end{aligned}$$

hence, we can also write:

$$\begin{aligned} \hat{H} &= \begin{pmatrix} \frac{E_1+E_2}{2} + \hbar\omega & 0 \\ 0 & \frac{E_1+E_2}{2} - \hbar\omega \end{pmatrix} = \begin{pmatrix} \frac{E_1+E_2}{2} & 0 \\ 0 & \frac{E_1+E_2}{2} \end{pmatrix} + \begin{pmatrix} \hbar\omega & 0 \\ 0 & -\hbar\omega \end{pmatrix} = \\ &= [(E_1 + E_2)/2] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{E_1 + E_2}{2} I + \hbar\omega Z \end{aligned} \tag{3.7}$$

If we substitute the new expressions for E_1 and E_2 in ..., we have:

$$\begin{aligned} |\phi(t)\rangle &= \alpha_1(t)\,|\psi_1\rangle + \alpha_2(t)\,|\psi_2\rangle = \\ &= \alpha_1(0)e^{-\frac{i}{\hbar}(\frac{E_1+E_2}{2}+\hbar\omega)t}\,|\psi_1\rangle + \alpha_2(0)e^{-\frac{i}{\hbar}(\frac{E_1+E_2}{2}-\hbar\omega)t}\,|\psi_2\rangle = \\ &= e^{-i\frac{E_1+E_2}{2}t}\left[\alpha_1(0)e^{-i\omega t}\,|\psi_1\rangle + \alpha_2(0)e^{i\omega t}\,|\psi_2\rangle\right] \end{aligned} \tag{3.8}$$

Now we can change notation, representing $|\phi(t)\rangle$ by the coefficients $a_1(0)$ and $a_2(0)$ of its expansions in the basis of the eigenfunctions of energy:

$$|\phi(0)\rangle = \begin{pmatrix} \alpha_1(0) \\ \alpha_2(0) \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \tag{3.9}$$

In this way, we have a two-level system that can be used as a **qbit**.
Our qbit evolves with time according to the time dependent Schrödinger equation:

$$\hat{H}\,|\phi(t)\rangle = i\hbar\frac{\partial}{\partial t}\,|\phi(t)\rangle \tag{3.10}$$

which allows us to write:

$$|\phi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\phi(0)\rangle \tag{3.11}$$

Now, we have seen that, in matricial form, we have:

$$\hat{H} = \frac{E_1 + E_2}{2}\hat{I} + \hbar\omega\hat{Z} \tag{3.12}$$

and so:

$$|\phi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\phi(0)\rangle = e^{-\frac{i}{\hbar}\left(\frac{E_1+E_2}{2}\hat{I}+\hbar\omega\hat{Z}\right)t}|\phi(0)\rangle = e^{-\frac{i}{\hbar}\left(\frac{E_1+E_2}{2}\hat{I}\right)t}e^{-\frac{i}{\hbar}\left(\hbar\omega\hat{Z}\right)t}|\phi(0)\rangle =$$

$$= \begin{pmatrix} e^{-\frac{i}{\hbar}\left(\frac{E_1+E_2}{2}\right)t} & 0 \\ 0 & e^{-\frac{i}{\hbar}\left(\frac{E_1+E_2}{2}\right)t} \end{pmatrix} \begin{pmatrix} e^{i\omega t} & 0 \\ 0 & e^{-i\omega t} \end{pmatrix} \begin{pmatrix} \alpha_1(0) \\ \alpha_2(0) \end{pmatrix} = \begin{pmatrix} e^{-\frac{i}{\hbar}\left(\frac{E_1+E_2}{2}\right)t}e^{i\omega t}\alpha_1(0) \\ e^{-\frac{i}{\hbar}\left(\frac{E_1+E_2}{2}\right)t}e^{-i\omega t}\alpha_2(0) \end{pmatrix}$$

as expected from **??**

The first exponential term in 3.1 is an overall phase and can be neglected. So the evolution of the system is given by the *effective Hamiltonian*:

$$\hat{H} = \hbar\omega\hat{Z} \tag{3.14}$$

which is simply a phase flip (given by $\hat{Z}$) and a rotation with angular frequency ω. This last term also can be neglected if we rotate together with our system, at the same angular frequency ω. So, in order to perform an operation on our qbit we must change its Hamiltonian. On the other hand this change must preserve the unitarity of $\hat{H}$, which is essential to have a consistent time evolution of our system. We can satisfy these constraints by applying only a small perturbation to $\hat{H}$: in this way we are sure that unitarity is conserved, at least at the first order.

For instance, let us change $\hat{H}$ adding a small term $\delta U(x) = -U_o(t)\frac{9\pi^2}{16}\left(\frac{x}{L} - \frac{1}{2}\right)$ to the potential energy $U(x)$ in the interval where it is zero (i.e. for $0 < x < L$):

$$\hat{H}' = \frac{p^2}{2m} + \delta U(x) = \frac{p^2}{2m} - U_o(t)\frac{9\pi^2}{16}\left(\frac{x}{L} - \frac{1}{2}\right) \tag{3.15}$$

and let us see what is the effect of this term on the system.

Let us recall that that the matrix components Γ_{ik} of a generic operator $\hat{\Gamma}$ in a basis $\{|e_i\rangle\}$ can be found computing the expressions:

$$\Gamma_{ik} = \langle e_i|\hat{\Gamma}|e_k\rangle \tag{3.16}$$

Now, in our case, our system has a basis having only two components:

$$|\psi_1\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right) \tag{3.17}$$
$$|\psi_2\rangle = \sqrt{\frac{2}{L}}\sin\left(2\frac{\pi}{L}x\right)$$

so, in order to compute the new components of $\hat{H}'$, we must compute:

$$\begin{aligned} H'_{11} &= \langle\psi_1|\,\hat{H}'\,|\psi_1\rangle \\ H'_{12} &= \langle\psi_1|\,\hat{H}'\,|\psi_2\rangle \\ H'_{21} &= \langle\psi_2|\,\hat{H}'\,|\psi_1\rangle \\ H'_{22} &= \langle\psi_2|\,\hat{H}'\,|\psi_2\rangle \end{aligned} \tag{3.18}$$

It is evident that, for instance:

$$H'_{11} = \langle\psi_1|\,\hat{H}'\,|\psi_1\rangle = \langle\psi_1|\,\hat{H}\,|\psi_1\rangle + \langle\psi_1|\,\delta\hat{U}(x)\,|\psi_1\rangle \tag{3.19}$$

so that the only terms that have changed, after the perturbation of the Hamiltonian $\hat{H}$ are:

$$\begin{aligned} \delta U(x)_{11} &= \langle\psi_1|\,\delta\hat{U}(x)\,|\psi_1\rangle \\ \delta U(x)_{12} &= \langle\psi_1|\,\delta\hat{U}(x)\,|\psi_2\rangle \\ \delta U(x)_{21} &= \langle\psi_2|\,\delta\hat{U}(x)\,|\psi_1\rangle \\ \delta U(x)_{22} &= \langle\psi_1|\,\delta\hat{U}(x)\,|\psi_1\rangle \end{aligned} \tag{3.20}$$

Let us compute explicitly these terms:

$$\begin{aligned} \delta U(x)_{11} &= \langle\psi_1|\,\delta\hat{U}(x)\,|\psi_1\rangle = \\ &= \int_{-\infty}^{\infty} \psi_1^* \delta\hat{U}\psi_1 dx = \\ &= \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) \left[-U_o \frac{9\pi^2}{16}\left(\frac{x}{L}-\frac{1}{2}\right)\right] \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) dx = \\ &= -\frac{2}{L}U_o\frac{9\pi^2}{16}\int_0^L \sin^2\left(\frac{\pi}{L}x\right)\left(\frac{x}{L}-\frac{1}{2}\right) dx \\ &= -U_o\frac{9\pi^2}{8L}\left[\frac{1}{L}\int_0^L x\sin^2\left(\frac{\pi}{L}x\right) dx - \frac{1}{2}\int_0^L \sin^2\left(\frac{\pi}{L}x\right) dx\right] \end{aligned} \tag{3.21}$$

The two integrals between square parentheses can be evaluated remembering that:

$$\int \sin^2(ax)dx = \frac{x}{2} - \frac{\sin(2ax)}{4a} \tag{3.22}$$

$$\int x\sin^2(ax)dx = \frac{x^2}{4} - \frac{x\sin(2ax)}{4a} - \frac{\cos(2ax)}{8a^2} \tag{3.23}$$

and we have:

$$\begin{aligned} \delta U(x)_{11} &= \langle\psi_1|\,\delta\hat{U}(x)\,|\psi_1\rangle = \\ &= -U_o\frac{9\pi^2}{8L}\left\{\frac{1}{L}\left[\frac{x^2}{4} - \frac{x\sin(2(\pi/L)x}{4(\pi/L)} - \frac{\cos(2(\pi/L)x}{8(\pi/L)^2}\right]_0^L - \frac{1}{2}\left[\frac{x}{2} - \frac{\sin(2(\pi/L)x)}{4(\pi/L)}\right]_0^L\right\} = \\ &= -U_o\frac{9\pi^2}{8L}\left\{\frac{1}{L}\left[\frac{L^2}{4}\right] - \frac{1}{2}\left[\frac{L}{2}\right]\right\} = 0 \end{aligned} \tag{3.24}$$

Of course we get the same result also for $\delta U(x)_{22}$, and so we have:

$$\delta U(x)_{11} = \delta U(x)_{22} = 0 \tag{3.25}$$

We can now compute $\delta U(x)_{12} = \langle\psi_1|\,\delta\hat{U}(x)\,|\psi_2\rangle$ and $\delta U(x)_{21} = \langle\psi_2|\,\delta\hat{U}(x)\,|\psi_2\rangle$: let us begin with $\delta U(x)_{12}$:

$$\begin{aligned}\delta U(x)_{12} &= \langle\psi_1|\,\delta\hat{U}(x)\,|\psi_2\rangle = &(3.26)\\ &= \int_0^L \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right)\left[-U_o\frac{9\pi^2}{16}\left(\frac{x}{L}-\frac{1}{2}\right)\right]\sqrt{\frac{2}{L}}\sin\left(2\frac{\pi}{L}x\right)dx = \\ &= -U_o\frac{9\pi^2}{8L}\left[\frac{1}{L}\int_0^L x\sin\left(\frac{\pi}{L}x\right)\sin\left(2\frac{\pi}{L}x\right)dx - \frac{1}{2}\int_0^L \sin\left(\frac{\pi}{L}x\right)\sin\left(2\frac{\pi}{L}x\right)dx\right]\end{aligned}$$

This equation shows clearly that in our case is $\delta U(x)_{12} = \delta U(x)_{21}$, being both $|\psi_1\rangle$ and $|\psi_2\rangle$ real. On the other hand, the first integral in **??** can be evaluated considering that:

$$\sin(ax)\sin(2ax) = \frac{1}{2}\left[\cos(ax-2ax)-\cos(ax+2ax)\right] = \frac{1}{2}\left[\cos(ax)-\cos(3ax)\right] \tag{3.27}$$

so that we can write:

$$\begin{aligned}\int x\sin(ax)\sin(2ax)dx &= \int x\frac{1}{2}\left[\cos(ax)-\cos(3ax)\right]\,dx &(3.28)\\ &= \frac{1}{2}\left[\int x\cos(ax)dx - \int x\cos(3ax)dx\right]\end{aligned}$$

Considering that:

$$\int x\cos(ax)dx = \frac{\cos ax}{a^2} + \frac{x\sin ax}{a} \tag{3.29}$$

we have, for the first integral in **??**:

$$\begin{aligned}&\int_0^L x\sin\left(\frac{\pi}{L}x\right)\sin\left(2\frac{\pi}{L}x\right)dx = &(3.30)\\ &= \frac{1}{2}\left[\int_0^L x\cos(\frac{\pi}{L}x)dx - \int_0^L x\cos(3\frac{\pi}{L}x)dx\right] = \\ &= \frac{1}{2}\left[\frac{\cos\frac{\pi}{L}x}{\left(\frac{\pi}{L}\right)^2} + \frac{x\sin\frac{\pi}{L}x}{\frac{\pi}{L}}\right]_0^L - \frac{1}{2}\left[\frac{\cos\frac{3\pi}{L}x}{\left(\frac{3\pi}{L}\right)^2} + \frac{x\sin\frac{3\pi}{L}x}{\frac{3\pi}{L}}\right]_0^L = \\ &= \frac{1}{2}\left[-2\frac{L^2}{\pi^2} + 2\frac{L^2}{9\pi^2}\right] = -\frac{8}{9}\frac{L^2}{\pi^2} &(3.31)\end{aligned}$$

Using **??** we can compute easily also the second integral in **??**:

$$\begin{aligned}&-\frac{1}{2}\int_0^L \sin\left(\frac{\pi}{L}x\right)\sin\left(2\frac{\pi}{L}x\right)dx = -\frac{1}{2}\int_0^L \left[\cos(\frac{\pi}{L}x) - \cos(3\frac{\pi}{L}x)\right] = &(3.32)\\ &= -\frac{1}{2}\left[\frac{\sin(\frac{\pi}{L}x)}{\frac{\pi}{L}} - \frac{\sin(3\frac{\pi}{L}x)}{3\frac{\pi}{L}}\right]_0^L = 0\end{aligned}$$

According to these results, we can now conclude that:

$$\delta U_{12} = \delta U_{21} = -U_o \frac{9\pi^2}{8L}\left[\frac{1}{L}\left(-\frac{8}{9}\frac{L^2}{\pi^2}\right) - \frac{1}{2}\times 0\right] = U_o \tag{3.33}$$

so that the matrix form of the perturbation term to the initial Hamiltonian is:

$$\begin{pmatrix} 0 & U_o \\ U_o & 0 \end{pmatrix} = U_o \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = U_o X \tag{3.34}$$

The time evolution of this perturbation of the Hamiltonian $\delta U(t)$ represents a rotation of the qbit around the x axis. So, by a perturbation of the potential, we have implemented an operation on our single qbit, preserving also the unitarity of the Hamiltonian.

Of course this is not enough to have a real universal quantum computer. In the following chapter we shall make a further step towards this goal by considering a physical system that we have already encountered in ....: a quantum particle in the potential of a Harmonic Oscillator.

3.2 Harmonic Oscillator as a Quantum Computer

Let us recall the main features of the behaviour of a particle in a harmonic oscillator potential, according to the time independent Schrödinger equation:

$$\left(\frac{p^2}{2m} + U(x)\right)\psi = \left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi = E\psi \tag{3.35}$$

To solve this equation, we consider that the solution must approach 0 for $x \to \pm\infty$: a possible function having this property is:

$$\psi(x) = Ae^{-ax^2} \tag{3.36}$$

with $a > 0$.

We can now insert this tentative form of $\psi(x)$ in the Schrödinger equation, to see if we can find a solution:

$$\begin{aligned} \left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi =& E\psi \\ \left(-\frac{\hbar^2}{2m}(-2aAe^{-ax^2} + 4a^2x^2Ae^{-ax^2}) + \frac{1}{2}m\omega^2x^2\right)Ae^{-ax^2} =& EAe^{-ax^2} \\ \frac{\hbar^2 a}{m} - \frac{2a^2\hbar^2}{m}x^2 + \frac{1}{2}m\omega^2x^2 =& E \\ \left(-\frac{2a^2\hbar^2}{m}x^2 + \frac{1}{2}m\omega^2\right)x^2 + \left(\frac{\hbar^2 a}{m} - E\right) =& 0 \end{aligned} \tag{3.37}$$

in order for $\psi(x) = Ae^{-ax^2}$ to be a solution, the equation above must be valid for any x, and so the following relations must be valid:

$$
\begin{aligned}
-\frac{2a^2\hbar^2}{m} + \frac{1}{2}m\omega^2 &= 0 \\
\frac{\hbar^2 a}{m} - E &= 0
\end{aligned}
$$

The result is:

$$a = \frac{m\omega}{2\hbar} \tag{3.38}$$

$$E = \frac{1}{2}\hbar\omega \tag{3.39}$$

This result means that the function $\psi_0(x) = Ae^{-ax^2} = Ae^{-\frac{m\omega}{2\hbar}x^2}$ is a state of the system with energy $E_0 = \frac{1}{2}\hbar\omega$. The index 0 that we have added comes from the fact that indeed this is the lowest energy state (or *ground state*) of the Harmonic Oscillator. We shall proof this statement in the following. The coefficient A can be found imposing the normalization condition on ψ_0:

$$\int_{-\infty}^{+\infty} |\psi_0(x)|^2 dx = 1$$

$$2A^2 \frac{1}{2}\sqrt{\frac{\pi\hbar}{m\omega}} = 1$$

$$\implies A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \implies \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \tag{3.40}$$

We can now reconsider equation 3.35 on the base of our new knowledge of quantum mechanics: we recognise that both $\hat{p}$ and $\hat{x}$ are operators corresponding to the observables momentum and position, respectively. In particular, it can be shown that the operator for the momentum p in one dimension is:

$$\hat{p} = -i\hbar\frac{d}{dx} \tag{3.41}$$

while in 3 dimensions is:

$$\hat{p} = -i\hbar\nabla \tag{3.42}$$

where, as usual, $\nabla := (\frac{\partial}{\partial x}; \frac{\partial}{\partial y}; \frac{\partial}{\partial z})$.

We can also identify in the Schrödinger equation above the *Hamiltonian* operator $\hat{H}$:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{3.43}$$

which allows us to write eq. 3.35 in the more compact form:

$$\hat{H}\psi = E\psi \tag{3.44}$$

which shows again that the quantized energy values of the system are simply the eigenvalues of the Hamiltonian operator.

The Hamiltonian 3.43 can also be written in a different form as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \frac{1}{2m}\left[\hat{p}^2 + (m\omega\hat{x}^2)\right] \tag{3.45}$$

which can be easily factorised defining two new operators:

$$\hat{a} := \frac{1}{\sqrt{2m\omega\hbar}}\left(m\omega\hat{x} + i\hat{p}\right) \qquad \textit{Annihilation Operator} \tag{3.46}$$

$$\hat{a}^\dagger := \frac{1}{\sqrt{2m\omega\hbar}}\left(m\omega\hat{x} - i\hat{p}\right) \qquad \textit{Creation Operator} \tag{3.47}$$

which are related to $\hat{x}$ and $\hat{p}$ by:

$$\hat{x} := \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \tag{3.48}$$

$$\hat{p} := -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^\dagger) \tag{3.49}$$

Using this two new operators, the Hamiltonian can be written as:

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger) \tag{3.50}$$

This expression can be further simplified using the commutator between $\hat{a}$ and $\hat{a}^\dagger$, which can be easily computed knowing the commutator between $\hat{x}$ and $\hat{p}$ (see Box 2.1):

$$\begin{aligned}
[\hat{a}, \hat{a}^\dagger] &= \frac{\hbar}{2m\omega}\left[(m\omega\hat{x} + i\hat{p})(m\omega\hat{x} - i\hat{p}) - (m\omega\hat{x} - i\hat{p})(m\omega\hat{x} + i\hat{p})\right] = \\
&= \frac{i}{2\hbar}\left[-\hat{x}\hat{p} + \hat{p}\hat{x} + \hat{p}\hat{x} - \hat{x}\hat{p}\right] = \\
&= \frac{i}{2\hbar}2\left[\hat{p}, \hat{x}\right] = \frac{i}{2\hbar}2(-i\hbar) = 1 \implies \hat{a}\hat{a}^\dagger = [\hat{a}, \hat{a}^\dagger] + \hat{a}^\dagger\hat{a} = 1 + \hat{a}^\dagger\hat{a}
\end{aligned} \tag{3.51}$$

Box 2.1 The Commutator between $\hat{x}$ and $\hat{p}$

In the following we shall explicitly compute the commutator between position and momentum $[\hat{p}, \hat{x}]$. To do this, let us apply the commutator to a generic function $f(x)$:

$$\begin{aligned}
[\hat{p}, \hat{x}]f(x) &= \left(-i\hbar\frac{d}{dx}\hat{x} + i\hbar\hat{x}\frac{d}{dx}\right)f(x) = \\
&= i\hbar\left(\hat{x}\frac{d}{dx} - \frac{d}{dx}\hat{x}\right)f(x) = \\
&= i\hbar\left(\hat{x}\frac{df(x)}{dx} - \frac{d}{dx}\left(\hat{x}f(x)\right)\right) = \\
&= i\hbar\left(\hat{x}\frac{df(x)}{dx} - \frac{d\hat{x}}{dx}f(x) - \hat{x}\frac{df(x)}{dx}\right) = \\
&= -i\hbar f(x) \implies [\hat{p}, \hat{x}] = -i\hbar
\end{aligned} \tag{3.52}$$

From the equations above we find that:

$$\begin{aligned}\hat{H} &= \frac{\hbar\omega}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger) \\ &= \frac{\hbar\omega}{2}(2\hat{a}^\dagger\hat{a} + 1) = \\ &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\end{aligned} \tag{3.53}$$

So now we can write eq.3.44 as:

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\psi = E\psi \implies \hat{a}^\dagger\hat{a}\psi = \left(\frac{E}{\hbar\omega} - \frac{1}{2}\right)\psi \tag{3.54}$$

which, defining the new operator $\hat{N} := \hat{a}^\dagger\hat{a}$, can be written as:

$$\hat{N}\psi = \left(\frac{E}{\hbar\omega} - \frac{1}{2}\right)\psi \tag{3.55}$$

The new operator $\hat{N}$ has the same eigenfunctions of the Hamiltonian $\hat{H}$, and eigenvalues given by $\left(\frac{E}{\hbar\omega} - \frac{1}{2}\right)$, which are simply related to the values of E.

From our initial treatment of the Quantum Harmonic Oscillator, we have affirmed that ground state of this system, ψ_0 has energy $E_0 = \frac{1}{2}\hbar\omega$. This is also the lowest value (or ground state value) for the eigenvalues of the Hamiltonian. From what we said above, ψ_0 is also an eigenfunction of $\hat{N}$, with eigenvalue $\left(\frac{E_0}{\hbar\omega} - \frac{1}{2}\right) = 0$, that is, the eigenvalue of $\hat{N}$ for the ground state is 0. On the other hand, having a negative value for the eigenvalues of $\hat{N}$ would give negative values for eigenvalues of the Hamiltonian, i.e. negative values of the energy, which are not allowed. Thus, 0 *is the lowest eigenvalue of* $\hat{N}$.

Now, before proceeding, let us compute some useful commutators between the new operators.

We start with the commutators $[\hat{N}, \hat{a}^\dagger]$ and $[\hat{N}, \hat{a}]$. Recalling the general rule for commutators:

$$[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}] \tag{3.56}$$

it is easy to see that:

$$\begin{aligned}\left[\hat{N}, \hat{a}^\dagger\right] &= [\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \\ &= [\hat{a}^\dagger, \hat{a}^\dagger]\hat{a} + \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] = \\ &= 0 \cdot \hat{a} + \hat{a}^\dagger \cdot 1 = \hat{a}^\dagger\end{aligned} \tag{3.57}$$

and:

$$\begin{aligned}\left[\hat{N}, \hat{a}\right] &= [\hat{a}^\dagger\hat{a}, \hat{a}] = \\ &= [\hat{a}^\dagger, \hat{a}]\hat{a} + \hat{a}^\dagger[\hat{a}, \hat{a}] = \\ &= -1 \cdot \hat{a} + \hat{a}^\dagger \cdot 0 = -\hat{a}\end{aligned} \tag{3.58}$$

Now, we compute the commutators $[\hat{H}, \hat{a}^\dagger]$ and $[\hat{H}, \hat{a}]$.

$$
\begin{aligned}
[\hat{H}, \hat{a}] &= [\hbar\omega(\hat{a}\hat{a}^\dagger - \frac{1}{2}), \hat{a}] = \\
&= \hbar\omega[\hat{a}\hat{a}^\dagger, \hat{a}] = \\
&= \hbar\omega(\hat{a}[\hat{a}^\dagger, \hat{a}] + [\hat{a}, \hat{a}]\hat{a}^\dagger) = -\hbar\omega\hat{a}
\end{aligned} \tag{3.59}
$$

and:

$$
\begin{aligned}
\left[\hat{H}, \hat{a}^\dagger\right] &= [\hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}), \hat{a}^\dagger] = \\
&= \hbar\omega[\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \\
&= \hbar\omega([\hat{a}^\dagger, \hat{a}^\dagger]\hat{a} + \hat{a}^\dagger[\hat{a}, \hat{a}]\hat{a}^\dagger) = \hbar\omega\hat{a}^\dagger
\end{aligned} \tag{3.60}
$$

Keeping in mind these results, let us see what happens if we apply in succession the two operators $\hat{a}^\dagger$ and $\hat{H}$ to ψ_o, the eigenfunction corresponding to the ground state energy of the Hamiltonian, $E_o = \frac{1}{2}\hbar\omega$:

$$
\begin{aligned}
\hat{H}\hat{a}^\dagger\psi_o &= \left(\left[\hat{H}, \hat{a}^\dagger\right] + \hat{a}^\dagger\hat{H}\right)\psi_o = \\
&= (\hbar\omega\hat{a}^\dagger + \hat{a}^\dagger E_o)\psi_o = \\
&= (\hbar\omega + E_o)\hat{a}^\dagger\psi_o
\end{aligned} \tag{3.61}
$$

These equations show that $\hat{a}^\dagger\psi_o$ is an eigenfunction of $\hat{H}$ with eigenvalue $(\hbar\omega + E_o)$, that is, it is a state with energy larger than E_o by a term $(\hbar\omega$.

If we apply again in succession $\hat{a}^\dagger$ and $\hat{H}$ to the new eigenfunction $\hat{a}^\dagger\psi_o$, we get:

$$
\begin{aligned}
\hat{H}\hat{a}^\dagger(\hat{a}^\dagger\psi_o) &= \left(\left[\hat{H}, \hat{a}^\dagger\right] + \hat{a}^\dagger\hat{H}\right)(\hat{a}^\dagger\psi_o) = \\
&= (\hbar\omega\hat{a}^\dagger + \hat{a}^\dagger\hat{H})(\hat{a}^\dagger\psi_o) = \\
&= (\hbar\omega + \hbar\omega + E_o)(\hat{a}^\dagger\hat{a}^\dagger\psi_o) = \\
\hat{H}(\hat{a}^\dagger\hat{a}^\dagger\psi_o) &= (2\hbar\omega + E_o)(\hat{a}^\dagger\hat{a}^\dagger\psi_o)
\end{aligned} \tag{3.62}
$$

Here we can se that again $\hat{a}^\dagger\hat{a}^\dagger\psi_o$ is an eigenfunction of $\hat{H}$ with an eigenvalue of energy $(2\hbar\omega + E_o)$. Again, the energy state of the oscillator has been increased by a quantity $\hbar\omega$. This can be generalized in the following way: every time that we apply the operator $\hat{a}^\dagger$ to a generic eigenfunction ψ_n of the generic energy level E_n, we increase the energy of the system by one step $\hbar\omega$, and the state of the system jumps to the next highest level. That is:

$$
\begin{aligned}
&\hat{H}\hat{a}^\dagger\psi_o = (\hbar\omega + E_o)\hat{a}^\dagger\psi_o = E_1\psi_1 \\
&\hat{H}\hat{a}^\dagger\psi_1 = \hat{H}(\hat{a}^\dagger\hat{a}^\dagger\psi_o) = (2\hbar\omega + E_o)\hat{a}^\dagger\hat{a}^\dagger\psi_o = (\hbar\omega + E_1)\hat{a}^\dagger\psi_1 = E_2\psi_2
\end{aligned}
$$

in general (3.63)

$$
\hat{H}\hat{a}^\dagger\psi_n = \hat{H}((\hat{a}^\dagger)^n\psi_o) = (n\hbar\omega + E_0)\hat{a}^\dagger\psi_n = (\hbar\omega + E_n)\hat{a}^\dagger\psi_n = E_{(n+1)}\psi_{(n+1)} \tag{3.64}
$$

So, we can conclude that:

$$
\hat{a}^\dagger\psi_n = C\psi_{n+1} \tag{3.65}
$$

where C is a constant that must be found imposing the usual normalization condition on each ψ_n: that is, the action of the operator $\hat{a}^\dagger$ is to rise the state of the system up by one energy level $\hbar\omega$.

Applying the same procedure we can find that:

$$\begin{aligned}
\hat{H}\hat{a}\psi_n &= \left([\hat{H},\hat{a}] + \hat{a}\hat{H}\right)\psi_n = \\
&= (-\hbar\omega\hat{a} + \hat{a}E_n)\psi_n = \\
&= (E_n - \hbar\omega +)\hat{a}\psi_n \implies \qquad (3.66)\\
&\implies \psi_{n-1} = \hat{a}\psi_n \qquad (3.67)
\end{aligned}$$

that is, the action of the operator $\hat{a}$ is to lower the state of the system down by one energy level $\hbar\omega$.

Resuming, if ψ_n are the eigenfunction of the energy operator $\hat{H}$ in the Schrödinger time independent equation $\hat{H}\psi_n = E_n\psi_n$, than their eigenvalues, that is the allowed energy states of the systems, E_n, are all separated by steps of energy $\hbar\omega$ and are given by $E_n = (n + \frac{1}{2})\hbar\omega$. The operator $\hat{a}^\dagger$ rises the state of the system by one step, that is, the state wave function changes from ψ_n to ψ_{n+1}, and the energy level changes from E_n to $E_{n+1} = E_n + \hbar\omega$. In the same way, the operator $\hat{a}$ lowers the state of the system by one step.

We can now also easily identify the physical quantity associated with the operator $\hat{N} := \hat{a}^\dagger\hat{a}$: this operator has the same eigenfunctions ψ_n of the Hamiltonian, and has eigenvalues given by $\left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right) = n$, **i.e. the quantum number giving the energy level of the system**.

We can now verify that indeed the solution of the Schrödinger Equation that we have found at the beginning of this chapter (3.60) is the wave function of the ground level of the system, that is the wave function for $n = 0$. To prove that, we argue that the action of the lowering operator $\hat{a}$ on the ground level eigenfunction must be 0, because no lower level is present, that is: $\hat{a}\psi_0 = 0$. If we write down this condition, using the explicit the form of $\hat{a}$, we get the equation:

$$\begin{aligned}
\hat{a}\psi_0 &= \frac{1}{\sqrt{2m\omega\hbar}}\left(m\omega\hat{x} + i\hat{p}\right)\psi_0 = 0 \\
&\implies \left(\frac{m\omega}{\hbar}x + \frac{d}{dx}\right)\psi_0 = 0 \qquad (3.68)
\end{aligned}$$

This equation can be solved separating the variables:

$$\begin{aligned}
\int \frac{d\psi_0}{\psi_0} &= -\int \frac{m\omega}{\hbar}xdx \\
\implies ln\psi_0 &= \frac{m\omega}{2\hbar}x^2 + C
\end{aligned} \qquad (3.69)$$

which indeed has the solution:

$$\psi_0(x) = Ae^{-\frac{m\omega}{2\hbar}x^2} \qquad (3.70)$$

where we obtain the solution that we found at the beginning of this chapter.

Having understood that $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$ is the ground state of our system, with eigenvalue $E_0 = \frac{1}{2}\hbar\omega$, we can now obtain all other eigenfunctions, with their eigenvalues, using the rising operator $\hat{a}^\dagger$.

Usually, the state $|\psi_n\rangle$ is simply written as $|n\rangle$, so that, for instance:

$$\hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle \tag{3.71}$$

Let us find with this simplified notation the normalization factors when $\hat{a}$ and $\hat{a}^\dagger$ are applied to $|n\rangle$. Let us start with $\hat{a}$. When applied to $|n\rangle$ we have: $\hat{a}|n\rangle = C_n |n-1\rangle$. with C_n a constant that keeps the new state function $|n-1\rangle$ normalized. Its value can be found considering that:

$$\begin{aligned}
&\hat{a}|n\rangle = \langle n| \hat{a}^\dagger \implies \\
&\implies \langle n| \hat{a}^\dagger \hat{a} |n\rangle = \\
&\quad = \langle n-1| C_n^* C_n |n-1\rangle = C_n^2 \langle n-1| |n-1\rangle = C_n^2
\end{aligned} \tag{3.72}$$

On the other hand, we can read $\hat{a}^\dagger \hat{a}$ in 3.72 as $\hat{N}$:

$$\begin{aligned}
&\langle n| \hat{a}^\dagger \hat{a} |n\rangle = \\
&\langle n| \hat{N} |n\rangle = n \langle n| |n\rangle = n
\end{aligned} \tag{3.73}$$

which finally gives:

$$\begin{aligned}
&\langle n| \hat{a}^\dagger \hat{a} |n\rangle = C_n^2 = n \implies \\
&\implies C_n = \sqrt{n}
\end{aligned} \tag{3.74}$$

The same procedure can be used to find the normalization constant in $\hat{a}^\dagger |n\rangle = C_n^{'} |n+1\rangle$. However, knowing 3.74 and 3.71, a simpler method can now be used:

$$\begin{aligned}
\hat{a}^\dagger \hat{a} |n\rangle &= n |n\rangle \\
\hat{a}^\dagger \sqrt{n} |n-1\rangle &= n |n\rangle \\
\hat{a}^\dagger |n-1\rangle &= \sqrt{n} |n\rangle \implies \\
\implies \hat{a}^\dagger |n\rangle &= \sqrt{n+1} |n+1\rangle
\end{aligned} \tag{3.75}$$

To resume:

$$\hat{a}|n\rangle = \sqrt{n} |n-1\rangle \tag{3.76}$$

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \tag{3.77}$$

$$\hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle \tag{3.78}$$

3.2.1 Quantum Computation with a Quantum Harmonic Oscillator

In the following we shall see how to use the quantum states of a harmonic oscillator to perform a C-NOT quantum gate. First of all, we perform the following encoding of *Logical* states (with subscript L) to the physical states of the harmonic oscillator:

$$\begin{aligned}
|00\rangle_L &= |0\rangle \\
|01\rangle_L &= |2\rangle \\
|10\rangle_L &= (|4\rangle + |1\rangle)/\sqrt{2} \\
|11\rangle_L &= (|4\rangle - |1\rangle)/\sqrt{2}
\end{aligned} \tag{3.79}$$

To perform a C-NOT on the logical states above, we must implement the transformations:

$$\begin{aligned}
|00\rangle_L &\rightarrow |00\rangle_L \\
|01\rangle_L &\rightarrow |01\rangle_L \\
|10\rangle_L &\rightarrow |10\rangle_L \\
|11\rangle_L &\rightarrow |10\rangle_L
\end{aligned} \tag{3.80}$$

This is possible, if we make, for instance, the states ref eq:HOHam16 evolve with time until $t = \pi/\omega$.

According to **??** the time evolution of the state $|n\rangle$ can be written as:

$$|n(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t} |n(0)\rangle \tag{3.81}$$

substituting for $t = \pi/\omega$ we have:

$$|n(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}\frac{\pi}{\omega}} |n(0)\rangle \tag{3.82}$$

We can substitute for $\hat{H}$ the expression 3.53:

$$\begin{aligned}
|n(t)\rangle &= e^{-\frac{i}{\hbar}\hat{H}\frac{\pi}{\omega}} |n(0)\rangle \\
&= e^{-\frac{i}{\hbar}\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\frac{\pi}{\omega}} |n(0)\rangle \\
&= e^{-i\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\pi} |n(0)\rangle \\
&= e^{-i\left(n+\frac{1}{2}\right)\pi} |n(0)\rangle = \\
&= e^{-i\frac{1}{2}\pi}e^{-ni\pi} |n(0)\rangle = \\
&= (-1)^n |n\rangle
\end{aligned} \tag{3.83}$$

where we have recalled that $\hat{a}^\dagger\hat{a}\,|n\rangle = n\,|n\rangle$ and we have neglected the overall phase factor $e^{-i\pi/2}$.

It is easy to see that in this evolution the states with n even, that is $|0\rangle$, $|2\rangle$, $|4\rangle$ are not changed, while we have: $|1\rangle \rightarrow -|1\rangle$, verifying the transformations in 3.80

3.3 Quantum Annealing

3.4 IBM Quantum Computer