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Exercise 9.2 (Quantum search as quantum simulation, part 1)
Interestingly, the quantum search algorithm can be derived from a Schrödinger time evolution governed by a certain Hamiltonian H (cf. Tutorial 3). For simplicity, we assume that there is a single solution $x \in \{0, \dots, N-1\}$ to the search problem with N elements, and we start from an arbitrary initial state $|\psi\rangle$. It turns out that the Hamiltonian

$$H = |x\rangle\langle x| + |\psi\rangle\langle\psi|$$

achieves a transition from $|\psi\rangle$ to $|x\rangle$, that is, $\mathrm{e}^{-iHt^*}|\psi\rangle = |x\rangle$ for a certain time t^* (up to a phase factor, which is not relevant here). In part 1 we analyze the time evolution theoretically, and part 2 (next exercise sheet) discusses the simulation of the Hamiltonian.

To understand the transition from $|\psi\rangle$ to $|x\rangle$, first note that the time dynamics under H never leaves the two-dimensional space spanned by $|x\rangle$ and $|\psi\rangle$. Let the vector $|y\rangle$ be chosen such that $\{|x\rangle, |y\rangle\}$ forms an orthonormal basis of this subspace, and represent $|\psi\rangle = \alpha|x\rangle + \beta|y\rangle$ for some coefficients $\alpha, \beta \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 = 1$. For simplicity, we can assume that the phases of $|x\rangle$, $|y\rangle$ and $|\psi\rangle$ are such that α and β are real.

(a) Show that the matrix representation of H within this subspace is given by

$$H = I + \alpha(\beta X + \alpha Z).$$

Hint: The matrix entries of H restricted to a subspace with orthonormal basis $\{|u_j\rangle\}_{j=1,\dots,n}$ are $(\langle u_j| H |u_k\rangle)_{j,k}$.

(b) From the representation in (a), we thus obtain $\mathrm{e}^{-iHt} = \mathrm{e}^{-it}\,\mathrm{e}^{-i\alpha t(\beta X + \alpha Z)}$, where the phase factor e^{-it} stems from the identity matrix in the representation. Use the definition of the single-qubit rotation operators (see lecture) to verify that

$$\mathrm{e}^{-iHt} = \mathrm{e}^{-it}\left(\cos(\alpha t) I - i\sin(\alpha t)(\beta X + \alpha Z)\right).$$

(c) Show that $(\beta X + \alpha Z)|\psi\rangle = |x\rangle$. Together with (b), we thus arrive at

$$\mathrm{e}^{-iHt}|\psi\rangle = \mathrm{e}^{-it}\left(\cos(\alpha t)|\psi\rangle - i\sin(\alpha t)|x\rangle\right).$$

(d) Specify a time t^* such that $\mathrm{e}^{-iHt^*}|\psi\rangle = |x\rangle$ up to a phase factor.

(e) Since the required time t^* depends on $\alpha = \langle x|\psi\rangle$ and thus seemingly on the (a priori unknown) solution x, a natural question is how to determine t^*. To resolve this question, one can choose $|\psi\rangle$ to be the equal superposition state. Compute α in this case, assuming that $|\psi\rangle$ is normalized.

Solution

(a) We insert $|\psi\rangle = \alpha|x\rangle + \beta|y\rangle$ into the definition of H:

$$\begin{aligned} H &= |x\rangle\langle x| + \big(\alpha|x\rangle + \beta|y\rangle\big)\big(\alpha\langle x| + \beta\langle y|\big) \\ &= |x\rangle\langle x| + \alpha^2|x\rangle\langle x| + \alpha\beta|x\rangle\langle y| + \alpha\beta|y\rangle\langle x| + \underbrace{\beta^2}_{1-\alpha^2}|y\rangle\langle y| \\ &= \big(|x\rangle\langle x| + |y\rangle\langle y|\big) + \alpha\big(\beta(|x\rangle\langle y| + |y\rangle\langle x|) + \alpha(|x\rangle\langle x| - |y\rangle\langle y|)\big). \end{aligned}$$

From this expression we can read off the matrix representation of H within the subspace:

$$\begin{pmatrix} \langle x|H|x\rangle & \langle x|H|y\rangle \\ \langle y|H|x\rangle & \langle y|H|y\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \alpha\left(\beta\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \alpha\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right) = I + \alpha(\beta X + \alpha Z),$$

as required.

(b) We recall from the lecture the following formula for the rotation operator around an axis $\vec{v} \in \mathbb{R}^3$ with angle θ:

$$R_{\vec{v}}(\theta) = \mathrm{e}^{-i\theta(\vec{v}\cdot\vec{\sigma})/2} = \cos(\theta/2) I - i\sin(\theta/2)(\vec{v}\cdot\vec{\sigma}).$$

Here $\frac{\theta}{2} = \alpha t$ and $\vec{v} = (\beta, 0, \alpha)$, which has norm 1 since $\alpha^2 + \beta^2 = 1$. Inserted into the formula for the rotation operator directly leads to

$$\mathrm{e}^{-i\alpha t(\beta X + \alpha Z)} = \cos(\alpha t) I - i\sin(\alpha t)(\beta X + \alpha Z),$$

as required.

(c) The vector representation of $|\psi\rangle$ with respect to the $\{|x\rangle, |y\rangle\}$ basis is (α, β). Thus

$$(\beta X + \alpha Z)|\psi\rangle = \begin{pmatrix} \alpha & \beta \\ \beta & -\alpha \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha^2 + \beta^2 \\ \beta\alpha - \alpha\beta \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |x\rangle .$$

(d) Setting $t^* = \frac{\pi}{2\alpha}$ satisfies $\cos(\alpha t^*) = 0$ and $\sin(\alpha t^*) = 1$, and thus

$$\mathrm{e}^{-iHt^*}|\psi\rangle = \mathrm{e}^{-it^*}(\cos(\alpha t^*)|\psi\rangle - i\sin(\alpha t^*)|x\rangle) = -i\,\mathrm{e}^{-i\pi/(2\alpha)}|x\rangle .$$

(e) The normalized equal superposition state is defined as

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{z=0}^{N-1} |z\rangle .$$

All computational basis states are equally likely, and $\alpha = \langle x|\psi\rangle = \frac{1}{\sqrt{N}}$, independent of x.