Reaching Fleming’s discrimination bound

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Abstract. Any rule for identifying a quantum system’s state within a set of two non-orthogonal pure states by a single measurement is flawed. It has a non-zero probability of either yielding the wrong result or leaving the query undecided. This also holds if the measurement of an observable $A$ is repeated on a finite sample of $n$ state copies. We formulate a state identification rule for such a sample. This rule’s probability of giving the wrong result turns out to be bounded from above by $1/n\delta_A^2$ with $\delta_A = |\langle A \rangle_1 - \langle A \rangle_2| / (\Delta_1 A + \Delta_2 A)$. A larger $\delta_A$ results in a smaller upper bound. Yet, according to Fleming, $\delta_A$ cannot exceed $\tan \theta$ with $\theta \in (0, \pi/2)$ being the angle between the pure states under consideration. We demonstrate that there exist observables $A$ which reach the bound $\tan \theta$ and we determine all of them.

1. Introduction

The transmission of a binary sequence through a sequence of quantum systems whose states are to be chosen from a given set $\{\rho_1, \rho_2\}$ makes it necessary for the recipient to identify the states $\rho_1$ and $\rho_2$ with as little an error as possible. If each single bit is transmitted as a single system, an error minimizing strategy is needed in order to identify this system’s state from one single measurement.

If it is to be discriminated between two non-orthogonal states $\rho_1$ and $\rho_2$ through the measurement of an observable a certain positive lower bound for the probability of either wrong or inconclusive state identification cannot be underrun. Such limitations of individual state identification have been investigated extensively in theory and experiment. For a review see e.g. [1].

If in contrast each bit is transmitted as a sample of $n$ identical systems, all of them in the same state $\rho \in \{\rho_1, \rho_2\}$, the minimum error in reading the message correctly reduces beyond the limit established for $n = 1$. More generally, the sequence of values, obtained by measuring an arbitrary, perhaps non-optimal observable $A$ on each of the sample’s members, can be used to lower the probability of an erroneous state identification below the one obtained for a single measurement of $A$.

We will describe a rule of state identification from the mean value of a general observable $A$ in an $n$-sample. For this rule we derive an upper bound for the probability
Reaching Fleming’s discrimination bound

of error from Chebyshev’s inequality associated with the mean value of $A$. It turns out that our rule of state identification produces the wrong result with a probability not greater than $1/n\delta_A^2$. Here the dimensionless parameter $\delta_A > 0$ not only depends on the two states $\rho_1, \rho_2$ but also on the observable $A$ to be measured on the sample’s elements. It is given by

$$\delta_A = \frac{|\langle A \rangle_{\rho_1} - \langle A \rangle_{\rho_2}|}{\Delta_{\rho_1} A + \Delta_{\rho_2} A}.$$ (1)

This number therefore quantifies how well the states $\rho_1$ and $\rho_2$ can be distinguished from each other by means of measuring the observable $A$.

We will address the issue of which observable $A$, for given states $\rho_1, \rho_2$, leads to the largest possible value of $\delta_A$. Such a choice then minimizes the upper bound $1/n\delta_A^2$ of the probability of error for a given sample size $n$, yet it does not need to minimize the actual error itself. For arbitrary pure states $\rho_1$ and $\rho_2$ we find the maximum of $\delta_A$ over the set of all linear, bounded and self-adjoint operators $A$. We prove that

$$\max_A \delta_A = \tan \theta,$$ (2)

where $\theta$ with $0 < \theta < \pi/2$ denotes the angle between the states $\rho_1$ and $\rho_2$. Furthermore, among all bounded observables $A$ we explicitly specify those which maximize $\delta_A$.

The plan of the paper is as follows. In section 2 we summarize some results concerning optimal state discrimination for single systems and exhibit their relation to our minimization problem. In section 3 we derive the law of large numbers which motivates our quest for maximizing $\delta_A$. In section 4 we slightly adapt Fleming’s derivation of the estimate $\delta_A \leq \tan \theta$ to our goals. This proof will then be used first in section 5 to demonstrate that the upper bound $\tan \theta$ can be attained and afterwards in section 6 to identify those observables $A$ which actually reach this bound.

2. State identification for a single system

How is the state $\rho$ of a single quantum system to be identified within a given set $\{\rho_1, \rho_2\}$ of two different yet non-orthogonal pure states $\rho_1$ and $\rho_2$? Is there an observable $A$ which when measured upon $\rho$ allows for identifying the state as either $\rho_1$ or $\rho_2$ most ‘reliably’?

One way to render this question more precisely has been specified by Jaeger and Shimony. It meanwhile bears the title ‘minimum error state discrimination’. Assume that the spectrum of the observable $A$ consists of two eigenvalues $a_1, a_2$ only. If the system, whose state is to be identified, is in the state $\rho_i$ with probability $p_i$, then a measurement of a fixed observable $A$ upon a randomly chosen state yields a random

‡ Since we will vary $A$ and keep the states fixed we refrain from using the more suggestive but cumbersome notation $\delta_A (\rho_1, \rho_2)$.

§ The notation seems obvious and it is spelled out in sect. 2.

∥ This means that $\text{tr} (\rho_1 \rho_2) = \cos^2 \theta$ holds.
trial with the composite event space \( \Omega^A = \{\rho_1, \rho_2\} \times \{a_1, a_2\} \) and with the probability measure \( W^A \) whose distribution function \( p^A \) obeys
\[
p^A(\rho_i, a_j) = p_i \cdot \text{tr} \left( \rho_i P^A_{a_j} \right).
\]

Here \( P^A_{a} \) denotes the orthogonal projection onto the eigenspace of \( A \) corresponding to the eigenvalue \( a \in \{a_1, a_2\} \). The positive numbers \( p_1, p_2 \) have to obey \( p_1 + p_2 = 1 \). In order to correlate the measurement outcome \( a_i \) with the random state \( \rho_i \) as strongly as possible one has to search for an observable \( A \) which maximizes the probability
\[
W^A(D) = \sum_{i=1}^{2} p_i \cdot \text{tr} \left( \rho_i P^A_{a_i} \right)
\]
of the 'detection event' \( D = \{(\rho_1, a_1), (\rho_2, a_2)\} \).

Since the states \( \rho_1, \rho_2 \) are supposed to be pure, there exist unitvectors \( \psi_i \in \mathcal{H} \) such that \( \rho_i = \psi_i \langle \psi_i, \cdot \rangle \) for \( i \in \{1, 2\} \). Assume now tentatively that \( \text{tr} \left( \rho_i P^A_{a_j} \right) = 0 \) for all pairs \( (i, j) \) with \( i \neq j \). This implies \( P^A_{a_i} \psi_j = 0 \) for \( i \neq j \) and therefore \( A \psi_i = a_i \psi_i \) for all \( i \). But this leads to \( \langle \psi_1, \psi_2 \rangle = 0 \) which contradicts the assumed non-orthogonality \( \text{tr} (\rho_1 \rho_2) \neq 0 \). Therefore the detection event \( D \) cannot be certain whatever choice of \( A \) is made. Rather Jaeger and Shimony have proven in [2] that the maximum of \( W^A(D) \) obeys
\[
\max_A \{ W^A(D) \} = \frac{1}{2} \left( 1 + \sqrt{1 - 4p_1 p_2 \cdot \cos^2 \theta} \right)
\]
with \( \theta \in (0, \pi/2) \) such that \( \cos^2 \theta = |\langle \psi_1, \psi_2 \rangle|^2 = \text{tr}(\rho_1 \rho_2) \). Here the maximum is taken over all linear, bounded and self-adjoint operators \( A : \mathcal{H} \to \mathcal{H} \) whose spectrum consists of two fixed (unequal) eigenvalues \( a_1, a_2 \) only. It comes with little surprise that \( \max_A \{ W^A(D) \} \) does not depend on the choice of eigenvalues \( (a_1, a_2) \).

A related maximization problem is the following one. Find a linear, bounded and self-adjoint operator \( A : \mathcal{H} \to \mathcal{H} \) such that firstly the spectrum of \( A \) consists of the eigenvalues \( a_1 = a > 0, a_2 = -a \) and secondly \( A \) maximizes the weighted difference of expectation value, i.e. \( \Delta := p_1 \langle A \rangle_1 - p_2 \langle A \rangle_2 \) with \( \langle A \rangle_i = \text{tr} (\rho_i A) \). Because of
\[
\Delta = a p^A(\rho_1, a) + a p^A(\rho_2, -a) - a p^A(\rho_1, -a) - a p^A(\rho_2, a)
\]
\[
= a \cdot (2W^A(D) - 1)
\]
this maximization problem for constant \( a \) is equivalent to the previous one of maximizing \( W^A(D) \).

A genuinely alternative maximization problem is posed by the following one, which is known as 'unambiguous state discrimination'. [3] Assume now that the spectrum of the observable \( A \) consists of three (different) eigenvalues \( a_0, a_1, a_2 \). Then the above probability space \( (\Omega^A, W^A) \) is replaced by the event space \( \Omega^A = \{\rho_1, \rho_2\} \times \{a_0, a_1, a_2\} \) with the modified probability measure \( W^A \) whose distribution function \( p^A \) obeys
\[
p^A(\rho_i, a_j) = p_i \cdot \text{tr} \left( \rho_i P^A_{a_j} \right).
\]

\( \text{Reaching Fleming’s discrimination bound} \)
If one now chooses $A$ in such a way that
\[ p^A(\rho_1, a_2) = 0 = p^A(\rho_2, a_1), \tag{8} \]
then, whenever the event $\{\rho_1, \rho_2\} \times \{a_1\}$ occurs, it follows that $\rho = \rho_i$. Thus, under these provisions, the state can be determined with certainty, whenever a measurement of $A$ yields one of the values $a_1$ or $a_2$. Note that for $D = \{(\rho_1, a_1), (\rho_2, a_2)\}$ holds
\[ W^A(D) = W^A\left(\{\rho_1, \rho_2\} \times \{a_1, a_2\}\right) = 1 - W^A\left(\{\rho_1, \rho_2\} \times \{a_0\}\right). \tag{9} \]
Yet, as above, the event $D = \{(\rho_1, a_1), (\rho_2, a_2)\}$, allowing for a correct state-identification, cannot be certain. Therefore one is led to search for those observables $A$, for which in addition to the validity of equation (8) the probability $W^A(D)$ is maximal.

Jaeger and Shimony \[2\] have proven for $\dim(\mathcal{H}) \geq 3$ that
\[ \max_A \{W^A(D)\} = \begin{cases} 
1 - 2\sqrt{p_1p_2} \cdot \cos \theta & \text{for } \sqrt{\frac{\min\{p_1,p_2\}}{\max\{p_1,p_2\}}} \geq \cos \theta \\
\max\{p_1,p_2\} \sin^2 \theta & \text{for } \sqrt{\frac{\min\{p_1,p_2\}}{\max\{p_1,p_2\}}} < \cos \theta
\end{cases} \tag{10} \]
Here the maximization is performed over all those linear, bounded operators $A$, whose spectrum contains three different eigenvalues only, and which obey equation (8).

In this work we shall consider a third maximization problem. Among all linear, bounded and self-adjoint operators $A : \mathcal{H} \rightarrow \mathcal{H}$ we determine those which maximize the number $\delta_A$ given by equation (11) for two arbitrary but fixed non-orthogonal, non-identical, pure state density operators $\rho_1, \rho_2 : \mathcal{H} \rightarrow \mathcal{H}$. Here
\[ \Delta_\rho A = \sqrt{\langle A^2 \rangle_\rho - \langle A \rangle_\rho^2} \text{ with } \langle X \rangle_\rho = \operatorname{tr}(\rho X) \tag{11} \]
denotes the uncertainty of $A$ in the state $\rho$. The number $\delta_A$ is invariant under the shift $A \rightarrow A + \mu \cdot 1d_\mathcal{H}$ for any real $\mu$ and also under the rescaling $A \rightarrow \lambda A$ for any non-zero real $\lambda$. It relates the distance between the states’ expectation values to their uncertainties and therefore has been proposed by Fleming \[4\] as a quantifier of the distinguishability of the states $\rho_1$ and $\rho_2$ by means of measuring $A$ on a finite sample.

Part of our result is
\[ \max_A \{\delta_A\} = \tan \theta, \tag{12} \]
where $A$ is allowed to run through the set of all linear, bounded, self-adjoint operators $A : \mathcal{H} \rightarrow \mathcal{H}$. Observe that no further restriction on the spectrum of $A$ is imposed. In particular, the spectrum of $A$ may include a continuous part.

Among the observables $A$ maximizing $\delta_A$ we shall identify one which also maximizes $\langle A \rangle_{\rho_1} - \langle A \rangle_{\rho_2}$. It is given by $A = (\rho_1 - \rho_2) / \sin \theta$. This operator therefore also maximizes the probability of correct state identification $W(D)$ for $p_1 = p_2 = 1/2$ from equation (5). Its value is given by
\[ \max_A \{W^A(D)\} = \frac{1}{2} \left(1 + \sin \theta\right). \tag{13} \]
\[ \downarrow \] The spectrum of $A$ is $\{1, -1, 0\}$ if $\dim(\mathcal{H}) \geq 3$ and $\{1, -1\}$ if $\dim(\mathcal{H}) = 2$. 

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*Reaching Fleming’s discrimination bound*
In deriving equation (12) we make use of a powerful estimate due to Fleming [4], that is conceived purely by general algebraic deliberations. Fleming called it a 'quantum master inequality', because he was able to derive a host of other well known quantum theoretical facts from it. Besides taking the orthogonality of two eigenvectors to different eigenvalues of an observable to a more general and quantitative level, Fleming’s quantum master inequality also implies Robertson’s generalized uncertainty relation \(2\Delta A\Delta B \geq |<[A,B]>|\). [5]

Fleming’s quantum master inequality states that, whenever \(\Delta \rho_1 A + \Delta \rho_2 A > 0\), then \(\delta_A \leq \tan \theta\). We shall first prove that Fleming’s upper bound can be reached and then identify necessary and sufficient conditions on \(A\) for \(\delta_A = \tan \theta\) to hold.

Before entering the problem of maximizing \(\delta_A\) we will clarify the role of \(\delta_A\) in identifying the state from an \(n\)-sample of states \(\rho \in \{\rho_1, \rho_2\}\). We shall do so in the more general context of identifying a probability measure \(W\) on the real line within a set of two options \(\{W_1, W_2\}\).

3. State identification for an \(n\)-sample

Let \(W\) denote a probability measure on the real line with finite expectation value \(X := \mathbb{E}_W (\text{id}_\mathbb{R})\) and variance \(\Delta^2 := \mathbb{E}_W ((\text{id}_\mathbb{R} - X)^2)\). Chebyshev’s inequality states that for any \(t \in \mathbb{R}_{>0}\) holds

\[
W \left( \{ x \in \mathbb{R} : |x - X| \geq t \} \right) \leq \left( \frac{\Delta}{t} \right)^2. \tag{14}
\]

The product space \(\mathbb{R}^n\) together with the product measure \(W^n = W \times \ldots \times W\) corresponds to the random experiment of drawing \(n\) real numbers independently and each one distributed by \(W\). The mean value of such a sample \((x_1, \ldots x_n) \in \mathbb{R}^n\) is given by the function \(m_n : \mathbb{R}^n \rightarrow \mathbb{R}\) with

\[
m_n (x_1, \ldots x_n) = \frac{1}{n} \sum_{i=1}^{n} x_i. \tag{15}
\]

For the expectation value and the variance of the random variable \(m_n\) under the measure \(W^n\) holds

\[
\mathbb{E}_{W^n} (m_n) = X \text{ and } \mathbb{V}_{W^n} (m_n) = \frac{\Delta^2}{n}. \tag{16}
\]

Application of Chebyshev’s inequality to \(m_n\) thus yields the following law of large numbers

\[
W^n \left( \{ \omega \in \mathbb{R}^n : |m_n (\omega) - X| \geq t \} \right) \leq \frac{1}{n} \cdot \left( \frac{\Delta}{t} \right)^2. \tag{17}
\]

The probability that the mean value of a random sample \(\omega \in \mathbb{R}^n\) of the distribution \(W^n\) deviates from the expectation value by at least a fixed value \(t > 0\) converges to 0 when \(n\) goes to \(\infty\).

Now, let \(W_1\) and \(W_2\) denote two different probability measures on the real line of the above type. Their expectation values \(X_i\) are assumed to be unequal and without
loss of generality we may assume \( X_2 > X_1 \). We also suppose that at least one of the probability measures \( W_i \) has non-zero variance, i.e. that \( \Delta_1 + \Delta_2 > 0 \).

A sample \( \omega \in \mathbb{R}^n \) of \( n \) real numbers is supposed to be generated by either the distribution \( W_1^n \) or \( W_2^n \). From the sample’s mean value one may try to guess whether the sample has been generated by \( W_1^n \) or \( W_2^n \). To this end, observe first that as a consequence of Chebyshev’s inequality (17) we have for all \( t \)

\[
W_1^n (\{ \omega \in \mathbb{R}^n : m_n (\omega) \geq X_1 + t_1 \}) \leq \frac{1}{n} \cdot \left( \frac{\Delta_1}{t_1} \right)^2, \tag{18a}
\]

\[
W_2^n (\{ \omega \in \mathbb{R}^n : m_n (\omega) \leq X_2 - t_2 \}) \leq \frac{1}{n} \cdot \left( \frac{\Delta_2}{t_2} \right)^2. \tag{18b}
\]

Choosing now the numbers \( t_i \) according to

\[
t_i = \Delta_i \cdot \delta \text{ with } \delta = \frac{X_2 - X_1}{\Delta_1 + \Delta_2} > 0 \tag{19}
\]

the estimates (18a) and (18b) turn into

\[
W_1^n (\{ \omega \in \mathbb{R}^n : m_n (\omega) \geq X_0 \}) \leq \frac{1}{n} \cdot \left( \frac{1}{\delta} \right)^2, \tag{20a}
\]

\[
W_2^n (\{ \omega \in \mathbb{R}^n : m_n (\omega) \leq X_0 \}) \leq \frac{1}{n} \cdot \left( \frac{1}{\delta} \right)^2. \tag{20b}
\]

Here the point

\[
X_0 = \frac{\Delta_2}{\Delta_1 + \Delta_2} X_1 + \frac{\Delta_1}{\Delta_1 + \Delta_2} X_2 \tag{21}
\]

divides the interval \([X_1, X_2] \) into a portion of length \( \frac{\Delta_1}{\Delta_1 + \Delta_2} \cdot (X_2 - X_1) \) to the left of \( X_0 \) and another one of length \( \frac{\Delta_2}{\Delta_1 + \Delta_2} \cdot (X_2 - X_1) \) to the right of \( X_0 \). Observe that

\[
X_1 + \frac{\Delta_1}{\Delta_1 + \Delta_2} \cdot (X_2 - X_1) = X_2 - \frac{\Delta_2}{\Delta_1 + \Delta_2} \cdot (X_2 - X_1) = X_0. \tag{22}
\]

Let a sample \( \omega \in \mathbb{R}^n \) be generated with probability \( p_1 > 0 \) through the measure \( W_1^n \) or with probability \( p_2 = 1 - p_1 > 0 \) through the measure \( W_2^n \). This corresponds to the composite random trial with event space \( \Omega = \{ 1, 2 \} \times \mathbb{R}^n \) with the product measure \( W \) which obeys for all measurable \( Z \subset \mathbb{R}^n \)

\[
W (\{ i \} \times Z) = p_i \cdot W_i^n (Z). \tag{23}
\]

Let \( E \) denote the event that the sample \( \omega \) is either generated by \( W_2^n \) and yields a value \( m_n (\omega) \leq X_0 \) or is generated by \( W_1^n \) and has a mean value \( m_n (\omega) \geq X_0 \). Then this event’s probability is bounded by

\[
W (E) \leq p_1 \cdot \frac{1}{n} \cdot \left( \frac{1}{\delta} \right)^2 + p_2 \cdot \frac{1}{n} \cdot \left( \frac{1}{\delta} \right)^2 = \frac{1}{n} \cdot \left( \frac{1}{\delta} \right)^2. \tag{24}
\]

Hence, by increasing \( n \), this event’s probability can be made arbitrarily small.

Thus we have the result: The event that \( \omega \) is generated by \( W_1^n \) and has a mean value \( m_n (\omega) \leq X_0 \) or that \( \omega \) is generated by \( W_2^n \) and has a mean value \( m_n (\omega) \geq X_0 \)
Reaching Fleming’s discrimination bound

has a probability greater or equal to \(1 - \frac{1}{n} \cdot \left(\frac{1}{\delta}\right)^2\). For \(n \delta^2 > 1/\varepsilon \gg 1\) this implies that the event \(m_n(\omega) \leq X_0\) is caused by \(W_1^n\) and \(m_n(\omega) \geq X_0\) is caused by \(W_2^n\) has probability greater than \(1 - \varepsilon\) and so is virtually certain. This fact justifies the identification of a sample’s generating distribution by means of the following criterion: if the sample’s mean value obeys \(m_n(\omega) < X_0\), then the sample \(\omega\) is assumed to have been generated by \(W_1^n\). If, however, \(m_n(\omega) \geq X_0\), then the sample is assumed to have been generated by \(W_2^n\).

Besides the sample’s size \(n\) the positive real number

\[
\delta = \frac{|X_1 - X_2|}{\Delta_1 + \Delta_2}
\]

(25)

is decisive for the correct identification of the sample-generating distribution \(W_i^n\) from the sample’s value \(m_n(\omega)\) with high probability. The two distributions \(W_1^n\) and \(W_2^n\) are identified correctly with the higher a probability the larger the value of \(\delta\). One might call the parameter \(\delta\) of two probability measures \(W_1\) and \(W_2\) on the real line their discernibility.

As is well known, any pair \((\rho, A)\) of a quantum state \(\rho : \mathcal{H} \to \mathcal{H}\) and a bounded observable \(A : \mathcal{H} \to \mathcal{H}\) defines a probability measure \(W^A_{\rho}\) on \(\mathbb{R}\), which has its support on the spectrum of \(A\). For any measurable set \(Z \subset \mathbb{R}\) the number \(W^A_{\rho}(Z)\) equals the probability that when \(A\) is measured on \(\rho\) the measured value belongs to \(Z\). The expectation value and variance of \(\rho\) under \(W^A_{\rho}\) equal \(\text{tr}(\rho A) = \langle A \rangle_{\rho}\) and \(\text{tr}(\rho A^2) - \text{tr}(\rho A)^2 = (\Delta_{\rho A})^2\). Thus the rule of identifying a probability measure \(W \in \{W_1, W_2\}\) from an \(n\)-sample of measured values \((\omega_1, \ldots, \omega_n)\) can be taken over in a straightforward manner to the quantum case by replacing \(W_i\) with the probability measure \(W^A_{\rho_i}\). Identification of \(W_i\) then amounts to an identification of \(\rho_i\) and the discernibility \(\delta\) specializes to the expression given by equation (1).

4. Fleming’s quantum master inequality

Let \(\mathcal{H}\) denote a separable Hilbert space and let the linear mapping \(A : \mathcal{H} \to \mathcal{H}\) be bounded and self-adjoint. The expectation value of \(A\) in the pure state represented by a unit vector \(v \in \mathcal{H}\) is denoted as \(\langle A \rangle_v\). The following quantum master inequality (QMIE) relates two pure states through their first two moments of an observable. It has been given by Fleming in [4].

**Proposition 1** For any two unit vectors \(v, w \in \mathcal{H}\) and any linear, bounded and self-adjoint operator \(A : \mathcal{H} \to \mathcal{H}\) there holds

\[
|\langle A \rangle_w - \langle A \rangle_v| \cdot |\langle w, v \rangle| \leq (\Delta_v A + \Delta_w A) \cdot \sqrt{1 - |\langle w, v \rangle|^2}.
\]

(26)

\(^+\) Thus \(\langle A \rangle_v = \langle v, Av \rangle\), and \(\Delta_v A = \sqrt{\langle A^2 \rangle_v - \langle A \rangle_v^2}\) denotes the uncertainty of \(A\) in the state represented by \(v\).
Before proving this estimate we discuss a few of its consequences. Observe first that there exists a unique \( \theta \in [0, \pi/2] \) such that \(|\langle w, v \rangle| = \cos \theta \). Squaring the inequality (26) and slightly rearranging terms yields

\[
\left[ (\langle A \rangle w - \langle A \rangle v)^2 + (\Delta_v A + \Delta_w A)^2 \right] \cos^2 \theta \leq (\Delta_v A + \Delta_w A)^2.
\]

Whenever the term in the square brackets is non-zero, then (26) is equivalent to

\[
\cos^2 \theta \leq \frac{(\Delta_v A + \Delta_w A)^2}{(\langle A \rangle w - \langle A \rangle v)^2 + (\Delta_v A + \Delta_w A)^2}.
\]

For \( \Delta_v A + \Delta_w A > 0 \) inequality (28) is equivalent to

\[
\cos^2 \theta \leq \frac{1}{1 + \delta^2} \quad \text{with} \quad \delta = \frac{|\langle A \rangle w - \langle A \rangle v|}{\Delta_v A + \Delta_w A} \geq 0.
\]

The bound (29) for \( \cos^2 \theta \) is strictly monotonically decreasing from 1 to 0 when \( \delta \) moves from 0 to \( \infty \). The number \( \delta \) quantifies the distinguishability of the states represented by \( v \) and \( w \) through measuring \( A \). For non-orthogonal vectors \( v \) and \( w \) the inequality (29) is equivalent to

\[
\delta^2 \leq \frac{1}{\cos^2 \theta} - 1 = \tan^2 \theta.
\]

Thus, for \( \cos \theta > 0 \) and \( \Delta_v A + \Delta_w A > 0 \) the estimate (26) is equivalent to

\[
\delta \leq \tan \theta.
\]

If \( v \) and \( w \) are parallel, then both sides of the inequality (26) take the value 0 due to \( \langle A \rangle w = \langle A \rangle v \) and \( |\langle w, v \rangle| = 1 \). The inequality (26) is thus saturated in this case for any \( A \). If \( v \) and \( w \) are orthogonal, the estimate (26) reduces to

\[
0 \leq \Delta_v A + \Delta_w A.
\]

This estimate is saturated if and only if \( \Delta_v A = 0 = \Delta_w A \), which in turn holds if and only if both \( v \) and \( w \) are eigenvectors of \( A \).

We shall now give a proof of Fleming’s quantum master inequality (26).

**Proof.** In a first step we decompose the vector \( Av \) into a vector parallel to \( v \) and one orthogonal to \( v \). This unique decomposition reads

\[
Av = \langle A \rangle v + (Av - \langle A \rangle v), \tag{33}
\]

since \( \langle v, Av - \langle A \rangle v \rangle = 0 \). Observe that the component \( v_A = Av - \langle A \rangle v \) of \( Av \) orthogonal to \( v \) has the norm \( \Delta_v A \) since

\[
|v_A|^2 = \langle Av - \langle A \rangle v, Av - \langle A \rangle v \rangle = (\Delta_v A)^2. \tag{34}
\]

We thus have

\[
\langle w, Av \rangle = \langle A \rangle w \langle w, v \rangle + \langle w, v_A \rangle. \tag{35}
\]

The analogous decomposition of \( Aw = \langle A \rangle w w + w_A \) with \( w_A = Aw - \langle A \rangle w w \) yields

\[
\langle Aw, v \rangle = \langle A \rangle w \langle w, v \rangle + \langle w, v_A \rangle. \tag{36}
\]
Since \( \langle w, Av \rangle = \langle Aw, v \rangle \) we obtain
\[
(\langle A \rangle_w - \langle A \rangle_v) \langle w, v \rangle = \langle w, v_A \rangle - \langle w_A, v \rangle. \tag{37}
\]
Taking the absolute value from both sides and applying the triangle inequality on \( \mathbb{C} \) gives the estimate
\[
|\langle A \rangle_w - \langle A \rangle_v| \cos \theta = |\langle w, v_A \rangle - \langle w_A, v \rangle| \leq |\langle w, v \rangle| + |\langle w_A, v \rangle|, \tag{38}
\]
where \( \theta \in [0, \pi/2] \) is uniquely defined through \( \cos \theta = |\langle w, v \rangle| \).

Since \( v_A \) is orthogonal to \( v \), by means of the decomposition of \( w \) into a vector from \( \mathbb{C} \cdot v \) and one from its orthogonal complement \( (\mathbb{C} \cdot v)^\perp \) according to
\[
w = \langle v, w \rangle v + (w - \langle v, w \rangle v), \tag{39}
\]
we obtain the equality
\[
\langle w, v_A \rangle = \langle w - \langle v, w \rangle v, v_A \rangle. \tag{40}
\]
After taking the absolute value from both sides the Cauchy-Schwarz inequality in \( \mathcal{H} \) gives
\[
|\langle w, v_A \rangle| = |\langle w - \langle v, w \rangle v, v_A \rangle| \leq |w - \langle v, w \rangle v| |v_A| = \sin \theta \cdot \Delta_v A. \tag{41}
\]
Interchanging \( v \) and \( w \) leaves us with
\[
|\langle w_A, v \rangle| = |\langle w_A, v - \langle w, v \rangle w \rangle| \leq \sin \theta \cdot \Delta_w A. \tag{42}
\]
Inserting these bounds into the right-hand side of estimate (38) then leads to the statement of prop. 1,
\[
|\langle A \rangle_w - \langle A \rangle_v| \cos \theta \leq (\Delta_v A + \Delta_w A) \sin \theta. \tag{43}
\]

5. Conditions for saturating the QMIE

When \( H = \hbar h \) denotes a Hamiltonian, the estimate (28) with \( w = v_t := e^{-iht}v \) produces an upper bound for the survival probability \( P_v(t) := |\langle v, v_t \rangle|^2 \) of the initial state \( v \langle v, \cdot \rangle \) under the time evolution up to time \( t \), which is equivalent to
\[
0 \leq Q(t) := \frac{(\Delta_v A + \Delta_{v_t} A)^2}{(\Delta_v A + \Delta_{v_t} A)^2 + |\langle A \rangle_{v_t} - \langle A \rangle_v|^2} - P_v(t). \tag{44}
\]
Searching for an observable \( A \) which minimizes \( \int_0^T Q(t) \, dt \) for a period of time \( T \) of a spin-1/2-system, we have found the following necessary and sufficient conditions on \( A \) to saturate the QMIE. [6]

**Proposition 2** Let \( v, w \) be unit vectors in a Hilbert space \( \mathcal{H} \) with \( |\langle w, v \rangle| = \cos \theta \) for some \( \theta \in (0, \pi/2] \), i.e. \( v \) and \( w \) are assumed to be linearly independent. Let \( A : \mathcal{H} \to \mathcal{H} \) be a linear, bounded and self-adjoint. Then, the QMIE for the states \( \rho_1 = v \langle v, \cdot \rangle \) and \( \rho_2 = w \langle w, \cdot \rangle \) is saturated, i.e. the equation
\[
|\langle A \rangle_w - \langle A \rangle_v| \cos \theta = (\Delta_v A + \Delta_w A) \sin \theta \tag{45}
\]
holds, if and only if the conditions (i) and (ii) are fulfilled.
Reaching Fleming’s discrimination bound

(i) The operator $A$ leaves the subspace $\mathbb{C} \cdot v + \mathbb{C} \cdot w$ invariant.

(ii) The equation

$$\langle w, Av \rangle = \lambda \langle w, v \rangle$$  \hspace{1cm} (46)

holds for some $\lambda \in \mathbb{R}$ with

$$\min \{ \langle A \rangle_w, \langle A \rangle_v \} \leq \lambda \leq \max \{ \langle A \rangle_w, \langle A \rangle_v \}.$$  \hspace{1cm} (47)

For $\theta = 0$ the QMIE is saturated for any observable $A$ since both sides of the QMIE are zero. Thus, the proposition has to deal with the non-trivial case $0 < \theta \leq \pi/2$ only.

**Proof.** The proof of proposition 1 contains three estimates. The first one is (38). It uses the triangle inequality for complex numbers as follows

$$|\langle w, v_A \rangle - \langle w_A, v \rangle| \leq |\langle w, v_A \rangle| + |\langle w_A, v \rangle|.$$  \hspace{1cm} (48)

Here, equality holds if and only if the complex numbers $\langle w, v_A \rangle$ and $- \langle w_A, v \rangle$ as elements of $\mathbb{R}^2 \cong \mathbb{C}$ point into the same direction. This is the case if and only if there exists a pair $(\alpha, \beta) \in (\mathbb{R}_0 \times \mathbb{R}_0) \setminus (0,0)$ such that

$$\alpha \langle w, v_A \rangle + \beta \langle w_A, v \rangle = 0.$$  \hspace{1cm} (49)

The other two estimates are contained in (41) and (42). They employ the Cauchy-Schwarz inequality for the scalar product of two elements of $\mathcal{H}$. The estimate (41) thus is saturated if and only if the vector $v_A$ is a (complex) multiple of the (non-zero) vector $w - \langle v, w \rangle v$, i.e., if

$$v_A \in \mathbb{C} \cdot (w - \langle v, w \rangle v).$$  \hspace{1cm} (50)

Similarly, the estimate (42) is saturated if and only if

$$w_A \in \mathbb{C} \cdot (v - \langle w, v \rangle w).$$  \hspace{1cm} (51)

Therefore, the equality (45) holds if and only if all three conditions (49), (50), and (51) are fulfilled. The conditions (50) and (51) hold, if and only if $A$ maps the space which is spanned by $v$ and $w$ onto itself. This can be seen as follows: (50) implies that $Av \in \mathbb{C} \cdot v + \mathbb{C} \cdot w$ and (51) implies that $Aw \in \mathbb{C} \cdot v + \mathbb{C} \cdot w$. On the other hand, since $v_A$ is by definition orthogonal to $v$ and $w_A$ is orthogonal to $w$, the conditions (50) and (51) follow from $A (\mathbb{C} \cdot v + \mathbb{C} \cdot w) \subset (\mathbb{C} \cdot v + \mathbb{C} \cdot w)$.

We now have to address condition (49). This condition says that there exists a pair $(\alpha, \beta) \in (\mathbb{R}_0 \times \mathbb{R}_0) \setminus (0,0)$ such that

\begin{align*}
0 &= \alpha \langle w, Av - \langle A \rangle_v v \rangle + \beta \langle Aw - \langle A \rangle_w w, v \rangle \hspace{1cm} (52a) \\
&= \alpha \langle w, Av \rangle + \beta \langle Aw, v \rangle - \alpha \langle A \rangle_v \langle w, v \rangle - \beta \langle A \rangle_w \langle w, v \rangle \hspace{1cm} (52b) \\
&= (\alpha + \beta) \langle w, Av \rangle - (\alpha \langle A \rangle_v + \beta \langle A \rangle_w) \langle w, v \rangle. \hspace{1cm} (52c)
\end{align*}

* Due to $\theta > 0$ we have $w - \langle v, w \rangle v \neq 0 \neq v - \langle w, v \rangle w$.

‡ Observe that it is here that we need that $v$ and $w$ are linearly independent, i.e. that $\theta > 0$. In case of $\theta = 0$ a condition on $v_A$ does not follow from saturating estimate (41).
Reaching Fleming's discrimination bound

Since \( \alpha + \beta > 0 \), it follows that condition (49) holds if and only if there exists a pair \((\alpha, \beta) \in (\mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0}) \setminus (0, 0) \) such that

\[
\langle w, Av \rangle = \left( \frac{\alpha}{\alpha + \beta} \langle A \rangle_v + \frac{\beta}{\alpha + \beta} \langle A \rangle_w \right) \langle w, v \rangle.
\]  

(53)

Due to \( \left( \frac{\alpha}{\alpha + \beta}, \frac{\beta}{\alpha + \beta} \right) \in ([0, 1] \times [0, 1]) \setminus (0, 0) \), and \( \frac{\alpha}{\alpha + \beta} + \frac{\beta}{\alpha + \beta} = 1 \), the real number

\[
\lambda = \left( \frac{\alpha}{\alpha + \beta} \langle A \rangle_v + \frac{\beta}{\alpha + \beta} \langle A \rangle_w \right)
\]

is a convex combination of \( \langle A \rangle_v \) and \( \langle A \rangle_w \). Thus condition (49) holds if and only if \( \langle w, Av \rangle \) is a real multiple of \( \langle w, v \rangle \), where the factor belongs to the interval bounded by \( \langle A \rangle_v \) and \( \langle A \rangle_w \). Thus we have proven equation (46).

Observe that in case of \( \cos \theta = 0 \) the pair \((v, w)\) is an orthonormal basis of the space \( \mathbb{C} \cdot v + \mathbb{C} \cdot w \). Then, the equation (45) holds if and only if \( A \) stabilizes the subspace \( \mathbb{C} \cdot v + \mathbb{C} \cdot w \) and \( \langle w, Av \rangle = 0 \). This in turn is equivalent to the statement that \( v \) and \( w \) both are eigenvectors of \( A \), because of \( Av = \langle v, Av \rangle v + \langle w, Av \rangle w = \langle A \rangle_v v \) and similarly \( Aw = \langle A \rangle_w w \). If on the other hand for \( 0 < \theta < \pi/2 \) we have \( \Delta_v A + \Delta_w A = 0 \) it follows that \( \langle A \rangle_w = \langle A \rangle_v \) and that \( v \) and \( w \) are eigenvectors of \( A \) with the same eigenvalue.

Thus the nontrivial case of equation (45) is realized if \( 0 < \theta < \pi/2 \) and \( \Delta_v A + \Delta_w A > 0 \) is valid. In this case the equality \( \delta_A = \tan \theta \) holds if and only if the conditions (i) and (ii) are fulfilled.

6. Observables of maximal \( \delta_A \)

We shall now determine the set of observables \( A \) which for given states \( \rho_1 = v \langle v, \cdot \rangle \), and \( \rho_2 = w \langle w, \cdot \rangle \) obey \( \Delta_w A + \Delta_v A > 0 \) and \( \delta_A = \tan \theta \). Let \( v, w \in \mathcal{H} \) be unit vectors with \( 0 < |\langle v, w \rangle| < 1 \) and let \( A : \mathcal{H} \to \mathcal{H} \) be linear, bounded and self-adjoint. Without loss of generality we assume that \( \langle A \rangle_v \leq \langle A \rangle_w \) and that \( |\langle v, w \rangle| = \langle v, w \rangle \). According to prop. 2 the equation \( \delta_A = \tan \theta \) holds if and only if

(i) \( A \) stabilizes \( \mathbb{C} \cdot v + \mathbb{C} \cdot w \)

(ii) The quotient \( \frac{\langle w, Av \rangle}{\langle w, v \rangle} \) is real and obeys \( \langle A \rangle_v \leq \frac{\langle w, Av \rangle}{\langle w, v \rangle} \leq \langle A \rangle_w \).

Since \( A \) is self-adjoint, condition (i) implies that \( A \) stabilizes the orthogonal complement of \( \mathbb{C} \cdot v + \mathbb{C} \cdot w \) too. Therefore, the action of \( A \) on this complementary subspace \( [\mathbb{C} \cdot v + \mathbb{C} \cdot w]^\perp \) has no relevance to our problem and it is the restriction \( A_0 \) of \( A \) to \( \mathcal{H}_0 := \mathbb{C} \cdot v + \mathbb{C} \cdot w \) only which has to be studied.

Since \( \delta_{\lambda A + \mu d_{\mathcal{H}}} = \delta_A \) holds for all \( \lambda \in \mathbb{R} \setminus 0 \) and \( \mu \in \mathbb{R} \) and for all \( A \) with \( \Delta_w A + \Delta_v A > 0 \), we may use this freedom of shifting and rescaling \( A \) in such a way that the spectrum of \( A_0 \) obeys \( \sigma (A_0) = \{1, -1\} \). This is clearly equivalent to

\[
\text{tr} (A_0) = 0 \quad \text{and} \quad \det (A_0) = -1.
\]

(55)

Observe that, because of \( 0 < \Delta_w A + \Delta_v A = \Delta_w A_0 + \Delta_v A_0 \), a transformation into \( A_0 = id_{\mathcal{H}_0} \) is impossible.
Among the observables \( A_0 : \mathcal{H}_0 \to \mathcal{H}_0 \) which obey (55) we now search for those which satisfy

\[
\langle A_0 \rangle_v \leq \frac{\langle w, A_0 v \rangle}{\langle w, v \rangle} \leq \langle A_0 \rangle_w .
\] (56)

To do so we introduce the following orthonormal basis in \( \mathcal{H}_0 \):

\[
e_1 = \frac{v + w}{2 \cos \left( \frac{\theta}{2} \right)}, \quad e_2 = \frac{w - v}{2 \sin \left( \frac{\theta}{2} \right)}.
\] (57)

The vectors \( v \) and \( w \) thus have the decomposition

\[
w = \cos \left( \frac{\theta}{2} \right) \cdot e_1 + \sin \left( \frac{\theta}{2} \right) \cdot e_2 \quad \text{and} \quad v = \cos \left( \frac{\theta}{2} \right) \cdot e_1 - \sin \left( \frac{\theta}{2} \right) \cdot e_2.
\] (58)

The matrix elements of \( A_0 \) with respect to \( e = (e_1, e_2) \) are denoted as \( A_{ij} = \langle e_i, A_0 e_j \rangle \).

Clearly, \( A_{ii} \in \mathbb{R} \) and \( A_{12} \in \mathbb{C} \) with \( A_{21} = \bar{A}_{12} \). Condition (55) is equivalent to

\[
A_{11} = -A_{22} \quad \text{and} \quad A_{11}^2 + |A_{12}|^2 = 1.
\] (59)

For the matrix elements involved in (56) we find

\[
\langle v, Av \rangle = \cos (\theta) A_{11} - \sin (\theta) \Re (A_{12}), \quad (60a)
\]

\[
\langle w, Av \rangle = A_{11} - i \sin (\theta) \Im (A_{12}), \quad (60b)
\]

\[
\langle w, Aw \rangle = \cos (\theta) A_{11} + \sin (\theta) \Re (A_{12}). \quad (60c)
\]

Condition (56) therefore implies that

\[
\Im (A_{12}) = 0 \quad \text{and} \quad \Re (A_{12}) \geq 0.
\]

Due to \( A_{11}^2 + A_{12}^2 = 1 \) there exists a unique \( \alpha \in [0, \pi] \) with

\[
A_{11} = \cos \alpha \quad \text{and} \quad A_{12} = \sin \alpha.
\]

Using this parametrization the matrix elements of \( A_0 \) obey

\[
\langle v, Av \rangle = \cos (\theta + \alpha), \quad (61a)
\]

\[
\langle w, Av \rangle = \cos \alpha, \quad (61b)
\]

\[
\langle w, Aw \rangle = \cos (\theta - \alpha). \quad (61c)
\]

Condition (56) thus implies

\[
\cos (\theta) \cos (\theta + \alpha) \leq \cos \alpha \leq \cos (\theta) \cos (\theta - \alpha).
\] (62)

which, due to \( \cos (\theta) \cos (\theta + \alpha) = [\cos (\alpha) + \cos (2\theta + \alpha)]/2 \), is equivalent to

\[
\cos (2\theta + \alpha) \leq \cos \alpha \leq \cos (2\theta - \alpha).
\] (63)

On the domain \( (\theta, \alpha) \in (0, \pi/2) \times [0, \pi] \) condition (63) is equivalent to

\[
\theta \leq \alpha \leq \pi - \theta.
\] (64)

Finally, it is now easy to prove that for any linear, bounded and self-adjoint map \( A : \mathcal{H} \to \mathcal{H} \) which stabilizes \( \mathcal{H}_0 \) and whose restriction \( A_0 \) to \( \mathcal{H}_0 \) obeys

\[
A_0 = \cos (\alpha) [e_1 \langle e_1, \cdot \rangle - e_2 \langle e_2, \cdot \rangle] + \sin (\alpha) [e_1 \langle e_2, \cdot \rangle + e_2 \langle e_1, \cdot \rangle]
\] (65)
Reaching Fleming’s discrimination bound

for some \( \alpha \in [\theta, \pi - \theta] \) there holds \( \delta_A = \tan \theta \). To do so we first derive from (61a) and (61c)

\[ \langle w, Aw \rangle - \langle v, Av \rangle = 2 \sin (\theta) \sin (\alpha) \]  
(66)

and then observe that

\[ (\Delta_v A)^2 = 1 - \langle A \rangle_w^2 = \sin^2 (\theta + \alpha), \]  
(67)

\[ (\Delta_w A)^2 = 1 - \langle A \rangle_w^2 = \sin^2 (\theta - \alpha). \]  
(68)

From this it follows that

\[ \delta_A = \frac{\langle w, Aw \rangle - \langle v, Av \rangle}{\Delta_w A + \Delta_v A} = \frac{2 \sin (\theta) \sin (\alpha)}{\sqrt{\sin^2 (\theta - \alpha)} + \sqrt{\sin^2 (\theta + \alpha)}}. \]  
(69)

Since \( 0 \leq \alpha - \theta \leq \pi \) and \( 0 < \theta + \alpha \leq \pi \) we have

\[ \sqrt{\sin^2 (\theta - \alpha)} = \sin (\alpha - \theta) \]  
and

\[ \sqrt{\sin^2 (\theta + \alpha)} = \sin (\alpha + \theta) \]  
(70)

and therefore

\[ \delta_A = \frac{2 \sin (\theta) \sin (\alpha)}{2 \sin (\alpha) \cos (\theta)} = \tan (\theta). \]  
(71)

We may now summarize our result as follows.

**Proposition 3** Let \( v, w \) be unit vectors in a Hilbert space \( H \) with \( \langle v, w \rangle = \cos \theta \) for some \( \theta \in (0, \pi/2) \). A linear, bounded self-adjoint operator \( A : H \to H \) with \( \Delta_w A + \Delta_v A > 0 \) reaches Fleming’s bound, i.e. obeys

\[ \delta_A := \left| \frac{\langle A \rangle_w - \langle A \rangle_v}{\Delta_w A + \Delta_v A} \right| = \tan \theta, \]  
(72)

if and only if

(i) \( A \) stabilizes the subspace \( H_0 = \mathbb{C} \cdot v + \mathbb{C} \cdot w \subset H \) and

(ii) the restriction of \( A \) to \( H_0 \) is related to an operator \( A_0 \) from the set

\[ \{ \cos (\alpha) (E_{11} - E_{22}) + \sin (\alpha) (E_{12} + E_{21}) | \alpha \in [\theta, \pi - \theta] \} \]  
(73)

through \( A|_{H_0} = \lambda A_0 + \mu d_{H_0} \) for some \( \lambda \in \mathbb{R} \setminus 0 \) and \( \mu \in \mathbb{R} \). Here \( E_{ij} := e_i \langle e_j, \cdot \rangle \), with the vectors \( e_i \) from equation (57).

Observe from equation (66) that for \( \alpha = \pi/2 \) the expectation values’ difference \( \langle A \rangle_w - \langle A \rangle_v \) is maximal. The maximal difference has the value \( 2 \sin \theta \). From equation (66) we then obtain for \( p_1 = p_2 = 1/2 \) that

\[ \sin \theta = 2 W^A (D) - 1. \]  
(74)

Thus we have \( W^A (D) = \frac{1}{2} (1 + \sin \theta) \), which coincides with the result of Jaeger and Shimony [2] stated in equation (5). The corresponding observable \( A_0 \) has the following particularly simple form

\[ A_0 = e_1 \langle e_2, \cdot \rangle + e_2 \langle e_1, \cdot \rangle = \frac{w \langle w, \cdot \rangle - v \langle v, \cdot \rangle}{\sin \theta}. \]  
(75)
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