Chapter 5
Variational Quantum Algorithms

This class of algorithms employs a quantum and a classical computer to solve some optimisation problems. The quantum computer performs the quantum evolution of a state with respect to an Hamiltonian that is transformed, say from $\hat{H}_0$ to $\hat{H}_1$. The classical computer determines how such a transformation should take place employing the variational principle. Typically, the problem is to map the state from the ground state of $\hat{H}_0$ to that of $\hat{H}_1$, whose ground state is unknown. Thus, one wants to have a well-known $\hat{H}_0$. This is often taken as that of the Ising model.

5.1 The Ising model

In a combinatorial optimisation problem, one has a string of n bits and wants to optimise a particular problem. The problem is mapped in a minimisation (or maximisation) of a cost function $C : \{ 0, 1 \}^n \to \mathbb{R}$. Notably, the maximisation problem can be obtained from the minimisation one buy a minus sign: $C \to -C$.

To solve a combinatorial optimisation problem via a quantum algorithm, one needs to encode the problem onto a quantum system. In the following, we show how the Ising Hamiltonian can be used to embed such an optimisation problem.

The Ising model was developed to study the phase transition in magnetic materials. It consists in n spins that can be coupled via long-range interactions. The corresponding Hamiltonian is

$$\hat{H}_{\mathrm{C}} = -\sum_{i=1}^{n} h_i \hat{\sigma}_z^{(i)} - \sum_{1 \leq i < j \leq n} J_{ij} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)}, \tag{5.1}$$

where h_i are the single spin magnetic fields describing the single spin evolution and J_{ij} the spin-spin couplings. The choice of the latter encodes if the spins are encouraged to be aligned (ferromegnetic phase) or anti-aligned (antiferromagnetic phase). Since only $\hat{\sigma}_z$ are appearing in $\hat{H}_{\mathrm{C}}$, then its spectral decomposition can be expressed in the computational basis:

$$\hat{H}_{\mathrm{C}} = \sum_{z=0}^{2^n - 1} C(z) \left| z \right\rangle \left\langle z \right|, \tag{5.2}$$

where $C(z)$ is the energy of the specific spin configuration $|z\rangle$. Then, by properly mapping a combinatorial problem in the choice of $\{ h_i \}$ and $\{ J_{ij} \}$, one can find the optimal solution by minimizing the energy, i.e. by finding the configuration $|z\rangle$ that corresponds to minimal energy (or cost) $C(z)$.

5.2 Mapping combinatorial optimisation problems into the Ising model

Many problems can be mapped in the form in Eq. (5.1), and hence solve with a quantum computer, by choosing the appropriate values of $\{ h_i \}$ and $\{ J_{ij} \}$. Here we consider some explicit examples.

Subset sum problem. Given an integer number m (total value) and a set of N positive and negative integers $n = \{ n_1, \dots, n_N \}$, which is the subset of the latter integers whose sum gives m?

Example 5.1
Consider the case of $m = 7$ *and* $n = \{ -5, -3, 1, 4, 9 \}$. *The subset* $\{ -3, 1, 9 \}$ *solves the problem:* $-3+1+9 = 7 = m$.

Exercise 5.1
Consider the case of $m = 13$ *and* $n = \{ -3, 2, 8, 4, 20 \}$. *Show that the corresponding subset sum problem has no solution.*

The subset sum problem can be framed as an energy minimisation problem as follows. Consider the sum $\sum_{i=1}^{N} n_i z_i - m$, where n_i are the elements of n and $z_i \in \{ 0, 1 \}$ are weights that select or not the corresponding element n_i in the sum (effectively, this is the way to select a specific subsection). We define $\mathcal{E}(z)$ as the square of such a sum:

$$\mathcal{E}(z) = \mathcal{E}(z_1, \dots, z_N) = \left(\sum_{i=1}^{N} n_i z_i - m \right)^2 . \tag{5.3}$$

Then, if there is a subset solving the problem, one has that exists a value of $z = \{ z_1, \dots, z_N \}$ such that $\mathcal{E}(z) = 0$. Conversely, if all the possible values of z give $\mathcal{E}(z) \neq 0$, then there is no subset that can solve the subset sum problem. One can already see that the z corresponding to the solution of the problem is the one minimising $\mathcal{E}(z)$. We now show the connection with the Ising model. We introduce the classical spins $s_i = \pm 1$, which will be employed in place of the weights z_i. Namely, one uses

$$z_i = \tfrac{1}{2}(1 - s_i), \tag{5.4}$$

so that $s_i = +1$ (spin up) corresponds to $z_i = 0$ and $s_i = -1$ (spin down) to $z_i = 1$. We define the corresponding classical Hamiltonian

$$\begin{aligned} \mathcal{H}(s_1, \dots, s_N) &= \left(\sum_{i=1}^{N} n_i \tfrac{1}{2}(1 - s_i) - m \right)^2 , \\ &= \tfrac{1}{4} \sum_{i,j=1}^{N} n_i n_j s_i s_j - \sum_{i=1}^{N} \left(\tfrac{1}{2} \sum_{j=1}^{N} n_j - m \right) n_i s_i + \left(\tfrac{1}{2} \sum_{i=1}^{N} n_i - m \right)^2 , \end{aligned} \tag{5.5}$$

where the last term is independent from s_i and thus is a negligible constant of the problem. After having defined

$$J_{ij} = -\frac{n_i n_j}{4}, \quad \text{and} \quad h_i = \left(\tfrac{1}{2} \sum_{j=1}^{N} n_j - m \right) n_i, \tag{5.6}$$

the Hamiltonian becomes

$$\mathcal{H}(s_1, \dots, s_N) = - \sum_{1 \leq i < j \leq n} J_{ij} s_i s_j - \sum_{i=1}^{n} h_i s_i + \text{const}, \tag{5.7}$$

where

$$\text{const} = \left(\tfrac{1}{2} \sum_{i=1}^{N} n_i - m \right)^2 - \sum_{i=1}^{N} J_{ii} s_i^2, \tag{5.8}$$

is s_i independent since $s_i^2 = 1$ for any value of i. To solve the problem on a quantum computer, one quantises the Hamiltonian in Eq. (5.7) by substituting $s_i \to \hat{\sigma}_z^{(i)}$ and gets Eq. (5.1).

Number partitioning problem. Another combinatory problem that can be mapped in an Ising Hamiltonian is the number partitioning problem. It asks if a set of N integers $\{ n_1, \ldots, n_N \}$ can be partitioned in two subsets such that the sum of the elements in the individual subsets is equal.

> ***Example 5.2***
> *Consider the set* $n = \{ 1, 2, 3, 4, 6, 10 \}$. *In such a case, one can consider the case of* $\{ 1, 2, 4, 6 \}$ *and* $\{ 3, 10 \}$, *whose individual sums are both equal to 13.*

The classical Hamiltonian for this problem can be straightforwardly constructed as

$$\mathcal{H}(s_1, \ldots, s_N) = \left(\sum_{i=1}^{N} n_i s_i \right)^2, \tag{5.9}$$

with $s_i = \pm 1$. Clearly, the solution $s = \{ s_1, \ldots, s_N \}$ is such that $\mathcal{H}(s) = 0$. Expanding the square, we find

$$\mathcal{H}(s) = - \sum_{1 \leq i < j \leq N} J_{ij} s_i s_j - \text{Tr}\left[J_{ij} \right], \tag{5.10}$$

where

$$J_{ij} = -\frac{n_i n_j}{2}, \quad \text{and} \quad \text{Tr}\left[J_{ij} \right] = \sum_{i=1}^{N} J_{ii} s_i^2. \tag{5.11}$$

The classical Hamiltonian in Eq. (5.10) can be quantised and one obtains that in Eq. (5.1) with no need to introduce the magnetic fields, i.e. $h_i = 0$.

5.3 Adiabatic Theorem

Adiabatic quantum computation is based on the adiabatic theorem. The latter considers the case of a time dependent Hamiltonian, that changes from $\hat{H}_0$ at time $t = 0$ to $\hat{H}_1$ at time $t = \tau$. We also assume that the two Hamiltonians do not commute, i.e.$[\hat{H}_0, \hat{H}_1] \neq 0$. The theorem states that a system prepared in the n-th eigeinstate of $\hat{H}_0$ goes in the n-th eigeinstate of $\hat{H}_1$ if the transformation is made slowly enough, i.e. adiabatically. The application to quantum computation then is to take an initial Hamiltonian with a ground state that can be easily prepared and then adiabatically change the Hamiltonian to that of the problem one wants to optimise. If the system is initially in the ground state of $\hat{H}_0$, then will remain in the ground state of the target Hamiltonian $\hat{H}_1$ and it will encode the solution of the optimisation problem.

The proof of the adiabatic theorem is the following. Consider the instantaneous spectralisation of a time-dependent Hamiltonian $\hat{H}(t)$, which is

$$\hat{H}(t) \left| n(t) \right\rangle = E_n(t) \left| n(t) \right\rangle, \tag{5.12}$$

where $E_n(t)$ and $|n(t)\rangle$ are respectively the corresponding instantaneous eigeinvalues and eigeinstates. Given a state $|\psi(t)\rangle$ at time t, one can always express it as a superposition of the instantaneous eigeinstates as

$$\left| \psi(t) \right\rangle = \sum_n c_n(t) \left| n(t) \right\rangle, \tag{5.13}$$

where

$$c_n(t) = \langle n(t)|\psi(t)\rangle\,, \tag{5.14}$$

determine the probabilities $P_n(t) = |c_n(t)|^2$ of being in $|n(t)\rangle$ at time t. The evolution of $c_n(t)$ can be determined via

$$\begin{aligned}\dot{c}_n(t) &= \langle \dot{n}(t)|\psi(t)\rangle + \langle n(t)|\dot{\psi}(t)\rangle\,,\\ &= \langle \dot{n}(t)|\psi(t)\rangle - \tfrac{i}{\hbar}\langle n(t)|\hat{H}(t)|\psi(t)\rangle\,,\\ &= \langle \dot{n}(t)|\psi(t)\rangle - \tfrac{i}{\hbar}E_n(t)\langle n(t)|\psi(t)\rangle\,,\end{aligned} \tag{5.15}$$

where we defined $|\dot{n}(t)\rangle = \frac{\mathrm{d}}{\mathrm{d}t}|n(t)\rangle$, and we applied the Schrödinger equation and applied the Hamiltonian to its eigeinstate. Then, the imposing Eq. (5.13), we get

$$\dot{c}_n(t) = \sum_m c_m(t)\langle \dot{n}(t)|m(t)\rangle - \tfrac{i}{\hbar}E_n(t)c_n(t), \tag{5.16}$$

which determines a system of coupled differential equations. In complete generality, the evolution of $c_n(t)$ depends on $c_m(t)$ for all values of m. To determine the first term of Eq. (5.16), we consider the time derivative of Eq. (5.12) with $|n(t)\rangle$ subsituted with $|m(t)\rangle$ and projecting it on $\langle n(t)|$. This gives

$$\langle n(t)|\tfrac{\mathrm{d}}{\mathrm{d}t}\hat{H}(t)|m(t)\rangle + \langle n(t)|\hat{H}|\dot{m}(t)\rangle = \dot{E}_m(t)\delta_{nm} + E_m(t)\langle n(t)|\dot{m}(t)\rangle\,, \tag{5.17}$$

which can be recasted as

$$(E_n(t) - E_m(t))\langle n(t)|\dot{m}(t)\rangle = \dot{E}_m(t)\delta_{nm} - \langle n(t)|\tfrac{\mathrm{d}}{\mathrm{d}t}\hat{H}(t)|m(t)\rangle\,. \tag{5.18}$$

For $m \neq n$, one then has

$$\langle \dot{n}(t)|m(t)\rangle = \frac{\langle n(t)|\frac{\mathrm{d}}{\mathrm{d}t}\hat{H}(t)|m(t)\rangle}{(E_n(t) - E_m(t))}, \tag{5.19}$$

where we exploited that $\langle \dot{n}(t)|m(t)\rangle = -\langle n(t)|\dot{m}(t)\rangle$. Thus, by separating the case of $m = n$ and $m \neq n$ in Eq. (5.16), we have

$$\dot{c}_n(t) = \left(\langle \dot{n}(t)|n(t)\rangle - \tfrac{i}{\hbar}E_n(t)\right)c_n(t) + \sum_{m\neq n} c_m(t)\frac{\langle n(t)|\frac{\mathrm{d}}{\mathrm{d}t}\hat{H}(t)|m(t)\rangle}{(E_n(t) - E_m(t))}. \tag{5.20}$$

In the limit where the Hamiltonian $\hat{H}(t)$ changes slowly enough, i.e. for $\langle n(t)|\frac{\mathrm{d}}{\mathrm{d}t}\hat{H}(t)|m(t)\rangle \ll (E_n(t) - E_m(t))$ for all n and m, then one can neglect the last term in Eq. (5.20). This is the so-called adiabatic approximation, which gives the following solutions

$$c_n(t) = e^{i\theta_n(t)}e^{i\gamma_n(t)}c_n(0), \tag{5.21}$$

where we defined

$$\theta_n(t) = -\tfrac{1}{\hbar}\int_0^t \mathrm{d}s\, E_n(s), \quad \text{and} \quad \gamma_n(t) = -i\int_0^t \mathrm{d}s\,\langle \dot{n}(s)|n(s)\rangle\,. \tag{5.22}$$

In particular, $\gamma_n(t) \in \mathbb{R}$ is known as the Berry phase.

Importantly, under the adiabatic approximation, one has that the probabilities evolve as

$$P_n(t) = |c_n(t)|^2 = |c_n(0)|^2 = P_n(0), \tag{5.23}$$

which is the final proof of the theorem.

Remark 5.1. It is important to understand the limits in which the adiabatic approximation is valid. To prove it in complete generality, one should require that the time-scale τ of the transformation is such that

$$\tau \gg \max_{n\neq m} \max_{0\leq t\leq \tau} \left| \frac{\langle n(t)| \frac{\mathrm{d}}{\mathrm{d}t} \hat{H}(t) |m(t)\rangle}{(E_n(t) - E_m(t))} \right|. \tag{5.24}$$

For the perspective of quantum computation, one can restrict to the case of $n = 0$ and $m = 1$. This is the case where the system is initially prepared in the ground state $n = 0$ and one does not want a jump in the first excited state $m = 1$. In such a case, the approximation is valid if

$$\tau \gg \max_{0\leq t\leq \tau} \left| \frac{\langle \psi_0(t)| \frac{\mathrm{d}}{\mathrm{d}t} \hat{H}(t) |\psi_1(t)\rangle}{(E_0(t) - E_1(t))} \right|. \tag{5.25}$$

Notably, the more the energy gap $E_1 - E_0$ closes, the larger value of τ one has to consider. In the case of a linear transition between the initial $\hat{H}_0$ and final Hamiltonian $\hat{H}_1$ (i.e. $\hat{H}(t) = (1-t/\tau)\hat{H}_0 + t/\tau \hat{H}_1$), a necessary condition for keeping the energy gap open is that $[\hat{H}_0, \hat{H}_1] \neq 0$. Figure 5.1 represents graphically how the gap should remain open during the Hamiltonian change so that the initial state being the ground state of $\hat{H}_0$ is mapped to the ground state of $\hat{H}_1$, which encodes the solution of the problem.

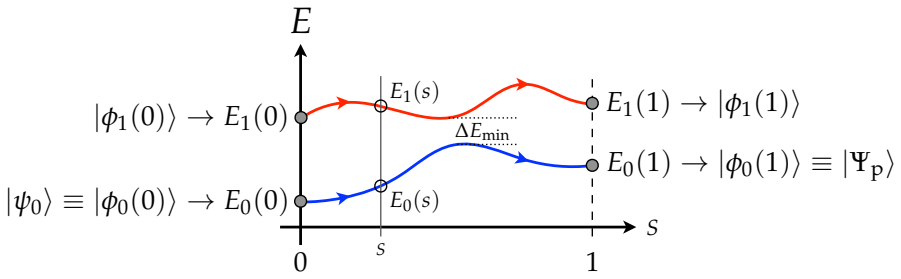

Fig. 5.1: Graphical representation of how the energy levels of $\hat{H}(t)$ change in time. As long as the minimum energy gap $\Delta E_{\min}$ is finite, one can employ the adiabatic theorem to go from the ground state of $\hat{H}_0$ (here denoted as $|\psi_0\rangle$) to that of $\hat{H}_1$ ($|\Psi_p\rangle$). Here, we used the parameter s to parametrise the time flow: $t = s\tau$.