**Assignment 3: selected solutions**

Problem 1: Show that the norm of a quantum state given by the density matrix $\rho$ remains unchanged if the state is subject to a unitary transformation $\hat{U}$.

Solution: Use the cyclic permutation invariance of the trace operation

$$\mathrm{tr}\,(U\rho U^{\dagger}) = \mathrm{tr}\,(U^{\dagger}U\rho) = \mathrm{tr}\,(\rho).$$

Problem 2: Derive the solution of the Schrödinger equation for the system characterised by a Hamiltonian that is time independent, and show that the resulting evolution operator is unitary if the Hamiltonian is self-adjoint.
Solution: use the separation of variables and integration

$$
\begin{aligned}
i\hbar\frac{\mathrm{d}|\psi(t)\rangle}{\mathrm{d}t} &= \hat{H}|\psi(t)\rangle \\
\frac{\mathrm{d}|\psi(t)\rangle}{|\psi(t)\rangle} &= -\frac{i}{\hbar}\hat{H}\mathrm{d}t \\
\int_0^T \frac{\mathrm{d}|\psi(t)\rangle}{|\psi(t)\rangle} &= -\frac{i}{\hbar}\hat{H}\int_0^T \mathrm{d}t \\
\ln|\psi(T)\rangle - \ln|\psi(0)\rangle &= -\frac{i}{\hbar}\hat{H}T \\
\ln\frac{|\psi(T)\rangle}{|\psi(0)\rangle} &= -\frac{i}{\hbar}\hat{H}T \\
|\psi(T)\rangle &= e^{-\frac{i}{\hbar}\hat{H}T}|\psi(0)\rangle
\end{aligned}
$$

Problem 3: Using the Taylor expansion, show that the evolution operator generated by the Hamiltonian $\hat{H} = \hbar\vec{n}\cdot\vec{\sigma}/2$ can be written as follows:

$$e^{-it\hat{H}/\hbar} \quad = \quad \cos\left(\frac{t}{2}\right)\,\hat{I} - i\sin\left(\frac{t}{2}\right)\,\vec{n}\cdot\vec{\sigma}$$

where $\vec{n} = \left(n_x, n_y, n_z\right)$ is a real unit vector and $\vec{\sigma}$ is the vector of Pauli matrices.

Solution: use properties of the Pauli matrices, specifically that they square to the identity and that they anticommute, to show

$$\begin{aligned}
(\vec{n}\cdot\vec{\sigma})^2 &= (n_x\sigma_x + n_y\sigma_y + n_z\sigma_z)^2 \\
&= (n_x^2 + n_y^2 + n_z^2)\hat{I} + n_xn_y(\sigma_x\sigma_y + \sigma_y\sigma_x) + n_xn_z(\sigma_x\sigma_z + \sigma_z\sigma_x) + n_yn_z(\sigma_y\sigma_z + \sigma_z\sigma_y) \\
&= \hat{I}
\end{aligned}$$

and consequently, $(\vec{n}\cdot\vec{\sigma})^{2n} = \hat{I}$ and $(\vec{n}\cdot\vec{\sigma})^{2n+1} = \vec{n}\cdot\vec{\sigma}$ for all $n \in \mathbb{N}$.

Now, use the Taylor series expansion to show

$$\begin{aligned}
e^{-it\hat{H}/\hbar} = e^{-it\vec{n}\cdot\vec{\sigma}/2} &= \sum_{n=0}^{\infty}(-i)^n\frac{(t/2)^n}{n!}(\vec{n}\cdot\vec{\sigma})^n \\
&= \left[\sum_{n=0}^{\infty}\frac{(-1)^n(t/2)^{2n}}{(2n)!}\right]\hat{I} - i\left[\sum_{n=0}^{\infty}\frac{(-1)^n(t/2)^{2n+1}}{(2n+1)!}\right](\vec{n}\cdot\vec{\sigma}) \\
&= \left[\cos\left(\frac{t}{2}\right)\right]\ \hat{I} - i\left[\sin\left(\frac{t}{2}\right)\right]\ (\vec{n}\cdot\vec{\sigma}).
\end{aligned}$$

Problem 4: Calculate the effect that a single qubit evolution operator $U(t)$, generated by the Hamiltonian $\hat{H} = \hbar\sigma_x/2$ has on a general single qubit pure state in the Bloch representation.

Solution: Evaluate the action of the evolution operator as follows

$$
\begin{aligned}
\rho(t) &= \hat{U}_t\,\rho(0)\,\hat{U}_t^\dagger = e^{-i\sigma_x t/2}\,\rho(0)\,e^{i\sigma_x t/2} \\
&= \frac{1}{2}\left[\hat{I} + \left(\cos\frac{t}{2}\,\hat{I} - i\sin\frac{t}{2}\,\sigma_x\right)\left(r_x\sigma_x + r_y\sigma_y + r_z\sigma_z\right)\left(\cos\frac{t}{2}\,\hat{I} + i\sin\frac{t}{2}\,\sigma_x\right)\right] \\
&= \frac{1}{2}\left[\hat{I} + r_x\,\sigma_x + (r_y\cos t - r_z\sin t)\,\sigma_y + (r_y\sin t + r_z\cos t)\,\sigma_z\right].
\end{aligned}
$$

Problem 5: Calculate the effect that a single qubit evolution operator $U(t)$, generated by the Hamiltonian given by $\hat{H} = \hbar\sigma_z/2$ has on a general single qubit pure state in the Bloch representation.

Solution: Evaluate the action of the evolution operator as follows

$$
\begin{aligned}
\rho(t) &= \hat{U}_t\,\rho(0)\,\hat{U}_t^\dagger = e^{-i\sigma_z t/2}\,\rho(0)\,e^{i\sigma_z t/2} \\
&= \frac{1}{2}\left[\hat{I} + \left(\cos\frac{t}{2}\,\hat{I} - i\sin\frac{t}{2}\,\sigma_z\right)\left(r_x\sigma_x + r_y\sigma_y + r_z\sigma_z\right)\left(\cos\frac{t}{2}\,\hat{I} + i\sin\frac{t}{2}\,\sigma_z\right)\right] \\
&= \frac{1}{2}\left[\hat{I} + (r_x\cos t - r_y\sin t)\,\sigma_x + (r_x\sin t + r_y\cos t)\,\sigma_y + r_z\,\sigma_z\right].
\end{aligned}
$$

Problem 6: Find the global phase with which one needs to multiply the Hadamard gate to convert it from an element of the group $U(2)$ to an element of the group $SU(2)$.

Solution: The Hadamard gate has $\det H = -1$, and hence the global phase is $\sqrt{\det H} = e^{i\pi/2}$. We can rewrite the gate as

$$H = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = e^{i\pi/2} \begin{pmatrix} \frac{e^{-i\pi/2}}{\sqrt{2}} & \frac{e^{-i\pi/2}}{\sqrt{2}} \\ \frac{e^{-i\pi/2}}{\sqrt{2}} & \frac{e^{i\pi/2}}{\sqrt{2}} \end{pmatrix}.$$

Problem 7: Propose a suitable Hamiltonian and determine a duration for which the Hamiltonian has to be turned on to generate the evolution operator which is equivalent up to a global phase to the Hadamard gate.

Solution: Up to the global phase, determined in the previous problem, we can expand the Hadamard gate into a superposition of the Pauli matrices

$$H = e^{i\pi/2}\begin{pmatrix} \frac{e^{-i\pi/2}}{\sqrt{2}} & \frac{e^{-i\pi/2}}{\sqrt{2}} \\ \frac{e^{-i\pi/2}}{\sqrt{2}} & \frac{e^{i\pi/2}}{\sqrt{2}} \end{pmatrix} = e^{i\pi/2}\begin{pmatrix} -\frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} = e^{i\pi/2}\left[0 - i\left(\frac{\sigma_x + \sigma_z}{\sqrt{2}}\right)\right]$$

and using the expression

$$e^{-it\hat{H}/\hbar} \;=\; \cos\left(\frac{t}{2}\right)\,\hat{I} - i\sin\left(\frac{t}{2}\right)\,\vec{n}\cdot\vec{\sigma}$$

we get

$$\begin{aligned} H &= e^{i\pi/2}\left[0 - i\left(\frac{\sigma_x + \sigma_z}{\sqrt{2}}\right)\right] \\ &= e^{i\pi/2}\left[\cos\frac{\pi}{2}\hat{I} - i\sin\frac{\pi}{2}\left(\frac{\sigma_x + \sigma_z}{\sqrt{2}}\right)\right] = e^{i\pi/2}e^{-i\pi\left(\frac{\sigma_x+\sigma_z}{\sqrt{2}}\right)/2} \end{aligned}$$

where $n_x = n_z = \frac{1}{\sqrt{2}}$ and time $t = \pi$ mod $2\pi$.

Problem 8: Show by calculation in the Bloch representation that the bit-flip $X$ and the Hadamard gate $H$ transform the Bloch vector of the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$ in the same way.

Solution: $X = \sigma_x$ and use the properties of Pauli matrices

$$X\,\rho\,X^{\dagger} = \sigma_x\,\rho\,\sigma_x = \frac{1}{2}\left[\hat{I} + \sigma_x\left(r_x\sigma_x + r_y\sigma_y + r_z\sigma_z\right)\sigma_x\right] = \frac{1}{2}\left[\hat{I} + r_x\,\sigma_x - r_y\,\sigma_y - r_z\,\sigma_z\right].$$

For the Hadamard gate, use $H = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)$

$$\begin{aligned} H\,\rho\,H^{\dagger} = H\,\rho\,H &= \frac{1}{2}\left[\hat{I} + \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)\left(r_x\sigma_x + r_y\sigma_y + r_z\sigma_z\right)\frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)\right] \\ &= \frac{1}{2}\left[\hat{I} + r_z\,\sigma_x - r_y\,\sigma_y + r_x\,\sigma_z\right]. \end{aligned}$$

Problem 9: Calculate the local invariants $g_1, g_2$ and $g_3$ for the two-qubit operations $CNOT_{12}$ and $CNOT_{21}$ and determine whether these are in the same local equivalence class.

Solution: $CNOT_{12}$

$$
\begin{aligned}
U_B &= U_Q^\dagger (CNOT_{12}) U_Q = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & -i & -i & 0 \\ 0 & 1 & -1 & 0 \\ -i & 0 & 0 & i \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & i \\ 0 & i & 1 & 0 \\ 0 & i & -1 & 0 \\ 1 & 0 & 0 & -i \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & -i & -i & 0 \\ 0 & 1 & -1 & 0 \\ -i & 0 & 0 & i \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & i \\ 0 & i & 1 & 0 \\ 1 & 0 & 0 & -i \\ 0 & i & -1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & i & -1 & i \\ -i & 1 & -i & -1 \\ -1 & i & 1 & i \\ -i & -1 & -i & 1 \end{pmatrix}
\end{aligned}
$$

$$m = U_B^T U_B = \begin{pmatrix} 1 & -i & -1 & -i \\ i & 1 & i & -1 \\ -1 & -i & 1 & -i \\ i & -1 & i & 1 \end{pmatrix} \begin{pmatrix} 1 & i & -1 & i \\ -i & 1 & -i & -1 \\ -1 & i & 1 & i \\ -i & -1 & -i & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

Using the local invariants defined for $U(4)$ and $\det(U) = -1$, we get

$$g_1 = \frac{Re\left[\mathrm{tr}^2(m)\right]}{16\det(U)} = 0, \quad g_2 = \frac{Im\left[\mathrm{tr}^2(m)\right]}{16\det(U)} = 0, \quad g_3 = \frac{\left[\mathrm{tr}^2(m) - \mathrm{tr}(m^2)\right]}{4\det(U)} = 1.$$

The transformation of $CNOT_{21}$ into the magic Bell basis produces the

$$U_B = U_Q^\dagger (CNOT_{12}) U_Q = \frac{1}{2} \begin{pmatrix} 1 & i & -1 & i \\ -1 & i & 1 & i \\ -i & -1 & -i & 1 \\ -i & 1 & -i & -1 \end{pmatrix}$$

which gives the same Maklin matrix as $CNOT_{12}$

$$m = U_B^T U_B = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

and thus the same local invariants

$$g_1 = \frac{Re\left[\mathrm{tr}^2(m)\right]}{16\,\det(U)} = 0, \qquad g_2 = \frac{Im\left[\mathrm{tr}^2(m)\right]}{16\,\det(U)} = 0, \qquad g_3 = \frac{\left[\mathrm{tr}^2(m) - \mathrm{tr}\,(m^2)\right]}{4\,\det(U)} = 1.$$

**Projective measurement**

A single measurement of an observable $\hat{M}$ can only yield one of its eigenvalues $\lambda_m$ which satisfy the eigenvalue equation

$$\hat{M}|\psi_m\rangle = \lambda_m|\psi_m\rangle$$

where $|\psi_m\rangle$ is the eigenvector associated with the eigenvalue $\lambda_m$.

The measurement operators correspond to the projectors $\hat{P}_m = |\psi_m\rangle\langle\psi_m|$ onto eigen-subspaces, which are associated with eigenvalues $\lambda_m$ and are spanned by the corresponding eigenvectors $|\psi_m\rangle$, in the spectral decomposition of the observable $\hat{M}$:

$$\hat{M} = \sum_m \lambda_m|\psi_m\rangle\langle\psi_m| = \sum_m \lambda_m\hat{P}_m.$$

If the state of the system before the measurement is $|\phi\rangle$, then the probability that the result $\lambda_m$ occurs is

$$p_m = \langle\phi|\hat{P}_m^\dagger \hat{P}_m|\phi\rangle = \langle\phi|\hat{P}_m^2|\phi\rangle = \langle\phi|\hat{P}_m|\phi\rangle$$

and the state immediately after the measurement is

$$|\psi\rangle = \frac{\hat{P}_m|\phi\rangle}{\||\hat{P}_m|\phi\rangle\||} = \frac{\hat{P}_m|\phi\rangle}{\sqrt{\langle\phi|\hat{P}_m^\dagger \hat{P}_m|\phi\rangle}} = \frac{\hat{P}_m|\phi\rangle}{\sqrt{\langle\phi|\hat{P}_m|\phi\rangle}} = \frac{\hat{P}_m|\phi\rangle}{\sqrt{p_m}}$$

Projective measurement allows us to easily calculate the expectation value of an observable $\hat{M}$ for the system in the state $|\phi\rangle$

$$< \hat{M} >= \langle\phi|\hat{M}|\phi\rangle = \langle\phi|\left(\sum_m \lambda_m \hat{P}_m\right)|\phi\rangle = \sum_m \lambda_m \langle\phi|\hat{P}_m|\phi\rangle = \sum_m \lambda_m p_m$$

**Projective measurements on states given by density matrices**

Consider a single qubit pure state $|\phi\rangle = c_0|0\rangle + c_1|1\rangle$:

$$\hat{\rho} = |\phi\rangle\langle\phi| = |c_0|^2|0\rangle\langle 0| + c_0 c_1^*|0\rangle\langle 1| + c_0^* c_1|1\rangle\langle 0| + |c_1|^2|1\rangle\langle 1|.$$

The norm is calculated as the trace of the density matrix, that is, the sum of its diagonal matrix elements

$$\mathrm{tr}\,\hat{\rho} = \langle 0|\hat{\rho}|0\rangle + \langle 1|\hat{\rho}|1\rangle = |c_0|^2 + |c_1|^2 = 1.$$

The operators for a measurement in the standard computational basis

$$\hat{P}_0 = |0\rangle\langle 0|, \qquad \hat{P}_1 = |1\rangle\langle 1|.$$

the probabilities of the measurement results $0$ and $1$:

$$\begin{aligned} p_0 &= \mathrm{tr}\left(\hat{P}_0|\phi\rangle\langle\phi|\hat{P}_0^\dagger\right) = \mathrm{tr}\left(\hat{P}_0\hat{\rho}\hat{P}_0^\dagger\right) = \mathrm{tr}\left(\hat{P}_0\hat{\rho}\hat{P}_0\right) = \mathrm{tr}\left(\hat{P}_0^2\hat{\rho}\right) = \mathrm{tr}\left(\hat{P}_0\hat{\rho}\right), \\ p_1 &= \mathrm{tr}\left(\hat{P}_1\hat{\rho}\hat{P}_1^\dagger\right) = \mathrm{tr}\left(\hat{P}_1\hat{\rho}\right). \end{aligned}$$

and the states after the measurement:

$$\rho_0 = \frac{\hat{P}_0\hat{\rho}\hat{P}_0^\dagger}{\mathrm{tr}\,(\hat{P}_0\hat{\rho}\hat{P}_0^\dagger)} = \frac{\hat{P}_0\hat{\rho}\hat{P}_0}{\mathrm{tr}\,(\hat{P}_0\hat{\rho})},$$
$$\rho_1 = \frac{\hat{P}_1\hat{\rho}\hat{P}_1^\dagger}{\mathrm{tr}\,(\hat{P}_1\hat{\rho}\hat{P}_1^\dagger)} = \frac{\hat{P}_1\hat{\rho}\hat{P}_1}{\mathrm{tr}\,(\hat{P}_1\hat{\rho})},$$

**Single-qubit measurements on multi-qubit systems**

Example: measurement operators for measurements of the second qubit in the standard computational basis on a two-qubit system:

$$\hat{P}_0^{(2)} = \hat{1} \otimes \hat{P}_0 = \hat{1} \otimes |0\rangle\langle 0|,$$
$$\hat{P}_1^{(2)} = \hat{1} \otimes \hat{P}_1 = \hat{1} \otimes |1\rangle\langle 1|.$$

where $\hat{1}$ is a $2 \times 2$ unit matrix acting on the first qubit which is not being measured.