University of Padova

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Homework for

Quantum Information and Computing

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Submitted to

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1 Exercise

Given: A qubit with basis states $\{|0\langle, |1\rangle\}$ and the operator

$$\hat{H} = \left[\Delta\omega\hat{\sigma}_z \quad \gamma\hat{\sigma}_x\right] \tag{1.1}$$

where $\Delta\omega,\ \gamma \in \mathbb{R}$ with the unit $[\frac{1}{\mathrm{s}}]$.

1. The operator

$$\hat{H} = \hbar \begin{pmatrix} \Delta\omega & \gamma \\ \gamma & -\Delta\omega \end{pmatrix} \tag{1.2}$$

is clearly linear, symmetric, and contains only real numbers; thus, it is also hermitian. As the Hamiltonian describes the energy state of the system, the units (in the SI system) have to be Joules, which is clearly the case since $\hbar$ has the unit [J s].

2. The eigenvalues of the Hamiltonian can be calculated by setting

$$\det \hat{H} - \lambda\mathbb{1} = (\hbar\Delta\omega - \lambda)\left(-\hbar\Delta\omega - \lambda\right) - \hbar^2\gamma^2 \tag{1.3}$$

$$= \lambda^2 - \hbar^2\left(\Delta\omega^2 + \gamma^2\right) \stackrel{!}{=} 0 \tag{1.4}$$

Introducing the following notation, the two eigenvalues $\lambda_{0,1}$ are thus:

$$\Omega = \sqrt{\Delta\omega^2 + \gamma^2} \tag{1.5}$$

$$\lambda_0 = \hbar\sqrt{\Delta\omega^2 + \gamma^2} = \hbar\Omega \tag{1.6}$$

$$\lambda_1 = -\hbar\sqrt{\Delta\omega^2 + \gamma^2} = -\hbar\Omega \tag{1.7}$$

With this, the corresponding eigenvectors $|E_{0,1}\rangle$ can be calculated. For λ_0 the following equation needs to hold:

$$\left(\hat{H} - \lambda_0\mathbb{1}\right)|E_0\rangle = \begin{pmatrix} \hbar\Delta\omega - \hbar\Omega & \hbar\gamma \\ \hbar\gamma & -\hbar\Delta\omega - \hbar\Omega \end{pmatrix} \begin{pmatrix} v_0 \\ v_1 \end{pmatrix} \stackrel{!}{=} \mathbf{0} \tag{1.8}$$

$$\Rightarrow \begin{pmatrix} \left(\Delta\omega - \Omega\right)v_0 + \gamma v_1 \\ \gamma v_0 - \left(\Delta\omega - \Omega\right)v_1 \end{pmatrix} = \mathbf{0} \tag{1.9}$$

$$\Rightarrow v_1 = \frac{\Omega - \Delta\omega}{\gamma} v_0 \tag{1.10}$$

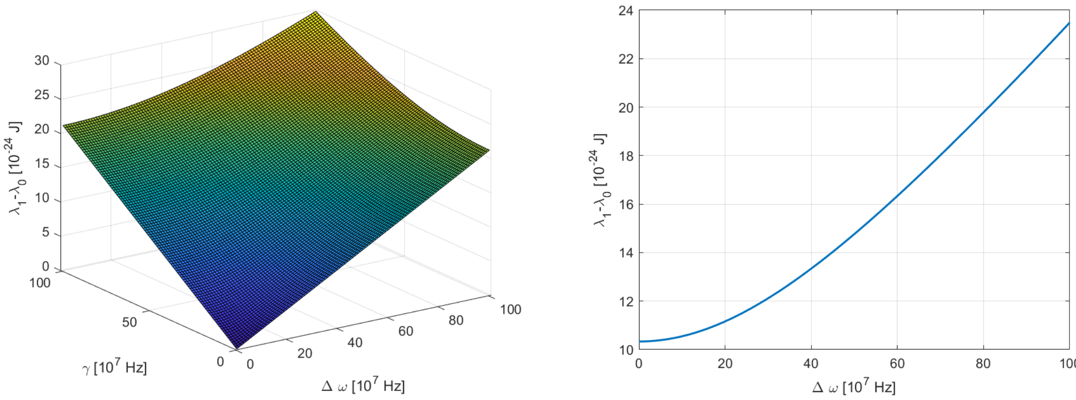
And therefore:

$$|E_0\rangle = |0\rangle + \frac{\Omega - \Delta\omega}{\gamma}|1\rangle \tag{1.11}$$

Following the same procedure, the eigenvalue for λ_1 is:

$$|E_1\rangle = |0\rangle - \frac{\Omega + \Delta\omega}{\gamma}|1\rangle \tag{1.12}$$

The energy gap $\lambda_1 - \lambda_0 = 2\hbar\Omega$ is depicted in Figure 1.1(a) as a function of both $\Delta\omega$ and γ, and in Figure1.1(b) as a function of $\Delta\omega$ only, with $\gamma = 5 \cdot 10^6$Hz.



(a) (b)

Figure 1.1: Plot of the energy gap.

3. The temporal evolution as defined by the Hamiltonian can be expressed as a unitary operator:

$$\hat{U}(t) = \exp\left\{-\frac{i}{\hbar}\hat{H}t\right\} \tag{1.13}$$

The Hamiltonian can be rewritten as a combination of Pauli matrices:

$$\hat{H} = \vec{n'}\vec{\sigma} \tag{1.14}$$

By normalizing

$$\vec{n'} = \hbar\begin{bmatrix}\gamma & 0 & \Delta\omega\end{bmatrix} \Rightarrow \vec{n} = \frac{\vec{n'}}{\hbar\Omega} \tag{1.15}$$

one obtains the unitary:

$$\hat{U}(t) = \exp\{-i\Omega\vec{n}\vec{\sigma}t\} \tag{1.16}$$

Expanding this using the power series and the properties of Pauli matrices, this can be expressed as:

$$\hat{U}(t) = \sum_{k=0}^{+\infty} \frac{\left(-i\Omega t\vec{n}\vec{\sigma}\right)^k}{k!} \tag{1.17}$$

$$= \sum_{k=0}^{+\infty} \frac{\left(-i\Omega t\right)^{2k}}{2k!} \left(\vec{n}\vec{\sigma}\right)^{2k} + \sum_{k=0}^{+\infty} \frac{\left(-i\Omega t\right)^{2k+1}}{(2k+1)!} \left(\vec{n}\vec{\sigma}\right)^{2k+1} \tag{1.18}$$

$$= \sum_{k=0}^{+\infty} \frac{\left(-i\Omega t\right)^{2k}}{2k!} \mathbb{1} + \sum_{k=0}^{+\infty} \frac{\left(-i\Omega t\right)^{2k+1}}{(2k+1)!} \vec{n}\vec{\sigma} \tag{1.19}$$

$$= \cos\left(\Omega t\right) \mathbb{1} - i\sin\left(\Omega t\right) \vec{n}\vec{\sigma} \tag{1.20}$$

The temporal evolution of the states $|\pm i\rangle$ can thus be expressed as:

$$\hat{U}(t)|\pm i\rangle = \left(\cos\left(\Omega t\right) \mathbb{1} - i\sin\left(\Omega t\right) \left(\frac{\gamma}{\Omega}\hat{\sigma}_x + \frac{\Delta\omega}{\Omega}\hat{\sigma}_x\right)\right) \left(\frac{1}{\sqrt{2}}\left(|0\rangle \pm |1\rangle\right)\right) \tag{1.21}$$

$$\begin{aligned} =&\frac{1}{\sqrt{2}}\cos\left(\Omega t\right)|0\rangle - \frac{i}{\sqrt{2}}\sin\left(\Omega t\right)\left(\frac{\gamma}{\Omega}|1\rangle + \frac{\Delta\omega}{\Omega}|0\rangle\right) \\ &\pm \frac{i}{\sqrt{2}}\cos\left(\Omega t\right)|1\rangle \pm \frac{1}{\sqrt{2}}\sin\left(\Omega t\right)\left(\frac{\gamma}{\Omega}|0\rangle - \frac{\Delta\omega}{\Omega}|1\rangle\right) \end{aligned} \tag{1.22}$$

$$\begin{aligned} =&\frac{1}{\sqrt{2}}\left(\left(\cos\left(\Omega t\right) \pm \frac{\gamma}{\Omega}\sin\left(\Omega t\right)\right) - i\sin\left(\Omega t\right)\frac{\Delta\omega}{\Omega}\right)|0\rangle \\ &+ \frac{1}{\sqrt{2}}\left(\mp\sin\left(\Omega t\right)\frac{\Delta\omega}{\Omega} \pm i\left(\cos\left(\Omega t\right) \mp \sin\left(\Omega t\right)\frac{\gamma}{\Omega}\right)\right)|1\rangle \end{aligned} \tag{1.23}$$

4. The components of the Bloch vectors $\vec{r}_{0,1}$ for generic states can be evaluated as follows:

$$|\psi\rangle = a|0\rangle + b|1\rangle \qquad \vec{r} = \begin{bmatrix} x & y & z \end{bmatrix} \tag{1.24}$$

$$\Rightarrow x = 2\,\mathrm{Re}\left(a'b\right) \tag{1.25}$$

$$y = 2\,\mathrm{Im}\left(a'b\right) \tag{1.26}$$

$$z = |a|^2 - |b|^2 \tag{1.27}$$

The expressions for the state evolutions from Equation 1.23 were implemented in MATLAB using the symbolic toolbox, and the expressions for x, y, and z were evaluated:

$$x_0 = -\frac{\Delta\omega}{\Omega}\sin\left(2\Omega t\right) \qquad x_1 = \frac{\Delta\omega}{\Omega}\sin\left(2\Omega t\right) \tag{1.28}$$

$$y_0 = \cos^2\left(\Omega t\right) - \sin^2(\Omega t) \qquad y_1 = 2\sin^2(\Omega t) - \cos^2\left(\Omega t\right) \tag{1.29}$$

$$z_0 = \frac{\gamma}{\Omega}\sin(2\Omega t) \qquad z_1 = -\frac{\gamma}{\Omega}\sin(2\Omega t) \tag{1.30}$$

The trajectories of the normalized vectors trace the same unit circle on the surface of the Bloch sphere. The vectors are always antiparallel, as the dot product between them is $\vec{r}_0 \cdot \vec{r}_1 = -1 \; \forall t$. They lie in the plane normal to $\vec{n}$. Figure 1.2 shows the traced circle for $\Delta\omega = \gamma$.

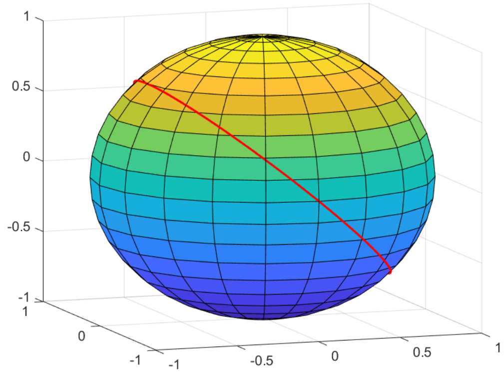


Figure 1.2: Trajectories of the Bloch vectors on the Bloch sphere.

5. From Equation 1.16, it is also possible to see that the unitary describing the temporal evolution is a rotation operator, rotating Bloch vectors around $\vec{n}$ with angular frequency 2Ω. Thus the states $|psi_{0,1}\rangle$ coincide with $|\pm i\rangle$ (each with their respective starting point) at the times $\frac{n}{2\Omega}$, $n \in \mathbb{N}$.

$$\hat{U}(t) = \exp\left(i\Omega\vec{n}\vec{\sigma}t\right) = \hat{R}_{\vec{n}}(2\Omega t) \tag{1.31}$$

2 Exercise

Given: A qubit system A, coupled with a qtrit system B, in the initial states $|\psi\rangle_A = \alpha|0\rangle + \beta|1\rangle$ and $|0\rangle_B$ and a unitary defining their interactions:

$$\hat{U}|00\rangle = \frac{1}{\sqrt{5}}(\sqrt{2}|10\rangle + |01\rangle + \sqrt{2}|02\rangle) \tag{2.1}$$

$$\hat{U}|10\rangle = \frac{1}{2}(|10\rangle - \sqrt{2}|01\rangle + |11\rangle) \tag{2.2}$$

1. The final joint state after the interaction is:

$$\begin{aligned}
|\Psi\rangle_{AB} &= \hat{U}(|\psi\rangle_A \otimes |0\rangle_B) &(2.3)\\
&= \hat{U}\left((\alpha|0\rangle_A + \beta|1\rangle_A) \otimes |0\rangle_B\right) &(2.4)\\
&= \hat{U}(\alpha|00\rangle + \beta|10\rangle) &(2.5)\\
&= \frac{\alpha}{\sqrt{5}}(|01\rangle + \sqrt{2}|02\rangle + \sqrt{2}|10\rangle) + \frac{\beta}{2}(-\sqrt{2}|01\rangle + |10\rangle + |11\rangle) &(2.6)\\
&= \left(\frac{\alpha}{\sqrt{5}} - \frac{\beta}{\sqrt{2}}\right)|01\rangle + \alpha\sqrt{\frac{2}{5}}|02\rangle + \left(\alpha\sqrt{\frac{2}{5}} + \frac{\beta}{2}\right)|10\rangle + \frac{\beta}{2}|11\rangle &(2.7)
\end{aligned}$$

2. The resulting state on the subsystem A can be evaluated by tracing out B. For notational convenience, the subscripts for the system are dropped in unambiguous cases. For clarity, joint states will be denoted by capital symbols. Also, the following complex numbers are defined:

$$a = \frac{\alpha}{\sqrt{5}} - \frac{\beta}{\sqrt{2}} \qquad c = \alpha\sqrt{\frac{2}{5}} + \frac{\beta}{2} \tag{2.8}$$

$$b = \alpha\sqrt{\frac{2}{5}} \qquad d = \frac{\beta}{2} \tag{2.9}$$

With these, the joint state can be expressed as:

$$|\Psi\rangle = a|01\rangle + b|02\rangle + c|10\rangle + d|11\rangle \tag{2.10}$$

The state of the subsystem A can be computed as:

$$\hat{\rho}_A = \mathrm{Tr}_B(|\Psi\rangle\langle\Psi|) = \sum_{n=0}^{2} {}_B\langle n|\Psi\rangle\langle\Psi|n\rangle_B \tag{2.11}$$

The ket-bra evaluates to:

$$\begin{aligned}
|\Psi\rangle\langle\Psi| = &|a|^2|01\rangle\langle 01| + ab'|01\rangle\langle 02| + ac'|01\rangle\langle 10| + ad'|01\rangle\langle 11|\\
&+ ba'|02\rangle\langle 01| + |b|^2|02\rangle\langle 02| + bc'|02\rangle\langle 10| + bd'|02\rangle\langle 11|\\
&+ ca'|10\rangle\langle 01| + cb'|10\rangle\langle 02| + |c|^2|10\rangle\langle 10| + cd'|10\rangle\langle 11|\\
&+ da'|11\rangle\langle 01| + db'|11\rangle\langle 02| + dc'|11\rangle\langle 10| + |d|^2|11\rangle\langle 11| \qquad (2.12)
\end{aligned}$$

The trace has the effect of singling out those contributions in which the part on B is equal, thus it evaluates to:

$$\hat{\rho}_A = (|a|^2 + |b|^2)\,|0\rangle\langle 0| + ad'\,|0\rangle\langle 1| + da'\,|1\rangle\langle 0| + (|c|^2 + |d|^2)\,|1\rangle\langle 1| \tag{2.13}$$

$$= \begin{pmatrix} |a|^2 + |b|^2 & ad' \\ da' & |c|^2 + |d|^2 \end{pmatrix} \tag{2.14}$$

3. Once the system B is measured in the computational basis, system A is affected by the generalized measurement operators $\hat{M}_n$, which can be calculated by:

$$|\Psi\rangle = \sum_{n=0}^{2} \hat{M}_n\,|\psi\rangle_A\,|n\rangle_B \tag{2.15}$$

$$\Rightarrow \langle k|\,\Psi\rangle = \langle k|\left(\sum_{n=0}^{2} \hat{M}_n\,|\psi\rangle\,|n\rangle\right) \tag{2.16}$$

$$= \sum_{n=0}^{2} \delta_{nk}\hat{M}_n\,|\psi\rangle \tag{2.17}$$

$$= \hat{M}_k\,|\psi\rangle \tag{2.18}$$

for $k = 0$:

$$\hat{M}_0\,|\psi\rangle = \hat{M}_0(\alpha\,|0\rangle + \beta\,|1\rangle) = \tag{2.19}$$

$$\langle 0|\,\Psi\rangle = c\,|1\rangle = \left(\alpha\sqrt{\frac{2}{5}} + \frac{\beta}{2}\right)|1\rangle \tag{2.20}$$

$$\Rightarrow \hat{M}_0 = \begin{pmatrix} 0 & 0 \\ \sqrt{\frac{2}{5}} & \frac{1}{2} \end{pmatrix} \tag{2.21}$$

for $k = 1$:

$$\hat{M}_1\,|\psi\rangle = \hat{M}_1(\alpha\,|0\rangle + \beta\,|1\rangle) = \tag{2.22}$$

$$\langle 1|\,\Psi\rangle = a\,|0\rangle + d\,|1\rangle = \left(\frac{\alpha}{\sqrt{5}} + \frac{\beta}{\sqrt{2}}\right)|0\rangle + \frac{\beta}{2}\,|1\rangle \tag{2.23}$$

$$\Rightarrow \hat{M}_1 = \begin{pmatrix} \frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{2} \end{pmatrix} \tag{2.24}$$

for $k = 2$:

$$\hat{M}_2\,|\psi\rangle = \hat{M}_2(\alpha\,|0\rangle + \beta\,|1\rangle) = \tag{2.25}$$

$$\langle 2|\,\Psi\rangle = b\,|0\rangle = \alpha\sqrt{\frac{2}{5}}\,|0\rangle \tag{2.26}$$

$$\Rightarrow \hat{M}_2 = \begin{pmatrix} \sqrt{\frac{2}{5}} & 0 \\ 0 & 0 \end{pmatrix} \tag{2.27}$$

4. The post measurement state of A after a measurement is obtained is given by:

$$|\psi_f\rangle = \frac{\hat{M}_k |\psi\rangle}{\sqrt{p_k}} \tag{2.28}$$

where the probability p_i for the measurement is given by:

$$\begin{aligned}
p_k &= \mathrm{Tr}\left(\hat{M}_k^\dagger \hat{M}_k |\psi\rangle \langle\psi|\right) && (2.29)\\
&= \mathrm{Tr}\left(\begin{pmatrix} \frac{2}{5} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} |\alpha|^2 & \alpha\beta' \\ \alpha'\beta & |\beta|^2 \end{pmatrix}\right) && (2.30)\\
&= \mathrm{Tr}\begin{pmatrix} \frac{2|\alpha|^2}{5} & \frac{2\alpha\beta'}{5} \\ 0 & 0 \end{pmatrix} && (2.31)\\
&= \frac{2|\alpha|^2}{5} && (2.32)
\end{aligned}$$

With this, the post measurement state is evaluated to:

$$|\psi_f\rangle = \frac{\alpha\sqrt{\frac{2}{5}}\,|0\rangle}{|\alpha|\sqrt{\frac{2}{5}}} = \frac{\alpha}{|\alpha|}\,|0\rangle \tag{2.33}$$

In this description, $\frac{\alpha}{|\alpha|}$ describes a global phase and can be disregarded. The final post measurement state is thus:

$$|\psi_f\rangle = |0\rangle \tag{2.34}$$

5. The POVM elements $\hat{F}_k$ can be derived from the generalized measurement operators and satisfy the completeness relation:

$$\begin{aligned}
\hat{F}_k &= \hat{M}_k^\dagger \hat{M}_k && (2.35)\\
\sum_{k=0}^{2} \hat{F}_k &= \mathbb{1} && (2.36)
\end{aligned}$$

for $k = 0$:

$$\begin{aligned}
\hat{F}_0 = \hat{M}_0^\dagger \hat{M}_0 &= \begin{pmatrix} 0 & \sqrt{\frac{2}{5}} \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ \sqrt{\frac{2}{5}} & \frac{1}{2} \end{pmatrix} && (2.37)\\
&= \begin{pmatrix} \frac{2}{5} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{10}} & \frac{1}{4} \end{pmatrix} && (2.38)
\end{aligned}$$

for $k = 1$:

$$\begin{aligned}
\hat{F}_1 = \hat{M}_1^\dagger \hat{M}_1 &= \begin{pmatrix} \frac{1}{\sqrt{5}} & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{2} \end{pmatrix} && (2.39)\\
&= \begin{pmatrix} \frac{1}{5} & -\frac{1}{\sqrt{10}} \\ -\frac{1}{\sqrt{10}} & \frac{3}{4} \end{pmatrix} && (2.40)
\end{aligned}$$

for $k = 2$:

$$\hat{F}_2 = \hat{M}_2^\dagger \hat{M}_2 = \begin{pmatrix} \sqrt{\frac{2}{5}} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{\frac{2}{5}} & 0 \\ 0 & 0 \end{pmatrix} \tag{2.41}$$

$$= \begin{pmatrix} \frac{2}{5} & 0 \\ 0 & 0 \end{pmatrix} \tag{2.42}$$

As a check, taking the sum yields:

$$\sum_{k=0}^{2} \hat{F}_k = \begin{pmatrix} \frac{2}{5} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{10}} & \frac{1}{4} \end{pmatrix} + \begin{pmatrix} \frac{1}{5} & -\frac{1}{\sqrt{10}} \\ -\frac{1}{\sqrt{10}} & \frac{3}{4} \end{pmatrix} + \begin{pmatrix} \frac{2}{5} & 0 \\ 0 & 0 \end{pmatrix} \tag{2.43}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1} \tag{2.44}$$

5. The probabilities for the measurements can be calculated in the same way as in equation 2.29. Given the state

$$\rho = \frac{1}{5} |0\rangle \langle 0| + \frac{4}{5} |1\rangle \langle 1| \tag{2.45}$$

for $k = 0$:

$$p_0 = \mathrm{Tr}\Big(\hat{F}_0 \rho\Big) = \mathrm{Tr}\left(\begin{pmatrix} \frac{2}{5} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{10}} & \frac{1}{4} \end{pmatrix} \begin{pmatrix} \frac{1}{5} & 0 \\ 0 & \frac{4}{5} \end{pmatrix} \right) \tag{2.46}$$

$$= \mathrm{Tr} \begin{pmatrix} \frac{2}{25} & \frac{4}{5\sqrt{10}} \\ \frac{1}{5\sqrt{10}} & \frac{4}{20} \end{pmatrix} = \frac{2}{25} + \frac{4}{20} = \frac{28}{100} \tag{2.47}$$

for $k = 1$:

$$p_1 = \mathrm{Tr}\Big(\hat{F}_1 \rho\Big) = \mathrm{Tr}\left(\begin{pmatrix} \frac{1}{5} & -\frac{1}{\sqrt{10}} \\ -\frac{1}{\sqrt{10}} & \frac{3}{4} \end{pmatrix} \begin{pmatrix} \frac{1}{5} & 0 \\ 0 & \frac{4}{5} \end{pmatrix} \right) \tag{2.48}$$

$$= \mathrm{Tr} \begin{pmatrix} \frac{1}{25} & -\frac{4}{5\sqrt{10}} \\ -\frac{1}{5\sqrt{10}} & \frac{12}{20} \end{pmatrix} = \frac{1}{25} + \frac{12}{20} = \frac{64}{100} \tag{2.49}$$

for $k = 2$:

$$p_2 = \mathrm{Tr}\Big(\hat{F}_2 \rho\Big) = \mathrm{Tr}\left(\begin{pmatrix} \frac{2}{5} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{5} & 0 \\ 0 & \frac{4}{5} \end{pmatrix} \right) \tag{2.50}$$

$$= \mathrm{Tr} \begin{pmatrix} \frac{2}{25} & 0 \\ 0 & 0 \end{pmatrix} = \frac{2}{25} = \frac{8}{100} \tag{2.51}$$

The sum of these probabilities equals 1.

3 Exercise

Given: Arbitrary spin observables $\hat{A} = a_x\hat{\sigma}_x + a_z\hat{\sigma}_z$ and $\hat{B} = b_x\hat{\sigma}_x + b_z\hat{\sigma}_z$ with $a_x^2 + a_z^2 = b_x^2 + b_z^2 = 1$ and a nonmaximally entangles state:

$$|\Phi(\theta)\rangle_{AB} = \cos\frac{\theta}{2}|0\rangle_A|0\rangle_B + \sin\frac{\theta}{2}|1\rangle_A|1\rangle_B$$

In the following the subscripts A and B will be dropped and the ordering maintained.

1. The eigenvalues of the operators can be calculated by expanding the Pauli matrices. For $\hat{A}$ it follows:

$$\hat{A} = \begin{pmatrix} a_z & a_x \\ a_x & -a_z \end{pmatrix} \tag{3.1}$$

$$\det\left(\hat{A} - \lambda\mathbb{1}\right) = (a_z - \lambda)(-a_z - \lambda) - a_x^2 \tag{3.2}$$

$$= \lambda^2 - (a_x^2 + a_z^2) = \lambda^2 - 1 \tag{3.3}$$

$$= 0 \text{ for } \lambda_{1,2} \pm 1 \tag{3.4}$$

2. The effects of the combination of Pauli matrices on the state can be calculated, recalling that $\hat{\sigma}_x$ "flips" the state from $|0\rangle$ to $|1\rangle$ and vice versa and that $\hat{\sigma}_z$ leaves $|0\rangle$ untouched, while reversing the sign of $|1\rangle$.

$$(\hat{\sigma}_x \otimes \hat{\sigma}_x)|\Phi(\theta)\rangle = \cos\frac{\theta}{2}\left(\hat{\sigma}_x|0\rangle \otimes \hat{\sigma}_x|0\rangle\right) + \sin\frac{\theta}{2}\left(\hat{\sigma}_x|1\rangle \otimes \hat{\sigma}_x|1\rangle\right)$$

$$= \cos\frac{\theta}{2}|11\rangle + \sin\frac{\theta}{2}|00\rangle \tag{3.5}$$

$$(\hat{\sigma}_x \otimes \hat{\sigma}_z)|\Phi(\theta)\rangle = \cos\frac{\theta}{2}|10\rangle - \sin\frac{\theta}{2}|01\rangle \tag{3.6}$$

$$(\hat{\sigma}_z \otimes \hat{\sigma}_x)|\Phi(\theta)\rangle = \cos\frac{\theta}{2}|01\rangle - \sin\frac{\theta}{2}|10\rangle \tag{3.7}$$

$$(\hat{\sigma}_z \otimes \hat{\sigma}_z)|\Phi(\theta)\rangle = \cos\frac{\theta}{2}|00\rangle + \sin\frac{\theta}{2}|11\rangle \tag{3.8}$$

3. To calculate the expectation value of the operators applied to the state, first, the tensor product of the operators is calculated:

$$\hat{A} \otimes \hat{B} = (a_x\hat{\sigma}_x + a_z\hat{\sigma}_z) \otimes (b_x\hat{\sigma}_x + b_z\hat{\sigma}_z) \tag{3.9}$$

$$= a_x b_x(\hat{\sigma}_x \otimes \hat{\sigma}_x) + a_x b_z(\hat{\sigma}_x \otimes \hat{\sigma}_z)$$

$$+ a_z b_x(\hat{\sigma}_z \otimes \hat{\sigma}_x) + a_z b_z(\hat{\sigma}_z \otimes \hat{\sigma}_z) \tag{3.10}$$

Using the results from task 3, the result of this operator applied to the state can be calculated:

$$
\begin{aligned}
(\hat{A} \otimes \hat{B})|\Phi(\theta)\rangle = a_x b_x &\left(\cos\frac{\theta}{2}|11\rangle + \sin\frac{\theta}{2}|00\rangle\right) \\
+ a_x b_z &\left(\cos\frac{\theta}{2}|10\rangle - \sin\frac{\theta}{2}|01\rangle\right) \\
+ a_z b_x &\left(\cos\frac{\theta}{2}|01\rangle - \sin\frac{\theta}{2}|10\rangle\right) \\
+ a_z b_z &\left(\cos\frac{\theta}{2}|00\rangle + \sin\frac{\theta}{2}|11\rangle\right)
\end{aligned} \tag{3.11}
$$

Taking the inner product of this with the state, it is immediate to see that the terms including $|01\rangle$ and $|10\rangle$ get canceled, and the result is:

$$
\begin{aligned}
\langle\Phi(\theta)|(\hat{A} \otimes \hat{B})|\Phi(\theta)\rangle &= \left(\cos\frac{\theta}{2}\langle 00| + \sin\frac{\theta}{2}\langle 11|\right) \\
&\cdot \left(a_x b_x \left(\cos\frac{\theta}{2}|11\rangle + \sin\frac{\theta}{2}|00\rangle\right) + a_z b_z \left(\cos\frac{\theta}{2}|00\rangle + \sin\frac{\theta}{2}|11\rangle\right)\right) && (3.12) \\
&= 2a_x b_x \cos\frac{\theta}{2}\sin\frac{\theta}{2} + a_z b_z \left(\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\right) && (3.13) \\
&= a_x b_x \sin\theta + a_z b_z && (3.14)
\end{aligned}
$$

4. To find the vectors $\vec{a}_0$, $\vec{a}_1, \vec{b}_0$ and $\vec{b}_1$ that allow for maximum violation of the CHSH inequality with the maximally entangled state $|\Phi(\frac{\pi}{2})\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle$, it is noted, that the expectation values are just the inner product of the vectors $\vec{a}_k$ and $\vec{b}_k$:

$$
\begin{aligned}
|\delta_{CHSH}| &= |\langle\hat{A}_0 \otimes \hat{B}_0\rangle + \langle\hat{A}_0 \otimes \hat{B}_1\rangle + \langle\hat{A}_1 \otimes \hat{B}_0\rangle - \langle\hat{A}_1 \otimes \hat{B}_1\rangle| && (3.15) \\
&= |\vec{a}_0\vec{b}_0 + \vec{a}_0\vec{b}_1 + \vec{a}_1\vec{b}_0 - \vec{a}_1\vec{b}_1| && (3.16)
\end{aligned}
$$

As proven many times, for instance in [1], the maximum value for entangled states is $2\sqrt{2}$. Together with the constraints on the magnitudes of the vectors, this yields five equations for eight unknowns, leading to infinite solutions. One of them is:

$$
\begin{aligned}
\vec{a}_0 &= \begin{bmatrix} 1 & 0 \end{bmatrix} & \qquad \vec{a}_1 &= \begin{bmatrix} 0 & 1 \end{bmatrix} \\
\vec{b}_0 &= \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} & \qquad \vec{b}_1 &= \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}
\end{aligned}
$$

Using these vectors with a variable value for θ now, one obtains:

$$\begin{aligned}|\delta_{CHSH}| &= (a_{x0}b_{x0}\sin\theta + a_{z0}b_{z0}) + (a_{x0}b_{x1}\sin\theta + a_{z0}b_{z1}) \\ &\quad + (a_{x1}b_{x0}\sin\theta + a_{z1}b_{z0}) - (a_{x1}b_{x1}\sin\theta + a_{z1}b_{z1}) \qquad (3.17)\\ &= \sqrt{2}\sin\theta + \sqrt{2} \overset{!}{>} 2 \qquad (3.18)\\ &\Rightarrow \sin\theta > \frac{2-\sqrt{2}}{\sqrt{2}} = \sqrt{2}-1 \qquad (3.19)\\ &\Rightarrow \theta > \arcsin\sqrt{2}-1 = 0.427\ \text{rad} \qquad (3.20)\end{aligned}$$

Due to the cyclicity of the sin function, the inequality is violated for:

$$\theta \in [0.427,\ \pi - 0.427] \cup [\pi + 0.427,\ 2\pi - 0.427] \qquad (3.21)$$

References

[1] Cirel'son, B. : *Quantum Generalizations of Bells' Inequality.* Leningrad, U.S.S.R : Lett Math Phys 4, 1980