Exercise 11.2

(a)

Recall that σ_j are the Pauli matrices: $\sigma_1 = X$, $\sigma_2 = Y$, $\sigma_3 = Z$. Since $\{I, \sigma_1, \sigma_2, \sigma_3\}$ forms a basis of 2×2 matrices, we can represent any density matrix ρ as

$$\rho = \alpha \, \mathbf{I} + \frac{1}{2} \, \left(r_1 \, \sigma_1 + r_2 \, \sigma_2 + r_3 \, \sigma_3 \right)$$

using suitable coefficients α , r_1 , r_2 , r_3 . These coefficients are real since any density matrix ρ and the Pauli matrices are Hermitian.

The Pauli matrices are traceless: $Tr[\sigma_j] = 0$, thus

$$Tr[\rho] = \alpha Tr[I] = 2 \alpha$$
.

Density matrices have trace 1, and therefore $\alpha = \frac{1}{2}$.

In summary, we arrive at the representation

$$\rho = \frac{\vec{I} + \vec{r} \cdot \vec{\sigma}}{2} \tag{1}$$

 $BlochDensity[r_] := \frac{1}{2} \left(IdentityMatrix[2] + Sum[r[i]] PauliMatrix[i], \{i, 3\} \right)$

Explicit matrix form:

BlochDensity[{r₁, r₂, r₃}] // MatrixForm

$$\begin{pmatrix} \frac{1}{2} (1 + r_3) & \frac{1}{2} (r_1 - i r_2) \\ \frac{1}{2} (r_1 + i r_2) & \frac{1}{2} (1 - r_3) \end{pmatrix}$$

Eigenvalues:

Eigenvalues[BlochDensity[$\{r_1, r_2, r_3\}$]]

$$\left\{\frac{1}{2}\left(1-\sqrt{r_1^2+r_2^2+r_3^2}\right),\ \frac{1}{2}\left(1+\sqrt{r_1^2+r_2^2+r_3^2}\right)\right\}$$

Density matrices are positive operators, i.e., their eigenvalues are non-negative. In particular,

$$\frac{1}{2}\left(1-\sqrt{r_1^2+r_2^2+r_3^2}\right)\geq 0,$$

which is equivalent to $\|\vec{r}\| \le 1$.

(b)

Recall that a density matrix ρ describes a pure state if and only if it can be written as $\rho = |\psi\rangle\langle\psi|$, equivalently if one eigenvalue of ρ is 1 and the others are all 0. Based on the two eigenvalues computed above, this is equivalent to $\|\vec{r}\| = 1$.

Alternative solution: in the lecture we have derived the criterion $Tr[\rho^2] = 1$ to characterize pure states. Inserting the representation in Eq. (1) leads to

$$Tr[\rho^{2}] = \frac{1}{4} Tr[(\mathbf{I} + \vec{r} \cdot \vec{\sigma})^{2}] = \frac{1}{4} Tr[\mathbf{I} + 2 \vec{r} \cdot \vec{\sigma} + (\vec{r} \cdot \vec{\sigma})^{2}] = \frac{1}{4} (Tr[\mathbf{I}] + Tr[(r_{1}^{2} + r_{2}^{2} + r_{3}^{2}) \mathbf{I}]) = \frac{1}{2} (1 + ||\vec{r}||^{2})$$
(2)

where we have used that the Pauli matrices are traceless and $(\vec{r} \cdot \vec{\sigma})^2 = (r_1^2 + r_2^2 + r_3^2) I$ (which one can check by direct computation). Directly from Eq. (2) one concludes that $Tr[\rho^2] = 1$ is equivalent to $\|\vec{r}\| = 1$.

(c)

$$\psi = e^{i\gamma} \left\{ \cos\left[\frac{\theta}{2}\right], e^{i\phi} \sin\left[\frac{\theta}{2}\right] \right\};$$

Compute $|\psi\rangle\langle\psi|$:

FullSimplify[KroneckerProduct[ψ , Conjugate[ψ]],

Assumptions $\rightarrow \{ \gamma \in \text{Reals}, \theta \in \text{Reals}, \phi \in \text{Reals} \}] // \text{MatrixForm}$

$$\begin{pmatrix} \cos\left[\frac{\theta}{2}\right]^2 & \frac{1}{2} e^{-i\phi} \sin[\theta] \\ \frac{1}{2} e^{i\phi} \sin[\theta] & \sin\left[\frac{\theta}{2}\right]^2 \end{pmatrix}$$

We now compute the vector \vec{r} implicitly defined via $|\psi\rangle\langle\psi| = (I + \vec{r} \cdot \vec{\sigma})/2$. First recall the definition of the Pauli matrices:

$$\sigma_1 = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Based on the diagonal entries, one concludes that

$$\cos\left[\frac{\theta}{2}\right]^2 = \frac{1+r_3}{2}$$
, $\sin\left[\frac{\theta}{2}\right]^2 = \frac{1-r_3}{2}$,

which has the solution $r_3 = Cos[\theta]$. Check:

$$\operatorname{FullSimplify} \left[\operatorname{Cos} \left[\frac{\theta}{2} \right]^2 - \frac{1 + \operatorname{Cos} [\theta]}{2} \right]$$

FullSimplify
$$\left[Sin \left[\frac{\theta}{2} \right]^2 - \frac{1 - Cos[\theta]}{2} \right]$$

0

From the off-diagonal entries, it follows that

$$\frac{1}{2} e^{-i\phi} \operatorname{Sin}[\theta] = \frac{1}{2} (r_1 - i r_2), \quad \frac{1}{2} e^{i\phi} \operatorname{Sin}[\theta] = \frac{1}{2} (r_1 + i r_2)$$

with solution (see Euler's formula)

$$r_1 = Cos[\phi] \times Sin[\theta], \quad r_2 = Sin[\phi] \times Sin[\theta].$$