4.5 Quantum Phase estimation

The framework of quantum phase estimation (QPE) is the following. Consider a unitary operation $\hat{U}$ where the state $|\psi\rangle$ is one of its eigenstates. In particular, one has

$$\hat{U}|\psi\rangle = e^{2\pi i\varphi}|\psi\rangle \,. \tag{4.39}$$

Then, the task is to determine the phase φ with a certain given precision.

4.5.1 Single-qubit quantum phase estimation

The Hadamard test described in Sec. 4.1.1 can be used to implement a single qubit phase estimation. Indeed, from Eq. (4.39) one gets that

$$\langle\psi|\hat{U}|\psi\rangle = e^{2\pi i\varphi}. \tag{4.40}$$

Then, by merging with Eq. (4.21) one has

$$P(|0\rangle) = \tfrac{1}{2}(1+\cos(2\pi\varphi)), \tag{4.41}$$

which implies

$$\varphi = \pm\frac{\arccos\left(1-2P(|0\rangle)\right)}{2\pi} + 2\pi k, \tag{4.42}$$

where $k \in \mathbb{N}$. Notice that such a circuit cannot distinguish the sign of φ. Conversely, using both Eq. (4.21) and Eq. (4.24), one has

$$\varphi = \arctan\left(\frac{1-2P(|0\rangle)}{1-2\tilde{P}(|0\rangle)}\right), \tag{4.43}$$

where $\tilde{P}(|0\rangle)$ is the probability of measuring $|0\rangle$ in the imaginary Hadamard test.

Now, for the sake of simplicity, let us restrict to the case of $\varphi \in [0,1[$. Suppose we would like to estimate the value of φ with a single run of the circuit in Eq. (4.17). Then, if the outcome is $+1$ (i.e., the state collapses on $|0\rangle$), we have $P(|0\rangle) = 1$. Conversely, with the outcome being -1 we have $P(|0\rangle) = 0$. Then, by employing Eq. (4.42) we obtain

outcome	$P(\lvert 0\rangle)$	$\bar{\varphi}$	φ_v
$+1$	1	0	$[0, 1/2[$
-1	0	$1/2$	$[1/2, 1[$

(4.44)

where $\bar{\varphi}$ gives the best estimation for the real value of the phase φ_v. Since there are no other possible outcomes with a single run, the phase is estimated with an error $\epsilon = 1/2$, namely $\varphi_v \in [\bar{\varphi}, \bar{\varphi}+\epsilon[$. This is a really low accuracy for a deterministic algorithm. To improve this accuracy, one should run the algorithm several times (namely, a number of times that scales as $\mathcal{O}(1/\epsilon^2)$, where ϵ is the target error bound), or consider alternative methods, as the N-qubit quantum phase estimation described below.

4.5.2 Kitaev's method for single-qubit quantum phase estimation

In the fixed point representation, a natural number k can be represented with a real number $\varphi \in [0,1[$ by employing d bits, i.e.

$$\varphi = (.\varphi_{d-1}\dots\varphi_0), \tag{4.45}$$

where $\varphi_k \in \{0,1\}$, as far as $k \le 2^d - 1$.

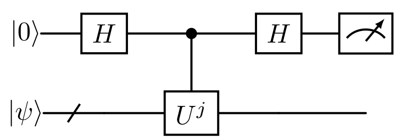
Example 4.3
To make an explicit example of the fixed point representation, the value of $k = 41$ corresponds to the $d = 6$ bit's string $[101001]$ and can be represented with $\varphi = 0.640625$ being equivalent to $(.101001)$. Indeed, by employing the following expression with the string $\varphi = (.\varphi_{d-1} \dots \varphi_0) = (.101001)$ one has

$$\sum_{i=0}^{d-1} \varphi_i 2^{i-d} = \varphi_5 2^{-1} + \varphi_4 2^{-2} + \varphi_3 2^{-3} + \varphi_2 2^{-4} + \varphi_1 2^{-5} + \varphi_0 2^{-6} = 2^{-1} + 2^{-3} + 2^{-6} = 0.640625. \quad (4.46)$$

Such a value, when multiplied by 2^6 gives exactly 41.

In the simplest scenario of $d = 1$, one has $\varphi = (.\varphi_0)$ with $\varphi_0 \in \{0, 1\}$. Thus, when performing once the real Hadamard test, one has $P(|0\rangle) = 1$ if $\varphi_0 = 0$ (i.e., $\bar{\varphi} = 0$), and $P(|0\rangle) = 0$ if $\varphi_0 = 1$ (i.e., $\bar{\varphi} = 1/2$).

Next, we consider the case of d bits, where $\varphi = (.0 \dots 0\varphi_0)$. Here, the first d bits are 0 and the last one is φ_0. To determined the value of φ_0 one needs to reach a precision of $\epsilon < 2^{-d}$. This would require $\mathcal{O}(1/\epsilon^2) = \mathcal{O}(2^{2d})$ repeated applications of the single-qubit quantum phase estimation, or number of queries to $\hat{U}$. The observation from Kitaev's method is that if we can have access to $\hat{U}^j$ for a suitable power j, then the number of queries to $\hat{U}$ can be reduced. If one substitutes $\hat{U}^j$ to $\hat{U}$, with the corresponding circuit being



(4.47)

then the probability changes in

$$P(|0\rangle) = \tfrac{1}{2}(1 + \cos(2\pi j \varphi)). \quad (4.48)$$

Importantly, every time one multiplies a number by a factor 2, the bits in the fixed point representation are shifted to the left. To make an example,

$$2 \times (.00\varphi_0) = (.0\varphi_0). \quad (4.49)$$

Then, one has that $2^{d-1}\varphi = 2^{d-1}(.0 \dots 0\varphi_0) = (.\varphi_0)$. Thus, applying the circuit in Eq. (4.47) with $j = d - 1$ to estimate $(.0 \dots 0\varphi_0)$ is equivalent to apply the circuit in Eq. (4.17) to estimate $(.\varphi_0)$.

This idea can be extended to general phases with d bits, i.e. $\varphi = (.\varphi_{d-1} \dots \varphi_0)$. Indeed, one has

$$\hat{U} e^{2\pi i \varphi} |\psi\rangle = \hat{U} e^{2\pi i (.\varphi_{d-1} \dots \varphi_0)} |\psi\rangle = e^{2\pi i (\varphi_{d-1} . \varphi_{d-2} \dots \varphi_0)} |\psi\rangle = e^{2\pi i \varphi_{d-1}} e^{2\pi i (.\varphi_{d-2} \dots \varphi_0)} |\psi\rangle, \quad (4.50)$$

but $e^{2\pi i \varphi_{d-1}} = 1$ independently from the value of φ_{d-1}. Thus

$$\hat{U} e^{2\pi i \varphi} |\psi\rangle = e^{2\pi i (.\varphi_{d-2} \dots \varphi_0)} |\psi\rangle, \quad (4.51)$$

i.e. the application of $\hat{U}$ shifts the bits and allows the evaluation of the first bit after the decimal point.

4.5.3 n-qubit quantum phase estimation

Notably, both the previous algorithms necessitate an important classical post-processing. Employing n ancillary qubits allow the reduction of such post-processing. This is based on the application of the Inverse Quantum Fourier Transform $\hat{F}^\dagger$.

Recall 4.1 (Quantum Fourier transform)
The discrete Fourier transform of a N-component vector with complex components $\{ f(0), \dots, f(N-1) \}$ *is a new complex vector* $\{ \tilde{f}(0), \dots, \tilde{f}(N-1) \}$*, defined as*

$$F(f(j), k) = \tilde{f}(k) = \tfrac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{2\pi i jk/N} f(j). \tag{4.52}$$

The Quantum Fourier transform (QFT) acts similarly: it acts as the unitary operator $\hat{F}$ *on a quantum register of* n *qubits, where* $N = 2^n$*, in the computational basis as*

$$\hat{F} |j\rangle = \tfrac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{2\pi i jk/2^n} |k\rangle , \tag{4.53}$$

where $|j\rangle = |j_{n-1} \dots j_0\rangle$ *and* $|k\rangle = |k_{n-1} \dots k_0\rangle$*. Namely, the application of the quantum Fourier transform* $\hat{F}$ *to the state* $|j\rangle = |j_{n-1} \dots j_0\rangle$ *gives*

$$\hat{F} |j\rangle = \tfrac{1}{\sqrt{2^n}} \Big(|0\rangle + e^{2\pi i (0.j_0)} |1\rangle \Big) \Big(|0\rangle + e^{2\pi i (0.j_1 j_0)} |1\rangle \Big) \dots \Big(|0\rangle + e^{2\pi i (0.j_{n-1} \dots j_0)} |1\rangle \Big) . \tag{4.54}$$

In the case of a superposition $|\psi\rangle = \sum_j f(j) |j\rangle$*, one has*

$$|\tilde{\psi}\rangle = \hat{F} |\psi\rangle = \sum_{k=0}^{2^n-1} \tilde{f}(k) |k\rangle , \tag{4.55}$$

where the coefficients $\tilde{f}(k)$ *are the discrete Fourier transform of the coeficients* $f(j)$*.*
The inverse quantum Fourier transform $\hat{F}^\dagger$ *acts as*

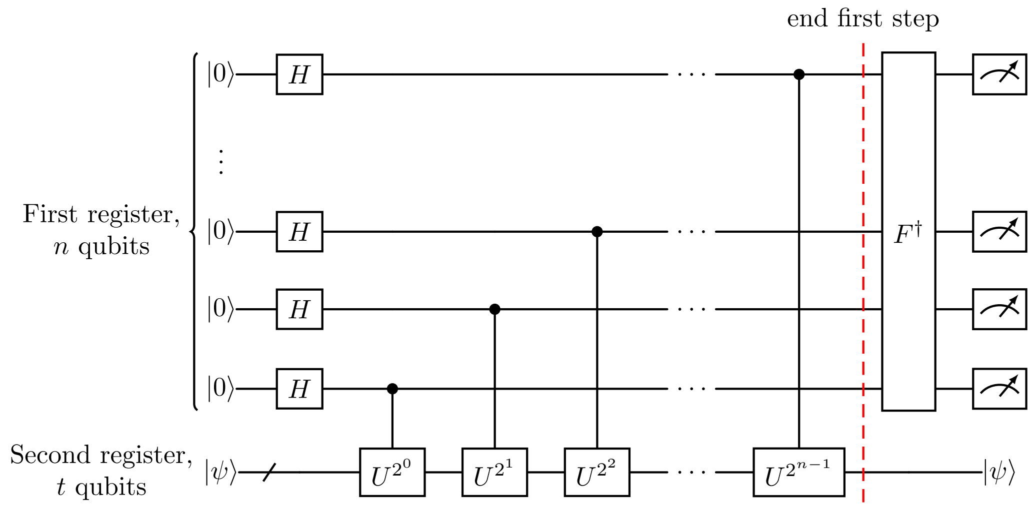
$$\hat{F}^\dagger |j\rangle = \tfrac{1}{\sqrt{2^n}} \sum_{j=0}^{2^n-1} e^{-2\pi i jk/2^n} |k\rangle , \tag{4.56}$$

in a completely similar way as Eq. (4.53) but with negative phases.

Example 4.4
The application of the quantum Fourier transform $\hat{F}$ *to the state* $|j\rangle = |10\rangle = |j_1 = 1, j_0 = 0\rangle$ *gives*

$$\begin{aligned} \hat{F} |j\rangle &= \tfrac{1}{2} \Big(|0\rangle + e^{2\pi i (0.j_0)} |1\rangle \Big) \Big(|0\rangle + e^{2\pi i (0.j_1 j_0)} |1\rangle \Big) , \\ &= \tfrac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \tfrac{1}{\sqrt{2}} (|0\rangle - |1\rangle). \end{aligned} \tag{4.57}$$

The algorithm implementing the (standard) quantum phase estimation uses a first register of n ancillary qubits and a second register of which we want to compute the phase. The first register is initially prepared in the $|0\rangle$ state for all the qubits. The circuit implementing the algorithm is the following



(4.58)

In particular, the state of the first register after the end of the first part of the algorithm (see red dashed line) reads

$$\frac{1}{\sqrt{2^n}}\left(|0\rangle + e^{2\pi i(2^{n-1}\varphi)}|1\rangle\right)\ldots\left(|0\rangle + e^{2\pi i(2^0\varphi)}|1\rangle\right). \tag{4.59}$$

Now, by considering the binary representation of $\varphi = (\varphi_{n-1}\ldots\varphi_0)$, the latter expression becomes

$$\frac{1}{\sqrt{2^n}}\left(|0\rangle + e^{2\pi i(0.\varphi_0)}|1\rangle\right)\left(|0\rangle + e^{2\pi i(0.\varphi_1\varphi_0)}|1\rangle\right)\ldots\left(|0\rangle + e^{2\pi i(0.\varphi_{n-1}\ldots\varphi_0)}|1\rangle\right), \tag{4.60}$$

which is exactly equal to $\hat{F}|j\rangle$ in Eq. (4.54) for $|j\rangle = |\varphi\rangle$. Thus, applying the inverse Fourier transform $\hat{F}^\dagger$ one gets $|\varphi\rangle$, which is then measured.

4.6 Harrow-Hassidim-Lloyd algorithm

The Harrow-Hassidim-Lloyd (HHL) algorithm allows for the resolution of linear system problems on a quantum computer. To be precise, the problem to be solved is described as finding the N_b complex entries of $\mathbf{x}$ that solve the following problem

$$A\mathbf{x} = \mathbf{b}, \tag{4.61}$$

where A is an hermitian and non-singular $N_b \times N_b$ matrix and $\mathbf{b}$ is a N_b vector, both defined on $\mathbb{C}$. Classically, the solution is given by

$$\mathbf{x} = A^{-1}\mathbf{b}. \tag{4.62}$$

The question is then how one can implement this on a quantum computer.

First, let us assume that the entries of $\mathbf{b}$ are such that $||\mathbf{b}|| = 1$. Then, $\mathbf{b}$ can be stored in a n_b-qubit state $|b\rangle$, through the following mapping:

$$\mathbf{b} = \begin{pmatrix} b_0 \\ \vdots \\ b_{N_b-1} \end{pmatrix} \leftrightarrow b_0|0\rangle + \cdots + b_{N_b-1}|N_b-1\rangle = |b\rangle, \tag{4.63}$$

where $N_b = 2^{n_b}$. For example, this can be done via a unitary operation $\hat{U}_\mathbf{b}$. Now, we define $|x\rangle = \hat{A}^{-1}|b\rangle$, where $\hat{A}$ in the computational representation gives the classical matrix A. Notably, the state $|x\rangle$ needs to be normalised to be stored in a quantum register. Thus, one has

$$|x\rangle = \frac{\hat{A}^{-1}|b\rangle}{||\hat{A}^{-1}|b\rangle||}, \tag{4.64}$$

where the normalisation problem can be tackled in a second moment.

Consider the spectral decomposition of $\hat{A}$:

$$\hat{A}|v_j\rangle = \lambda_j |v_j\rangle, \tag{4.65}$$

where λ_j and $|v_j\rangle$ are respectively the eigeinvalues and eigeinstates of $\hat{A}$. We also assume that the ordering of the eigeinvalues is such that

$$0 < \lambda_0 \leq \cdots \leq \lambda_{N_b-1} < 1. \tag{4.66}$$

In general this will not be the case, but one can remap the problem in order to fall within this case. We also assume that all the N_b eigeinvalues have an exact d-bit representation.

By applying what in Sec. 4.5, we can query $\hat{A}$ via an unitary operation $\hat{U} = e^{2\pi i \hat{A}}$ using QPE. For example, suppose $|b\rangle = |v_j\rangle$, then we have

$$\hat{U}_{\text{QPE}} |0\rangle^{\otimes d} |v_j\rangle = |\lambda_j\rangle |v_j\rangle. \tag{4.67}$$

In particular, the (not-normalised) solution of the linear system problem would be

$$\hat{A}^{-1}|b\rangle = \hat{A}^{-1}|v_j\rangle = \tfrac{1}{\lambda_j}|v_j\rangle. \tag{4.68}$$

More generally, one can decompose the state $|b\rangle$ on the basis of $\hat{A}$, i.e.

$$|b\rangle = \sum_{j=0}^{2^{n_b}-1} \beta_j |v_j\rangle, \tag{4.69}$$

where β_j are a linear combination of b_j. Then the QPE procedure gives

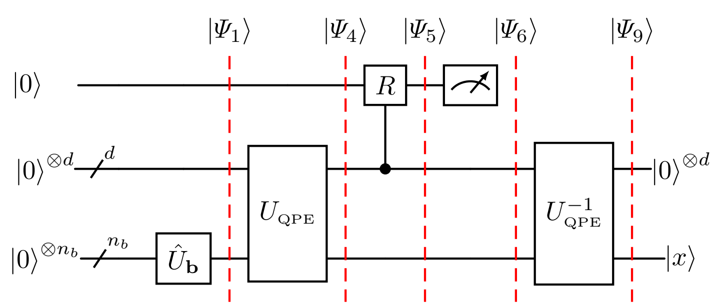
$$\hat{U}_{\text{QPE}} |0\rangle^{\otimes d} |b\rangle = \sum_j \beta_j |\lambda_j\rangle |v_j\rangle, \tag{4.70}$$

and the solution of the problem is given by

$$\hat{A}^{-1}|b\rangle = \sum_{j=0}^{2^{n_b}-1} \frac{\beta_j}{\lambda_j} |v_j\rangle. \tag{4.71}$$

The aim of the HHL algorithm is to generate the normalised version of the state in Eq. (4.71) from the general state $|b\rangle$ as shown in Eq. (4.69).

The algorithm works with three registers. The first one is an ancillary register made of a single qubit, the second is also an ancillary register but made of d qubits, the third register is made of n_b qubits and will encode the solution of the problem. The HHL circuit is the following



(4.72)

The algorithm works as the following. Initially, all the qubits are prepared in $|0\rangle$:

$$|\Psi_0\rangle = |0\rangle\,|0\rangle^{\otimes d}\,|0\rangle^{\otimes n_b}\,, \tag{4.73}$$

then the information about $\mathbf{b}$ is encoded in the last register:

$$|\Psi_1\rangle = \hat{\mathbb{1}} \otimes \hat{\mathbb{1}}^{\otimes d} \otimes \hat{U}_{\mathbf{b}}\,|\Psi_0\rangle = |0\rangle\,|0\rangle^{\otimes d}\,|b\rangle\,. \tag{4.74}$$

We apply the QPE procedure, which is here broke down in the corresponding three steps. The first is the application of the Hadamard gate:

$$|\Psi_2\rangle = \hat{\mathbb{1}} \otimes \hat{H}^{\otimes d} \otimes \hat{\mathbb{1}}\,|\Psi_1\rangle = |0\rangle\,\tfrac{1}{2^{d/2}}(|0\rangle + |1\rangle)^{\otimes d}\,|b\rangle\,. \tag{4.75}$$

This is followed by the controlled unitary $\hat{U}^j$:

$$|\Psi_3\rangle = \hat{\mathbb{1}} \otimes C(U^j)\,|\Psi_2\rangle = |0\rangle\,\tfrac{1}{2^{d/2}}\sum_{k=0}^{2^d-1} e^{2\pi i k\varphi}\,|k\rangle\,|b\rangle\,, \tag{4.76}$$

where $\hat{U}\,|b\rangle = e^{2\pi i\varphi}\,|b\rangle$ with $\varphi \in [0,1[$. Finally, we apply the inverse Fourier transform to the second register

$$\begin{aligned} |\Psi_4\rangle &= \hat{\mathbb{1}} \otimes \hat{F}^\dagger \otimes \hat{\mathbb{1}}^{\otimes n_b}\,|\Psi_3\rangle\,,\\ &= |0\rangle\,\tfrac{1}{2^{d/2}}\sum_{k=0}^{2^d-1} e^{2\pi i k\varphi}\hat{F}^\dagger\,|k\rangle\,|b\rangle\,,\\ &= |0\rangle\,\tfrac{1}{2^d}\sum_{k=0}^{2^d-1} e^{2\pi i k\varphi}\sum_{y=0}^{2^d-1} e^{-2\pi i yk/2^d}\,|y\rangle\,|b\rangle\,. \end{aligned} \tag{4.77}$$

However, one has that

$$\sum_{k=0}^{2^d-1} e^{2\pi i k(\varphi - y/2^d)} = \begin{cases} \sum_{k=0}^{2^d-1} e^0 = 2^d, & \text{if } \varphi = y/2^d,\\ 0, & \text{if } \varphi \neq y/2^d, \end{cases} \tag{4.78}$$

meaning that the k sum selects the value of $y = \varphi 2^d$. Thus,

$$|\Psi_4\rangle = |0\rangle\,|\varphi 2^d\rangle\,|b\rangle\,. \tag{4.79}$$

In general, $|b\rangle$ is in a superposition of $|v_j\rangle$, then

$$\hat{U}\,|v_j\rangle = e^{2\pi i\hat{A}}\,|v_j\rangle = e^{2\pi i\lambda_j}\,|v_j\rangle\,. \tag{4.80}$$

Then, the entire QPE gate maps

$$|\Psi_1\rangle = |0\rangle\,|0\rangle^{\otimes d}\sum_{j=0}^{2^{n_b}-1}\beta_j\,|v_j\rangle \xrightarrow{U_{\text{QPE}}} |\Psi_4\rangle = |0\rangle\sum_{j=0}^{2^{n_b}-1}\beta_j\,|\lambda_j 2^d\rangle\,|v_j\rangle\,. \tag{4.81}$$

We apply a controlled rotation on the first register, such that

$$|\Psi_5\rangle = C(R) \otimes \hat{\mathbb{1}}^{\otimes n_b}\,|\Psi_4\rangle = \sum_{j=0}^{2^{n_b}-1}\beta_j\left(\sqrt{1-\tfrac{C^2}{\lambda_j^2}}\,|0\rangle + \tfrac{C}{\lambda_j}\,|1\rangle\right)|\lambda_j 2^d\rangle\,|v_j\rangle\,, \tag{4.82}$$

where $C \in \mathbb{R}$ is an arbitrary constant. At this point we perform the measurement of the first register. If the outcome is $+1$ and the state collapses in $|0\rangle$ then we discard the run; if the outcome is -1 with the state collapsed in $|1\rangle$ then we retain the run. To increase the probabilities of having the outcome -1, we make C as large as possible. After the collapse of the first register in $|1\rangle$, the state of the second and third register is

$$|\Psi_6\rangle = \frac{1}{\left(\sum_{j=0}^{2^{n_b}-1} |\beta_j/\lambda_j|^2\right)^{1/2}} \sum_{j=0}^{2^{n_b}-1} \tfrac{\beta_j}{\lambda_j} |\lambda_j 2^d\rangle |v_j\rangle \,, \tag{4.83}$$

where we exploited that $C \in \mathbb{R}$. Now, we apply the inverse QPE, which has also three steps. The first is the application of the QFT:

$$\begin{aligned} |\Psi_7\rangle &= \hat{F} \otimes \hat{\mathbb{1}}^{\otimes n_b} |\Psi_6\rangle \,, \\ &= \frac{1}{\left(\sum_{j=0}^{2^{n_b}-1} |\beta_j/\lambda_j|^2\right)^{1/2}} \sum_{j=0}^{2^{n_b}-1} \tfrac{\beta_j}{\lambda_j} \hat{F} |\lambda_j 2^d\rangle |v_j\rangle \,, \\ &= \frac{1}{\left(\sum_{j=0}^{2^{n_b}-1} |\beta_j/\lambda_j|^2\right)^{1/2}} \sum_{j=0}^{2^{n_b}-1} \tfrac{\beta_j}{\lambda_j} \tfrac{1}{2^{d/2}} \sum_{y=0}^{2^d-1} e^{2\pi i y(\lambda_j 2^d)/2^d} |y\rangle |v_j\rangle \,. \end{aligned} \tag{4.84}$$

Then, we apply the controlled unitary $C(U^{-j})$, which gives

$$\begin{aligned} |\Psi_8\rangle &= C(U^{-j}) |\Psi_7\rangle \,, \\ &= \frac{1}{\left(\sum_{j=0}^{2^{n_b}-1} |\beta_j/\lambda_j|^2\right)^{1/2}} \sum_{j=0}^{2^{n_b}-1} \tfrac{\beta_j}{\lambda_j} \tfrac{1}{2^{d/2}} \sum_{y=0}^{2^d-1} e^{2\pi i y \lambda_j} |y\rangle \, e^{-2\pi i \lambda_j y} |v_j\rangle \,, \end{aligned} \tag{4.85}$$

where the two phases cancel and thus

$$|\Psi_8\rangle = \tfrac{1}{2^{d/2}} \sum_{y=0}^{2^d-1} |y\rangle \sum_{j=0}^{2^{n_b}-1} \tfrac{\beta_j}{\lambda_j} \frac{1}{\left(\sum_{j=0}^{2^{n_b}-1} |\beta_j/\lambda_j|^2\right)^{1/2}} |v_j\rangle \,. \tag{4.86}$$

Finally, the application of Hadamard's gates on the second register gives

$$|\Psi_9\rangle = \hat{H}^{\otimes d} \otimes \hat{\mathbb{1}}^{\otimes n_b} |\Psi_8\rangle = |0\rangle^{\otimes d} \sum_{j=0}^{2^{n_b}-1} \tfrac{\beta_j}{\lambda_j} \frac{1}{\left(\sum_{j=0}^{2^{n_b}-1} |\beta_j/\lambda_j|^2\right)^{1/2}} |v_j\rangle \,, \tag{4.87}$$

where the third register is exactly in the form in Eq. (4.71) after the proper normalisation. Thus,

$$|\Psi_9\rangle = |0\rangle^{\otimes d} |x\rangle \,, \tag{4.88}$$

embeds the solution of the linear system $A\mathbf{x} = \mathbf{b}$.