Spring 2024: Final Project
COM-308: Quantum Computing

Notations

We denote $|i\rangle$ the state in the computational basis corresponding to the binary decomposition of i. For example, with 4 qubits, $|5\rangle = |0101\rangle$.

The HHL Algorithm

The HHL (Harrow-Hassidim-Lloyd) algorithm is a quantum algorithm designed to solve systems of linear equations. Given a matrix $A \in \mathbb{C}^{2^n \times 2^n}$ and a vector $\mathbf{b} \in \mathbb{C}^{2^n}$, we want to find a vector $\mathbf{x} \in \mathbb{C}^{2^n}$ that verifies

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

The HHL algorithm is exponentially faster than classical methods when the matrix A is sparse. If s is the number of non-zero elements per row in A, then the quantum circuit can be constructed with $O(ns^2)$ gates whereas the best classical algorithm runs in $O(2^n s)$.

To solve the linear system $A\mathbf{x} = \mathbf{b}$ with a quantum circuit, we need to represent $\mathbf{b}$ and $\mathbf{x}$ by quantum states; thus, we need to scale them to unit length $\|\mathbf{b}\| = \|\mathbf{x}\| = 1$. Then $\mathbf{b}$ can be represented by a state $|b\rangle$ using n qubit such that $|b\rangle = \sum_{i=0}^{2^n-1} b_i |i\rangle$. Here, the b_i are the components of $\mathbf{b}$. The vector solution $\mathbf{x}$ can be then represented by the state $|x\rangle$ that verifies

$$|x\rangle = cA^{-1}|b\rangle, \quad c^{-1} = \|A^{-1}|b\rangle\| \tag{2}$$

where c ensures that the state is normalized.

The HHL algorithm uses quantum phase estimation to encode the solution $\mathbf{x}$ into a quantum state. To do so, the algorithm requires that the matrix A be Hermitian.

Question Theory 1: Show that if A is not Hermitian, we can still find a solution to the system by running the HHL algorithm on the larger system:

$$\tilde{A} = \begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix}, \quad \tilde{b} = \begin{pmatrix} b \\ 0 \end{pmatrix}. \tag{3}$$

Solution. First, note that $\tilde{A}$ is Hermitian. Also, observe that $\tilde{A}^{-1} = \begin{pmatrix} 0 & (A^\dagger)^{-1} \\ A^{-1} & 0 \end{pmatrix}$. Then, the solution of the larger system is given by

$$\tilde{x} = \begin{bmatrix} 0 & A \\ A^\dagger & 0 \end{bmatrix}^{-1} \begin{bmatrix} b \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & (A^\dagger)^{-1} \\ A^{-1} & 0 \end{bmatrix} \begin{bmatrix} b \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ A^{-1}b \end{bmatrix} = \begin{bmatrix} 0 \\ x \end{bmatrix}.$$

Hence, entries from $2^n + 1$ to 2^{n+1} in $\tilde{x}$ gives x. $\square$

So, from now on, we will assume that A is a Hermitian matrix, i.e. $A = A^\dagger$. Thus, by the spectral theorem (see Homework 1 Ex 3), there exists a set of orthogonal states $(|u_i\rangle)_{i=0,\dots,2^n-1}$ such that A can be written

$$A = \sum_{i=0}^{2^n-1} \lambda_i |u_i\rangle\langle u_i| \tag{4}$$

where the $\lambda_i \in \mathbb{R}$ are the eigenvalues of A. The $(|u_i\rangle)_{i=0,\dots,2^n-1}$ form an eigenbasis of A. The state $|b\rangle$ can also be written in the $(|u_i\rangle)_{i=0,\dots,2^n-1}$ basis and we denote

$$|b\rangle = \sum_{i=0}^{2^n-1} \beta_i |u_i\rangle . \tag{5}$$

Question Theory 2: Check that $|x\rangle = c\sum_{i=0}^{2^n-1} \frac{\beta_i}{\lambda_i} |u_i\rangle$ is solution to the system.

Solution. Note that we have $A^{-1} = \sum_{i=0}^{2^n-1} \frac{1}{\lambda_i} |u_i\rangle\langle u_i|$ (this can be verified using $AA^{-1} = I$). Hence,

$$\begin{aligned}
|x\rangle = cA^{-1}|b\rangle &= c\sum_{i=0}^{2^n-1} \frac{1}{\lambda_i} |u_i\rangle\langle u_i| \sum_{j=0}^{2^n-1} \beta_j |u_j\rangle , \\
&= c\sum_{i,j=0}^{2^n-1} \frac{1}{\lambda_i}\beta_j \langle u_i|u_j\rangle |u_i\rangle , \\
&= c\sum_{i,j=0}^{2^n-1} \frac{1}{\lambda_i}\beta_j\delta_{ij} |u_i\rangle , \\
&= c\sum_{i=0}^{2^n-1} \frac{\beta_j}{\lambda_i} |u_i\rangle .
\end{aligned}$$

□

The circuit

The HHL circuit is represented in Figure 1. The circuit uses three registers:

- The top register is 1 ancilla qubit initialized to $|0\rangle$.
- The middle register is a memory register that stores the eigenvalues λ_i of A. More precisely, we will store the binary representation of λ_i. The number of qubits m needed for this register will therefore depend on λ_i. This register is initialized to $|0\rangle^{\otimes m}$.
- The bottom register uses n qubits and is initialized with the state $|b\rangle$.

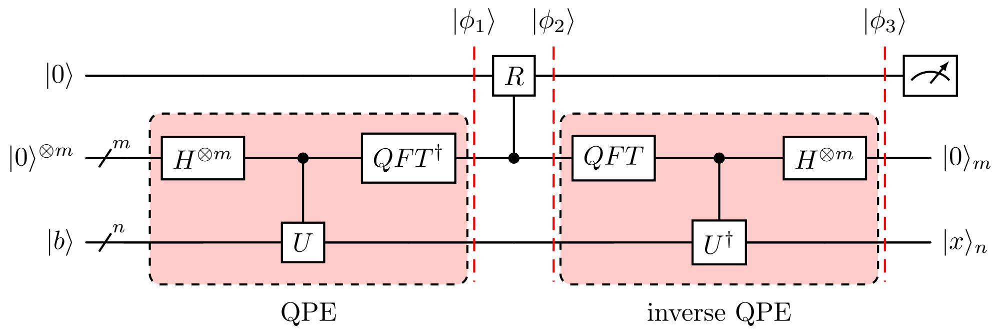

Figure 1: Quantum Circuit for HHL Algorithm

The circuit is composed of 4 steps, a quantum phase estimation (QPE), a controlled rotation, an inverse quantum phase estimation and a measurement. Let us detail the gates appearing in each part:

Quantum phase estimation: This part of the circuit is detailed in Figure 2. The circuit starts with a Hadamard gate on each qubit of the memory register. The unitary U is

$$U = e^{i2\pi \frac{A}{2^m}}. \tag{6}$$

Then we apply an inverse quantum Fourier transform on the memory register.

$$QFT^\dagger |k\rangle = \frac{1}{\sqrt{2^m}} \sum_{j=0}^{2^m-1} e^{-i2\pi \frac{kj}{2^m}} |j\rangle . \tag{7}$$

Controlled rotation: The gate R realizes the transformation

$$R(|0\rangle \otimes |\lambda\rangle) = \left(\sqrt{1 - \frac{1}{\lambda^2}} |0\rangle + \frac{1}{\lambda} |1\rangle \right) \otimes |\lambda\rangle . \tag{8}$$

Inverse QPE: We apply the **inverse** gates of the QPE in **reverse** order to set back the memory register to $|0\rangle^{\otimes m}$. The memory register is no longer entangled with the output register.

Measurement: The algorithm outputs $|x\rangle$ if the ancilla qubit is measured in state $|1\rangle$.

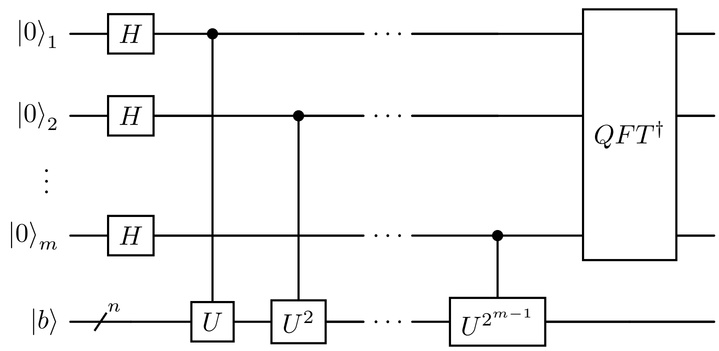

Figure 2: Detailed QPE

Analysis

We assume that the eigenvalues of A are positive integers, i.e. $\lambda_i \in \mathbb{N}^*$ and $\max_i(\lambda_i) < 2^m$. The circuit starts with a quantum phase estimation that stores the eigenvalues in the memory register.

Question Theory 3: Show that the state $|\phi_1\rangle$ defined in Figure 1 is

$$|\phi_1\rangle = |0\rangle \otimes \left(\sum_i \beta_i |\lambda_i\rangle \otimes |u_i\rangle \right). \tag{9}$$

Hint: Use the lecture notes on QPE. You can start by answering these questions:

- *What are the eigenvalues and eigenvectors of U ?*
- *What happens if $|b\rangle = |u_i\rangle$?*

Solution. Since the ancilla qubit is not involved in the Quantum Phase Estimation, we consider only the $m+n$ bit that are inputs the QPE circuit. Let CU denote the controlled U gate. Then, $QPE = (QFT^\dagger \otimes I)CU(H^{\otimes m} \otimes I)$. We have

$$\begin{aligned} |\phi_1\rangle &= I \otimes QPE \ |0\rangle \otimes (|0\rangle^{\otimes m} \otimes |b\rangle), \\ &= |0\rangle \otimes QPE \ |0\rangle^{\otimes m} \otimes \sum_{j=0}^{2^n-1} \beta_j |u_j\rangle, \\ &= |0\rangle \otimes \sum_{j=0}^{2^n-1} \beta_j QPE \ |0\rangle^{\otimes m} \otimes |u_j\rangle. \end{aligned} \tag{10}$$

For an integer $0 \leq x < 2^m$, let $(x_{m-1}, x_{m-2}, \cdots, x_0)$ be its binary expansion. Then, we can compute

$QPE\ |0\rangle^{\otimes m} \otimes |u_j\rangle$ as follows:

$$\begin{aligned}
QPE\ |0\rangle^{\otimes m} \otimes |u_j\rangle &= (QFT^\dagger \otimes I) CU (H^{\otimes m} \otimes I) |0\rangle^{\otimes m} \otimes |u_j\rangle\,, \\
&= (QFT^\dagger \otimes I) CU (H\,|0\rangle)^{\otimes m} \otimes |u_j\rangle\,, \\
&= (QFT^\dagger \otimes I) \frac{1}{2^{m/2}} \sum_{x=0}^{2^m-1} CU\ |x\rangle \otimes |u_j\rangle\,, \\
&= (QFT^\dagger \otimes I) \frac{1}{2^{m/2}} \sum_{x=0}^{2^m-1} |x\rangle \otimes U^{\sum_{i=0}^{m-1} x_i 2^i} |u_j\rangle\,, \\
&= (QFT^\dagger \otimes I) \frac{1}{2^{m/2}} \sum_{x=0}^{2^m-1} |x\rangle \otimes U^{x} |u_j\rangle\,, \\
&= (QFT^\dagger \otimes I) \frac{1}{2^{m/2}} \sum_{x=0}^{2^m-1} |x\rangle \otimes e^{i2\pi \frac{\lambda_j}{2^m} x} |u_j\rangle\,, \\
&= (QFT^\dagger \otimes I) \left(\frac{1}{2^{m/2}} \sum_{x=0}^{2^m-1} e^{i2\pi \frac{\lambda_j}{2^m} x} |x\rangle \right) \otimes |u_j\rangle\,, \\
&= (QFT^\dagger \otimes I)(QFT\,|\lambda_j\rangle) \otimes |u_j\rangle\,, \\
&= |\lambda_j\rangle \otimes |u_j\rangle\,.
\end{aligned}$$

Hence, substituting in (10), we get

$$|\phi_1\rangle = |0\rangle \otimes \left(\sum_i \beta_i \,|\lambda_i\rangle \otimes |u_i\rangle \right).$$

□

Then we apply a controlled rotation R to create the $\frac{1}{\lambda}$ factor.

Question Theory 4: Compute $|\phi_2\rangle$.

Solution. The state $|\phi_2\rangle$ is given by $(R \otimes I)\,|\phi_1\rangle$, where R is the controlled rotation acting on the first $m+1$ qubit. Thus,

$$\begin{aligned}
|\phi_2\rangle &= (R \otimes I)\,|\phi_1\rangle\,, \\
&= \sum_{j=0}^{2^n-1} \beta_j (R \otimes I)\,|0\rangle \otimes |\lambda_j\rangle \otimes |u_j\rangle\,, \\
&= \sum_{j=0}^{2^n-1} \beta_j \{R(|0\rangle \otimes |\lambda_j\rangle)\} \otimes |u_j\rangle\,, \\
&= \sum_{j=0}^{2^n-1} \beta_j \left(\sqrt{1 - \frac{1}{\lambda_j^2}}\,|0\rangle + \frac{1}{\lambda_j}\,|1\rangle \right) \otimes |\lambda_j\rangle \otimes |u_j\rangle\,.
\end{aligned}$$

□

We want to disentangle the memory register from the output state. Thus, we apply the inverse QPE.

Question Theory 5: Show that the state $|\phi_3\rangle$ defined in Figure 1 is

$$|\phi_3\rangle = \sum_i \beta_i \left(\sqrt{1 - \frac{1}{\lambda_i^2}} |0\rangle + \frac{1}{\lambda_i} |1\rangle \right) \otimes |0\rangle^{\otimes m} \otimes |u_i\rangle . \tag{11}$$

Hint: Start with $|b\rangle = |u_i\rangle$ and use the fact that gates are unitary.

Solution. In the solution to Question 3, we showed that $QPE \ \ |0\rangle^{\otimes m} \otimes |u_j\rangle = |\lambda_j\rangle \otimes |u_j\rangle$. Inverting, this gives $QPE^\dagger \ \ |\lambda_j\rangle \otimes |u_j\rangle = |0\rangle^{\otimes m} \otimes |u_j\rangle$. We can use this to simplify the computation of $|\phi_3\rangle$. We have

$$\begin{aligned}
|\phi_3\rangle &= (I \otimes QPE^\dagger) |\phi_2\rangle , \\
&= \sum_{j=0}^{2^n-1} \beta_j \left(\sqrt{1 - \frac{1}{\lambda_j^2}} |0\rangle + \frac{1}{\lambda_j} |1\rangle \right) \otimes (QPE^\dagger |\lambda_j\rangle \otimes |u_j\rangle), \\
&= \sum_{j=0}^{2^n-1} \beta_j \left(\sqrt{1 - \frac{1}{\lambda_j^2}} |0\rangle + \frac{1}{\lambda_j} |1\rangle \right) \otimes |0\rangle^{\otimes m} \otimes |u_j\rangle , \\
&= |0\rangle \otimes |0\rangle^{\otimes m} \otimes \sum_{j=0}^{2^n-1} \beta_j \sqrt{1 - \frac{1}{\lambda_j^2}} |u_j\rangle + |1\rangle \otimes |0\rangle^{\otimes m} \otimes \sum_{j=0}^{2^n-1} \frac{\beta_j}{\lambda_j} |u_j\rangle .
\end{aligned}$$

□

Question Theory 6: Show that the output of the circuit is a solution of the linear system if the result of the measurement is "1". What is the probability of obtaining this result? Use $\max_i(\lambda_i) < 2^m$ to lower bound this result.

Solution. When we measure 1, the output state is proportional to

$$(|1\rangle \langle 1| \otimes I) |\phi_3\rangle = |1\rangle \otimes |0\rangle^{\otimes m} \otimes \sum_{j=0}^{2^n-1} \frac{\beta_j}{\lambda_j} |u_j\rangle$$

Normalizing the state yields question 2 result. Hence, $|x\rangle_n$ is the solution to the linear system. The probability of measuring 1 is

$$\begin{aligned}
|(|1\rangle \langle 1| \otimes I) |\phi_3\rangle |^2 &= \sum_{j=0}^{2^n-1} \left| \frac{\beta_j}{\lambda_j} \right|^2 , \\
&\geq \frac{1}{2^{2m}} \sum_{j=0}^{2^n-1} |\beta_j|^2, \\
&= \frac{1}{2^{2m}}.
\end{aligned}$$

□

Question Implementation 1: Implement the HHL circuit on a simulator. Consider only the case where the eigenvalues of A are powers of 2. More detailed instructions are given in the notebook.

Measuring the solution

We want to measure $|x\rangle$ to learn its value. We are used to measuring states with projectors. The probability of a state $|\phi\rangle$ to be in state $|\psi\rangle$ is

$$P(|\psi\rangle) = \langle\phi| (|\psi\rangle\langle\psi|) |\phi\rangle = |\langle\phi |\psi\rangle |^2. \tag{12}$$

Question Implementation 2: On a simulator and a real device, run the HHL circuit to measure $|x\rangle$, the solution of the system

$$A = \frac{1}{2}\begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix} \text{ and } |b\rangle = \frac{1}{\sqrt{5}}(2\,|0\rangle - |1\rangle). \tag{13}$$

Compare it to the expected solution $\frac{A^{-1}\mathbf{b}}{\|A^{-1}\mathbf{b}\|}$. What is missing to fully reconstruct the solution?

Limitations

Although the HHL algorithm offers exponential speedup over classical methods, it has several limitations:

- It requires that the matrix A be sparse to reach the announced complexity. In our implementation, we do not pay attention to this requirement.
- We need to have some a priori knowledge of the eigenvalues λ_i to have an exact and efficient algorithm.
- The algorithm only gives a solution with some probability of error.
- The preparation of the quantum state for $|b\rangle$ is often difficult and requires additional resources.
- We do not have direct access to the result. We still need to measure $|x\rangle$ to learn the solution.
- On a real quantum noisy device, we will only have access to an approximate solution.

Bonus - Another measurement

If we measure our state $|x\rangle$ only in the computational basis, which means that we choose the set of projectors $|i\rangle\langle i|$, we will only obtain the norm of each amplitude in the computational basis. If the amplitude is complex, we will not be able to reconstruct the full state $|x\rangle$. Thus, we need another kind of measurement.

An observable O is a Hermitian matrix that represents a physical property we want to measure in our system. It can be the position, momentum, spin ... We are interested to know the average value of that property. As a Hermitian matrix, O can be decomposed into its eigenbasis, $O = \sum_k \mu_k |v_k\rangle\langle v_k|$. The expected value of O observed in the state $|\phi\rangle$ is then $\langle O\rangle = \langle\phi| O |\phi\rangle = \sum_k \mu_k \langle\phi| \big(|v_k\rangle\langle v_k| \big) |\phi\rangle = \sum_k \mu_k P(|v_k\rangle)$.

Remark that if we choose O to be a projector $|\psi\rangle\langle\psi|$, then O has only one non-zero eigenvalue which is 1 associated with the eigenvector $|\psi\rangle$. Therefore, the expected value of O is $P(|\psi\rangle)$.

We focus on the case where A is a 2×2 matrix and $\mathbf{b}$ is a vector of size 2. We denote by ρ the matrix $\rho = |x\rangle\langle x|$. The set of operators $P = \frac{1}{\sqrt{2}}\{I, X, Y, Z\}$ is a basis of the space of the 2×2 matrices. Thus, we can decompose ρ in this basis:

$$\rho = \frac{c_I I + c_X X + c_Y Y + c_Z Z}{\sqrt{2}} \tag{14}$$

Question Theory 7: Show that $c_\sigma = \mathrm{Tr}(\rho\sigma)$ for all $\sigma \in P$.

Hint: Show that for all $\sigma_i\sigma_j \in P$, $\mathrm{Tr}(\sigma_i\sigma_j) = 0$ if $j \neq i$ and 1 if $i = j$.

Solution. Pauli matrices are given by $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. It is direct to verify that, for any $\sigma_i, \sigma_j \in P$, $\mathrm{Tr}(\sigma_i\sigma_j) = 1$ if $i = j$ and 0 otherwise since their eigenvalues are ± 1. Then,

$$\mathrm{Tr}(\rho\tilde{\sigma}) = \mathrm{Tr}\left(\sum_{\sigma\in P} c_\sigma \sigma\tilde{\sigma}\right) = \sum_{\sigma\in P} c_\sigma \mathrm{Tr}(\sigma\tilde{\sigma}) = \sum_{\sigma\in P} c_\sigma \mathrm{Tr}(\sigma\tilde{\sigma}) = c_{\tilde{\sigma}}.$$

□

Pauli matrices are Hermitian and can be interpreted as observables. Therefore, by measuring each operator $\sigma \in P$, we can have access to their expected value $\langle\sigma\rangle = \langle x| \sigma |x\rangle = \mathrm{Tr}(\langle x| \sigma |x\rangle) = \mathrm{Tr}(\rho\sigma)$, and we can reconstruct the density matrix ρ

$$\rho = \frac{\langle I\rangle I + \langle X\rangle X + \langle Y\rangle Y + \langle Z\rangle Z}{2}. \tag{15}$$

Question Implementation 3: Run your HHL circuit on a simulator and a real quantum device and reconstruct completely the solution state for the system defined as

$$A = \frac{1}{9}\begin{pmatrix} 13 & 2+i4 \\ 2-i4 & 14 \end{pmatrix} \text{ and } |b\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i\,|1\rangle) \tag{16}$$

Observable measurements will be detailed in the notebook.

Solution. How to relate $\langle P_1 \otimes I^{\otimes m} \otimes \sigma\rangle$ to $\langle\sigma\rangle$ (here we take $\sigma \in \{I, X, Y, Z\}$):

$$\begin{aligned}
\langle \quad P_1 &\otimes I^{\otimes m} \otimes \sigma\rangle = Tr(|\phi_3\rangle\langle\phi_3|P_1 \otimes I^{\otimes m} \otimes \sigma) \\
&= \sum_{i,j} \beta_i\beta_j Tr\left(\left(\sqrt{1-\frac{1}{\lambda_i^2}}\,|0\rangle + \frac{1}{\lambda_i}\,|1\rangle\right)\left(\sqrt{1-\frac{1}{\lambda_j^2}}\,\langle 0| + \frac{1}{\lambda_j}\,\langle 1|\right) \otimes |0\rangle^{\otimes m}\langle 0|^{\otimes m} \otimes |u_i\rangle\langle u_j|\left(P_1 \otimes I^{\otimes m} \otimes \sigma\right)\right) \\
&= \sum_{i,j} \beta_i\beta_j Tr\left(\left(\sqrt{1-\frac{1}{\lambda_i^2}}\,|0\rangle + \frac{1}{\lambda_i}\,|1\rangle\right)\left(\sqrt{1-\frac{1}{\lambda_j^2}}\,\langle 0| + \frac{1}{\lambda_j}\,\langle 1|\right) P_1 \otimes |0\rangle^{\otimes m}\langle 0|^{\otimes m} \otimes |u_i\rangle\langle u_j|\,\sigma\right) \\
&= \sum_{i,j} \beta_i\beta_j Tr\left(\left(\sqrt{1-\frac{1}{\lambda_i^2}}\,|0\rangle + \frac{1}{\lambda_i}\,|1\rangle\right)\left(\sqrt{1-\frac{1}{\lambda_j^2}}\,\langle 0| + \frac{1}{\lambda_j}\,\langle 1|\right) P_1\right) Tr\left(|0\rangle^{\otimes m}\langle 0|^{\otimes m}\right) Tr\left(|u_i\rangle\langle u_j|\,\sigma\right) \\
&= \sum_{i,j} \frac{\beta_i\beta_j}{\lambda_j} Tr\left(\left(\sqrt{1-\frac{1}{\lambda_i^2}}\,|0\rangle + \frac{1}{\lambda_i}\,|1\rangle\right)\langle 1|\right) Tr\left(|u_i\rangle\langle u_j|\,\sigma\right) \\
&= \sum_{i,j} \frac{\beta_i\beta_j}{\lambda_i\lambda_j} Tr\left(|u_i\rangle\langle u_j|\,\sigma\right) \\
&= \frac{1}{c^2} Tr\left(|x\rangle\langle x|\,\sigma\right) = \frac{\langle\sigma\rangle}{c^2}
\end{aligned}$$

One could also use directly

$$\begin{aligned}
Tr(|\phi_3\rangle\langle\phi_3|P_1 \otimes I^{\otimes m} \otimes \sigma) &= Tr((\langle 1| \otimes I^{\otimes m} \otimes I)|\phi_3\rangle\langle\phi_3|(|1\rangle \otimes I^{\otimes m} \otimes \sigma)) \\
&= \frac{1}{c^2} Tr((|0\rangle^{\otimes m}\langle 0|^{\otimes m} \otimes |x\rangle\langle x|\,(I^{\otimes m} \otimes \sigma))) = \frac{\langle\sigma\rangle}{c^2}.
\end{aligned}$$

□