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Tutorial 6

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Problem 1

Consider a 2-dimensional Hamiltonian $\mathcal{H}$, where $|+_{\frac{\pi}{4}}\rangle$ is the eigenvector with 0 eigenvalue and $|-_{\frac{\pi}{4}}\rangle$ is the other eigenvector with eigenvalue 1. Recall that you can always write an operator as the sum of the product of an eigenvalue with the projection to the corresponding eigenspace.

a. Write the Hamiltonian in terms of the eigenvectors and in matrix form (in the computational basis).

Solution:

$$H = \mathbf{0}\,|+_{\frac{\pi}{4}}\rangle\langle+_{\frac{\pi}{4}}| + \mathbf{1}\,|-_{\frac{\pi}{4}}\rangle\langle-_{\frac{\pi}{4}}| = |-_{\frac{\pi}{4}}\rangle\langle-_{\frac{\pi}{4}}| = \frac{1}{2}\begin{pmatrix} 1 & -e^{-i\frac{\pi}{4}} \\ -e^{i\frac{\pi}{4}} & 1 \end{pmatrix}$$

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b. Express $\mathcal{H} = \sum_i c_i P_i$ in terms of Pauli matrices ($P_i \in \{I, X, Y, Z\}$) using the formula for calculating the coefficients c_i given in the lecture, and for simplicity here too: $c_i = \langle P_i, \mathcal{H}\rangle$, where $\langle A, B\rangle := \frac{Tr(A^\dagger B)}{2}$.

Solution:

$$\mathcal{H} = \sum_{i=0}^{3} \alpha_i P_i = \alpha_0 I + \alpha_1 X + \alpha_2 Y + \alpha_3 Z$$

To calculate the α_i coefficients, we use the above formula:

$$\alpha_0 = \langle I, \mathcal{H}\rangle = \frac{Tr(\mathcal{H})}{2} = \frac{1}{2}$$

$$\alpha_1 = \langle X, \mathcal{H}\rangle = \frac{Tr(X\,|-_{\frac{\pi}{4}}\rangle\langle-_{\frac{\pi}{4}}|)}{2} = \frac{1}{2}(\langle-_{\frac{\pi}{4}}|\,X\,|-_{\frac{\pi}{4}}\rangle)$$

$$\langle-_{\frac{\pi}{4}}|\,X\,|-_{\frac{\pi}{4}}\rangle = \frac{1}{2}(\langle 0| - e^{-i\frac{\pi}{4}}\langle 1|)(|1\rangle - e^{i\frac{\pi}{4}}|0\rangle) = \frac{1}{2}(-e^{i\frac{\pi}{4}} - e^{-i\frac{\pi}{4}}) = -\cos\frac{\pi}{4} = -\frac{\sqrt{2}}{2}$$

And the coefficient is:

$$\alpha_1 = -\frac{\sqrt{2}}{4}$$

For the Z operator we have:

$$Z\,|-_{\frac{\pi}{4}}\rangle = |+_{\frac{\pi}{4}}\rangle$$

We can calculate the fourth coefficient:

$$\alpha_3 = \langle Z, \mathcal{H}\rangle = \frac{Tr(Z\,|-_{\frac{\pi}{4}}\rangle\langle-_{\frac{\pi}{4}}|)}{2} = \frac{1}{2}(\langle-_{\frac{\pi}{4}}|\,Z\,|-_{\frac{\pi}{4}}\rangle) = \frac{1}{2}(\langle-_{\frac{\pi}{4}}|+_{\frac{\pi}{4}}\rangle) = 0$$

Finally, for Pauli $Y = -iZX$ we have:

$$\alpha_2 = \langle Y, \mathcal{H} \rangle = \frac{Tr(-iZX \left|-\tfrac{\pi}{4}\right\rangle \left\langle -\tfrac{\pi}{4}\right|)}{2} = \frac{-i}{2}(\left\langle -\tfrac{\pi}{4}\right| ZX \left|-\tfrac{\pi}{4}\right\rangle) = \frac{-i}{2\sqrt{2}}(\left\langle -\tfrac{\pi}{4}\right| Z(|1\rangle - e^{i\frac{\pi}{4}} |0\rangle))$$

$$\alpha_2 = \frac{-i}{4}(\langle 0| - e^{-i\frac{\pi}{4}} \langle 1|)(-|1\rangle - e^{i\frac{\pi}{4}} |0\rangle) = \frac{i}{4}(e^{i\frac{\pi}{4}} - e^{-i\frac{\pi}{4}}) = \frac{i}{4}(2i \sin\frac{\pi}{4}) = -\frac{\sin\frac{\pi}{4}}{2} = -\frac{\sqrt{2}}{4}$$

So the decomposition of the Hamiltonian will be:

$$\mathcal{H} = \frac{1}{2}(I - \frac{\sqrt{2}}{2}(X + Y))$$

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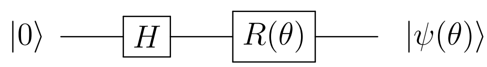
c. Evaluate the output state $|\psi(\theta)\rangle$ given by the following parametrised circuit :



Solution: The output of the circuit can be evaluated as follows:
After the first Hadamard gate, the $|0\rangle$ state will be transformed to $|+\rangle$. Then, by performing the $R(\theta)$ gate, we will have:

$$|\psi(\theta)\rangle = R(\theta)|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\theta}|1\rangle)$$

d. For any state express $E(\theta) := \langle\psi(\theta)| \mathcal{H} |\psi(\theta)\rangle$ by using part b, in terms of $\langle\psi(\theta)| P_i |\psi(\theta)\rangle$.
Solution:

$$E(\theta) = \langle\psi(\theta)| \mathcal{H} |\psi(\theta)\rangle = \frac{1}{4}\langle\psi(\theta)| (2I + (-\sqrt{2})(X+Y)) |\psi(\theta)\rangle =$$
$$\frac{1}{4}(2 + (-\sqrt{2})(\langle\psi(\theta)| X |\psi(\theta)\rangle + \langle\psi(\theta)| Y |\psi(\theta)\rangle))$$

First, note that $\sqrt{2}$ can be written as:

$$\sqrt{2} = 2\cos\frac{\pi}{4} = 2\sin\frac{\pi}{4}$$

Then, the expectation values of X and Y are:

$$\langle\psi(\theta)| X |\psi(\theta)\rangle = \frac{1}{2}(e^{-i\theta} + e^{i\theta}) = \cos\theta$$
$$\langle\psi(\theta)| Y |\psi(\theta)\rangle = \frac{-i}{2}(e^{i\theta} - e^{-i\theta}) = \sin\theta$$

If we replace the above equations in the expectation value $E(\theta)$, we get:

$$E(\theta) = \frac{1}{4}[2 - 2(\cos\theta\cos\frac{\pi}{4} + \sin\theta\sin\frac{\pi}{4})] = \frac{1-\cos(\theta - \frac{\pi}{4})}{2}$$

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e. Now find the ground state with the following steps:

- Start from $\theta_0 = 0$
- Estimate the gradient in each step using $\Delta(\theta_i) = E(\theta_i + \delta\theta) - E(\theta_i - \delta\theta)$ where $\delta\theta = \frac{\pi}{8}$
- Update θ accordingly by moving in the opposite direction of the gradient by a step $\delta\theta$, i.e. set $\theta_1 = \theta_0 \pm \delta\theta$ with the sign determined by the computed gradient
- Continue this for another two steps and find the value of θ which minimises $\langle\mathcal{H}\rangle$.

Solution: For $\theta_0 = 0$ and $\delta\theta = \frac{\pi}{8}$

$$\Delta(\theta_0) = E(\frac{\pi}{8}) - E(-\frac{\pi}{8}) = \frac{1}{2}(cos(\frac{\pi}{8} - \frac{\pi}{4}) - \cos(-\frac{\pi}{8} - \frac{\pi}{4})) = \frac{1}{2}(\cos(\frac{3\pi}{8}) - \cos(\frac{\pi}{8})) \approx -0.27$$

The gradient is negative. We move in the opposite direction of the gradient, so we need to go to larger values of θ. We update the θ as:

$$\theta_1 = \theta_0 + \delta\theta = \frac{\pi}{8}$$

Now we repeat the last step for θ_1 and we calculate the gradient:

$$\Delta(\theta_1) = E(\frac{\pi}{8} + \frac{\pi}{8}) - E(\frac{\pi}{8} - \frac{\pi}{8}) = E(\frac{\pi}{4}) - E(0) = \frac{1}{2}(-\cos(0) + \cos(-\frac{\pi}{4})) = \frac{1}{2}(-1 + \frac{\sqrt{2}}{2})$$

Again, the gradient is negative, so we update the θ with the larger value. The next θ is:

$$\theta_2 = \theta_1 + \delta\theta = \frac{\pi}{8} + \frac{\pi}{8} = \frac{\pi}{4}$$

And the gradient is:

$$\Delta(\theta_2) = E(\frac{\pi}{4} + \frac{\pi}{8}) - E(\frac{\pi}{4} - \frac{\pi}{8}) = E(\frac{3\pi}{8}) - E(\frac{\pi}{8}) = \frac{1}{2}(-\cos(\frac{\pi}{8}) + \cos(-\frac{\pi}{8})) = 0$$

The gradient is zero and we have found the minimum. $\theta = \frac{\pi}{4}$ minimizes the energy. This can also be checked by taking the derivation of $E(\theta)$ and finding the minimum value of the function.

Problem 2

Consider the cost function of a Binary Optimisation problem with up to cubic terms:

$$C(x) = \sum_i a_i x_i + \sum_{i,j} b_{ij} x_i x_j + \sum_{i,j,k} c_{ijk} x_i x_j x_k$$

Each of x_i is a binary variable $x_i \in \{0, 1\}$, and the index i runs from 1 to n. Finding the configuration with the smallest cost gives a general cubic, n-binary-variables optimisation problem. For a number of reasons, one may be interested in turning this problem to a Quadratic Unconstrained Binary Optimisation (QUBO) problem, i.e. restricting the cost function to a cost function that has at most quadratic terms (but no cubic terms).

a. Let $g(x, y) := (2 - x_i - x_j - x_k)y = 2y - x_i y - x_j y - x_k y$, where $y \in \{0, 1\}$ is another, new, binary variable. Show that the following functions are the same:

$$\begin{aligned} f(x) &= -x_i x_j x_k \\ &= \min_y g(x, y) \end{aligned}$$

This proves that we can replace cubic terms $-x_i x_j x_k$ with quadratic ones $(2 - x_i - x_j - x_k)y$ with the cost of introducing (in this case a single) extra variable y. Note, that we are interested in the minimum value of the cost function (i.e. we are taking the minimum of this expression over all binary variables, including the newly introduced y).

Solution: We will prove that for every possible configuration $x_i x_j x_k$ with $x_i \in \{0, 1\}$ the two functions above are equivalent. Let $x = (x_i, x_j x_k)$, then:

$$\begin{aligned}
x = (0,0,0) &\implies f(x) = 0 \text{ and } \min_y g(x,y) = \min_y 2y = 0 \\
x = (0,0,1) &\implies f(x) = 0 \text{ and } \min_y g(x,y) = \min_y (2y - y) = 0 \\
x = (0,1,0) &\implies f(x) = 0 \text{ and } \min_y g(x,y) = \min_y (2y - y) = 0 \\
x = (0,1,1) &\implies f(x) = 0 \text{ and } \min_y g(x,y) = \min_y (2y - y - y) = 0 \\
x = (1,0,0) &\implies f(x) = 0 \text{ and } \min_y g(x,y) = \min_y (2y - y) = 0 \\
x = (1,0,1) &\implies f(x) = 0 \text{ and } \min_y g(x,y) = \min_y (2y - y - y) = 0 \\
x = (1,1,0) &\implies f(x) = 0 \text{ and } \min_y g(x,y) = \min_y (2y - y - y) = 0 \\
x = (1,1,1) &\implies f(x) = -1 \text{ and } \min_y g(x,y) = \min_y (2y - y - y - y) = -1
\end{aligned}$$

Intuitively, we see that unless $x_i = x_j = x_k = 1$ the term $(2 - x_i - x_j - x_k)$ is non-negative, thus it is minimised when we multiply it with $y = 0$ giving cost 0 in agreement with the product of $-x_i x_j x_k$ (since at least one of the variables is zero). In the case that $x_i = x_j = x_k = 1$, then $(2 - x_i - x_j - x_k)$ is -1 and thus we get minimum when $y = 1$, leading to total cost of -1, again in agreement with $-x_i x_j x_k$ for the same case.

So we can see that we can replace every term $-x_i x_j x_k$ with quadratic ones $\min_y(2 - x_i - x_j - x_k)y$ with the cost of introducing (in this case a single) extra variable y. By doing so, we can reduce any cubic binary optimisation problem to a quadratic one.

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b. Find how we reduce the order of a cost function that has fourth order terms of the form $x_i x_j x_k x_l$ and make it quadratics (i.e. an expression with at most quadratic terms).

Solution: We define a new function $h(x, y) := (3 - x_i - x_j - x_k - x_l)y$. It's easy to see that:

$$\min_y h(x, y) = -x_i x_j x_k x_l$$

In fact, we can generalise and replace every term with n binary variables $-x_0 \dots x_{n-1}$ with the function:

$$h(x, y) = \left[(n - 1) - \sum_{i=0}^{n-1} x_i\right] y$$

that has only up to quadratic terms. Then:

$$\min_y h(x, y) = -x_0 \dots x_{n-1}$$

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c. Consider the cost function:

$$C(x) = -5x_1x_2x_3x_4 + x_2 + 2x_3$$

Using the result of b. reduce the order to quadratic. Then change the variables to spins using this $x_i = \frac{1-s_i}{2}$. Construct a Hamiltonian $\mathcal{H}_C$ by replacing each spin variable s_i with the Pauli Z_i gate. Finally, calculate the expectation value $\langle\psi| \mathcal{H}_C |\psi\rangle$ of the state $|\psi\rangle$ if $|\psi\rangle = a|00000\rangle + b|01011\rangle$ where the last qubit denotes the extra qubit, i.e. $|s_1 s_2 s_3 s_4 y\rangle$.

Solution: We start by mapping the cost function $C(x)$ to the cost function $C(x, y)$ by introducing an extra bit y and replacing the term $-5x_1x_2x_3x_4$:

$$C(x) \to C(x, y) = 5(3 - x_1 - x_2 - x_3 - x_4)y + x_2 + 2x_3$$
$$\implies C(x, y) = 15 - 5x_1y - 5x_2y - 5x_3y - 5x_4y + x_2 + 2x_3$$

Now, we can change every binary variable x_i to a spin variable s_i where $x_i = \frac{1-s_i}{2}$, i.e.:

$$C(s, s_y) = \frac{23}{2} + 5s_y + \frac{5}{4}s_1 + \frac{3}{4}s_2 + \frac{1}{4}s_3 + \frac{5}{4}s_4 - \frac{5}{4}(s_1 s_y + s_2 s_y + s_3 s_y + s_4 s_y)$$

Now, we can construct a Hamiltonian $\mathcal{H}_C$ by replacing each variable s_i with the Pauli Z_i gate. Thus:

$$\mathcal{H}_C = \frac{23}{2} + 5Z_y + \frac{5}{4}Z_1 + \frac{3}{4}Z_2 + \frac{1}{4}Z_3 + \frac{5}{4}Z_4 - \frac{5}{4}(Z_1 Z_y + Z_2 Z_y + Z_3 Z_y + Z_4 Z_y)$$

Recall that for a computational basis state $|x\rangle$, $Z|x\rangle = (-1)^x |x\rangle$. Initially, we will find the expectation value of the state $|00000\rangle$:

$$F_1 = \langle 00000| \mathcal{H}_C |00000\rangle = 15$$

Then, for the second state:

$$F_2 = \langle 01011| \mathcal{H}_C |01011\rangle = 6$$

So the total expectation value is:

$$\langle \psi | \mathcal{H}_C | \psi \rangle = 15|a|^2 + 6|b|^2$$