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

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

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: $\mathrm{Tr}[\sigma_j] = 0$, thus

$\mathrm{Tr}[\rho] = \alpha \mathrm{Tr}[I] = 2\alpha.$

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

In summary, we arrive at the representation

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

```
BlochDensity[r_] := 1/2 (IdentityMatrix[2] + Sum[r[[i]] PauliMatrix[i], {i, 3}])
```

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[{r1, r2, r3}]]
```

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

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 $\|\vec{r}\| \leq 1$.

(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 $\mathrm{Tr}[\rho^2] = 1$ to characterize pure states. Inserting the representation in Eq. (1) leads to

$$\mathrm{Tr}\left[\rho^2\right] = \frac{1}{4}\mathrm{Tr}\left[\left(\mathrm{I} + \vec{r}.\vec{\sigma}\right)^2\right] = \\ \frac{1}{4}\mathrm{Tr}\left[\mathrm{I} + 2\,\vec{r}.\vec{\sigma} + \left(\vec{r}.\vec{\sigma}\right)^2\right] = \frac{1}{4}\left(\mathrm{Tr}[\mathrm{I}] + \mathrm{Tr}\left[\left(r_1^2 + r_2^2 + r_3^2\right)\mathrm{I}\right]\right) = \frac{1}{2}\left(1 + \|\vec{r}\|^2\right) \tag{2}$$

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

(c)

```
ψ = ⅇ^(ⅈ γ) {Cos[θ/2], ⅇ^(ⅈ ϕ) Sin[θ/2]};
```

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

```
FullSimplify[KroneckerProduct[ψ, Conjugate[ψ]],
  Assumptions → {γ ∈ Reals, θ ∈ Reals, ϕ ∈ Reals}] // MatrixForm
```

$$\begin{pmatrix} \mathrm{Cos}\left[\frac{\theta}{2}\right]^2 & \frac{1}{2}e^{-i\phi}\,\mathrm{Sin}[\theta] \\ \frac{1}{2}e^{i\phi}\,\mathrm{Sin}[\theta] & \mathrm{Sin}\left[\frac{\theta}{2}\right]^2 \end{pmatrix}$$

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

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

Based on the diagonal entries, one concludes that

$$\mathrm{Cos}\left[\frac{\theta}{2}\right]^2 = \frac{1 + r_3}{2},\ \mathrm{Sin}\left[\frac{\theta}{2}\right]^2 = \frac{1 - r_3}{2},$$

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

```
FullSimplify[Cos[θ/2]^2 - (1 + Cos[θ])/2]
FullSimplify[Sin[θ/2]^2 - (1 - Cos[θ])/2]
```

```
0
```

```
0
```

From the off-diagonal entries, it follows that

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

with solution (see Euler’s formula)

$$r_1 = \mathrm{Cos}[\phi]\,\mathrm{Sin}[\theta],\ r_2 = \mathrm{Sin}[\phi]\,\mathrm{Sin}[\theta].$$