Extrema of discrete Wigner functions and applications

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We study the class of discrete Wigner functions proposed by Gibbons et al. [Phys. Rev. A 70, 062101 (2004)] to describe quantum states using a discrete phase-space based on finite fields. We find the extremal values for the discrete Wigner function in a quantum information application known as quantum random access codes. In section VI we introduce these codes with a simple example, and present a quantum random access code construction based on states that maximize the discrete Wigner function.

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I. INTRODUCTION

The Wigner function $W(q, p)$ was introduced by Wigner in 1932 [1] as a way to represent quantum states of one or more particles in phase-space. It is a quasi-probability distribution, which means it retains some of the geometrical properties akin to the properties of lines in usual geometry: for example, it can be negative in some regions in phase-space.

There were many proposals of analogues of $W(q, p)$ to represent quantum systems with discrete degrees of freedom such as spins (see [2] and references therein for a review). These discrete Wigner functions have been applied to visualize quantum states and operations in a quantum information application: a construction of quantum random access codes. These are constructed using the complete set of phase-space point operators to find encoding states and to obtain the codes’ average success rates for Hilbert space dimensions 2, 3, 4, 5, 7 and 8.

II. DEFINING A CLASS OF DISCRETE WIGNER FUNCTIONS

The discrete phase-space is a $d \times d$ grid in which we identify some particular sets of $d$ points called lines. Parallel lines are lines sharing no points in common. Following Gibbons et al. [2], a partition of the $d^2$ phase-space points into $d$ parallel lines of $d$ points each will be called a striation. The definition of lines and striations is done in such a way as to ensure, in this discrete geometry, some geometrical properties akin to the properties of lines in usual geometry:

i. given any two points, exactly one line contains both points;

ii. given a point $\alpha$ and a line $\lambda$ not containing $\alpha$, there is exactly one line parallel to $\lambda$ that contains $\alpha$;

iii. two non-parallel lines intersect at exactly one point.

In this paper we study properties and applications of the class of discrete Wigner functions defined by Gibbons et al. [2], which take values on a discrete phase-space built with finite fields. We start in sections III and IV by reviewing the definition of this class of functions. In section V we calculate the spectra of the phase-space point operators used to define the discrete Wigner functions. In section VI we describe how to use the spectra calculated to find encoding states and to obtain the codes’ average success rates for Hilbert space dimensions 2, 3, 4, 5, 7 and 8.

In [6] Wootters discusses different geometrical problems considering the discrete phase-space as a 2-dimensional vector space labelled by finite fields (for details, see [2]). In [3] we discuss different geometrical problems associated with this construction.

To define a discrete Wigner function, we need to associate a projector onto a quantum state to each line in discrete phase-space. These will be projectors onto a set of $d+1$ mutually unbiased bases (MUB). Consider two different orthonormal bases $B_1$ and $B_2$:

\begin{align}
B_1 &= \{|v_{1,1}\rangle, |v_{1,2}\rangle, ..., |v_{1,d}\rangle\}, |\langle v_{1,1}|v_{1,j}\rangle|^2 = \delta_{i,j}, \\
B_2 &= \{|v_{2,1}\rangle, |v_{2,2}\rangle, ..., |v_{2,d}\rangle\}, |\langle v_{2,1}|v_{2,j}\rangle|^2 = \delta_{i,j}.
\end{align}

These two bases $B_1$ and $B_2$ are mutually unbiased if

\begin{equation}
|\langle v_{i,j}|v_{k,l}\rangle|^2 = \frac{1}{d} \text{ if } i \neq k.
\end{equation}
Wootters and Fields showed that one can define \((d+1)\) such mutually unbiased bases for power-of-prime dimension \(d\) \cite{Wootters}. Mutually unbiased bases have been studied because of their use in a number of quantum information applications, for example quantum cryptography \cite{Bennett}, quantum state and process tomography \cite{Kelly} and in the construction of quantum t-designs \cite{Mezzadri}, used to estimate averages of functions over quantum states.

To define a discrete Wigner function (DWF) we pick a one-to-one map between the lines in discrete phase-space and the projectors onto a complete set of MUB in the following way:

- each basis set \(B_i\) is associated with one striation \(S_i\);
- each basis vector projector \(Q_{i,j} \equiv |v_{i,j}\rangle \langle v_{i,j}|\) is associated with a line \(\lambda_{i,j}\) (the \(j\)th line of the \(i\)th striation).

These maps define uniquely the values of the DWF \(W_\beta\) for all points \(\beta\) if we impose the following constraints:

\[
Tr(Q_{i,j} \rho) = \sum_{\alpha \in \lambda_{i,j}} W_\alpha, \tag{4}
\]

where \(\rho\) is the system's density matrix, and the sum is over phase-space points \(\alpha\) in the line \(\lambda\) associated with projector \(Q_{i,j}\). These requirements amount to demanding that the sum of the Wigner function over each line must be equal to the probability of projecting onto the basis vector associated with that line.

Note that there are multiple ways of making these associations. In general, this will lead to different definitions of the DWF using the same fixed set of MUB. The procedure outlined above then leads not to a single definition of \(W\), but to a class of Wigner functions instead.

We now define the phase-space point operator \(A_\beta\) associated with phase-space point \(\beta\):

\[
A_\beta \equiv \sum_{\lambda \supset \beta} Q_\lambda - I, \tag{5}
\]

where the sum is over projectors \(Q_\lambda\) associated to lines \(\lambda\) containing point \(\beta\), and \(I\) represents identity. The operators \(A_\beta\) appear naturally when we invert equations \(\ref{4}\) to write an expression for \(W_\beta\) in terms of the MUB projectors:

\[
W_\beta = \frac{1}{d} Tr(\rho A_\beta), \tag{6}
\]

The multiple ways of associating projectors with lines in phase-space result in multiple definitions for \(A_\beta\). While a single definition of \(W\) requires \(d^2\) operators \(A_\alpha\) (one for each phase-space point), the full set of \(A_\alpha\) one can define with the same fixed complete set of MUB has \(d^{d+1}\) elements. In section \(\text{IV}\) we will make use of the full set of phase-space point operators to obtain a construction for a quantum information application known as quantum random access codes.

### A. Negativity and non-classicality

Cormick et al. \cite{Cormick} have characterized the set of states which have non-negative Wigner functions. These states turn out to have some interesting properties, which we will review here, as they motivate the work reported in the remainder of this paper.

For a \(d\)-dimensional quantum system, one can find complete sets of \((d+1)\) mutually unbiased bases using the finite-field construction introduced in \cite{Wootters}. This construction is only valid for power-of-prime \(d\), since this is the necessary condition for a finite field to exist. One can then define the set \(C_d\) of \(d\)-dimensional states which have non-negative DWF in all definitions, that is, whose expectation values for all phase-space point-operators are non-negative.

In \cite{Cormick} it was shown that the only pure states in \(C_d\) are the MUB projectors, which can always be chosen to be stabilizer states. The stabilizer formalism \cite{Gottesman} provides a way to represent pure states in \(C_d\) using a number of bits which is polynomial in the number of qubits. Since general pure states require a description which is exponential-size, the set \(C_d\) is classical in the sense of having a short description.

For systems of prime dimensions, the two notions of classicality exactly coincide: the only pure states with non-negative DWF are exactly the stabilizer states. In this context, negativity of any DWF (as witnessed by negativity of one of the \(A_\alpha\) operators) indicates non-classicality in the sense of the absence of an efficient description using the stabilizer formalism. These results motivated us to investigate the extrema of the discrete Wigner functions.

Before proceeding, we need to review some constructions of complete sets of MUB for \(d\)-dimensional systems, as these are necessary to define DWF using eqs. \(\ref{4}\) and \(\ref{6}\).

### III. COMPLETE SETS OF MUTUALLY UNBIASED BASES

For prime dimension \(d\) there is a canonical construction of a complete set of \((d+1)\) MUB’s first proposed by Ivanovic \cite{Ivanovic}. To review this construction, let \(|v_{r,k}\rangle\rangle_j^j\) denote the \(j\)-th component of the \(k\)-th vector in the \(r\)-th basis, \(r = 0, 1, ..., d\). The vectors in the complete set of
IV. SPECTRA OF PHASE-SPACE POINT OPERATORS

As we have seen in the previous sections, the DWF is defined by eq. (10) using the phase-space point operators

\[ \lvert v_{d,k} \rangle = \frac{1}{\sqrt{d}} e^{\frac{2\pi i}{d} (d+1)j^k} \]

and the Hilbert space dimension is a prime power, there are different constructions of complete sets of MUB. Let us now review a simple construction of a complete set of MUB for \( n \) qubits (Hilbert space dimension \( d = 2^n \)) consisting solely of stabilizer states [14]. We start by considering the \( 4^n \) Pauli operators for \( n \) qubits, which are the tensor products of single-qubit Pauli operators \( X, Y, Z \) and identity. From this set, remove the identity operator. The remaining \( 4^n - 1 \) Pauli operators can be partitioned into \( 2^n + 1 \) sets, each containing \( 2^n - 1 \) mutually commuting Pauli operators. It was proven in [14] that the common eigenstates of the operators in each such set form a basis, and moreover that the \( 2^n + 1 \) bases thus defined are mutually unbiased.

We will now provide two examples of this construction, which will be useful to us later on. The first example is a set of 5 MUB for two qubits, each basis being formed by the common eigenstates of each row of operators in Table I In the table, operator \( XY \) for example stands for the tensor product of \( X \) on the first qubit by \( Y \) on the second.

The second example is a set of 9 MUB for three qubits, comprising the common eigenstates of the operators in each row of Table II.

V. EXTREMA OF DISCRETE WIGNER FUNCTIONS

Unlike probability distributions, we have seen that the discrete Wigner function can assume negative values. What are the extremal values that it can attain? Wootters conjectured that the minimal value \( \min(W) \) that the discrete Wigner function could assume would be \(-1/d\) for odd-prime Hilbert space dimension \( d \) [16]. He also showed that \( \min(W) = -0.183 \) for \( d = 2 \) [17], and together with Sussman [18] found a maximum value of \( \max(W) = 0.319 \) for some particular definitions of discrete Wigner functions for \( d = 8 \). In this section we calculate the spectra of \( A \) for the constructions of complete sets of MUB we reviewed in section III. The spectra we tabulate in Table III agree with the spectra calculated independently by Appleby et al. [15] for Hilbert space dimensions \( d = 3, 4, 5 \) and 7. In Table III we also report the number of phase-space point operators with each spectrum, an information which will be necessary for the quantum information application described in section VI.

We have calculated the full spectra of all \( d^{d+1} \) phase-space point operators for \( d = 2, 3, 4, 5, 7 \) and 8, but the latter two cases have too many different spectra for us to reproduce here. We would like to point out only one piece of information about these cases: the extremal eigenvalues found over all the \( A_y \). For \( d = 7 \) the largest eigenvalue is \( \lambda_{\max} = 2.4178 \) and the smallest is \( \lambda_{\min} = -1 \), whereas for \( d = 8 \) the largest is \( \lambda_{\max} = 2.5490 \) and the smallest is \( \lambda_{\min} = -0.9979 \).

For the case of two qubits (\( d = 4 \)) we calculated the spectra for all six different stabilizer MUB constructions of the kind described in [14], and the spectra found are identical to those of the MUB set in Table II. We have also established that for three qubits (\( d = 8 \)), one can find 960 different stabilizer constructions of this kind. Testing a few of those we found exactly the same spectra as for the example in Table II. Based on this, we conjecture that the phase-space point operator spectra is independent of which MUB set construction one uses.

| TABLE I: Set of 5 MUB for two qubits |
|--------------------------------------|
| 1 11 11 11 11 |
| 2 11 11 11 11 |
| 3 11 11 11 11 |
| 4 11 11 11 11 |
| 5 11 11 11 11 |

| TABLE II: Set of 9 MUB for three qubits |
|----------------------------------------|
| 1 11 11 11 11 11 11 11 11 |
| 2 11 11 11 11 11 11 11 11 |
| 3 11 11 11 11 11 11 11 11 |
| 4 11 11 11 11 11 11 11 11 |
| 5 11 11 11 11 11 11 11 11 |
| 6 11 11 11 11 11 11 11 11 |
| 7 11 11 11 11 11 11 11 11 |
| 8 11 11 11 11 11 11 11 11 |
| 9 11 11 11 11 11 11 11 11 |
describe a general method for finding the extrema among all discrete Wigner functions definable with a fixed complete set of MUB, and use it to explicitly calculate the extrema for \( d = 2, 3, 4, 5, 7 \) and 8.

Recall that the phase-space point operator \( A_\alpha \) associated with the phase-space point \( \alpha \) is given as the sum over MUB projectors associated with lines \( \lambda \) containing point \( \alpha \), and \( I \) represents identity.

Given a phase-space point operator \( A_\alpha \), we want to find the minimum of its expectation value

\[
\min \langle A_\alpha \rangle = \min \left( \text{Tr} \left( \sum_{\lambda \supset \alpha} Q_\lambda |\psi\rangle \langle \psi| \right) \right) - 1. 
\]

The minimum results when \( |\psi\rangle \) is the eigenvector associated with the smallest eigenvalue \( \lambda_\text{min} \) of \( A_\alpha \) (see the Appendix for a proof). We can evaluate the spectrum of \( A_{\alpha} \) to find its smallest eigenvalue \( \lambda_\text{min}^\alpha \). Then, using eq. \( 16 \), the most negative value for the discrete WF at point \( \alpha \) will be given by

\[
\min(W_\alpha) = \frac{1}{d} \min \langle A_\alpha \rangle = \frac{1}{d} \lambda_\text{min}^\alpha. \tag{17}
\]

To find the most negative value for the function, one needs to find all eigenvalues of all possible phase-space point operators. For a \( d \)-dimensional system there are \( d^{d+1} \) different phase-space point operators, only \( d^2 \) of which appear in any single definition of a DWF. Minimizing over \( \alpha \), we can use eq. \( 17 \) to obtain the smallest value that the function can attain.

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**TABLE III: Spectra of phase-space point operators**

| \( d \) | Number | Spectrum |
|-------|-------|---------|
| 2     | 8     | \( \frac{1}{2} + \frac{\alpha}{2}, \frac{-1}{2} - \frac{\alpha}{2} \) |
| 3     | 9     | \{-1, 1, 1\} |
|       | 72    | \( \{0, \frac{1}{2} + \alpha, \frac{1}{2} - \alpha\} \) |
| 4     | 320   | \{-0.50000, -0.50000, 0.13397, 1.86603\} |
|       | 320   | \{-0.86603, -0.50000, 0.86603, 1.50000\} |
|       | 384   | \{-0.89680, -0.14200, 0.27877, 1.76007\} |
| 5     | 1000  | \{-0.70281, -0.61803, -0.13294, 0.48666, 1.96712\} |
|       | 2000  | \{-0.79859, -0.36221, 0.00000, 0.10661, 2.05419\} |
|       | 2000  | \{-0.83607, -0.81000, 0.00000, 1.05469, 1.59139\} |
|       | 3000  | \{-0.83726, -0.58152, -0.09576, 0.62870, 1.88584\} |
|       | 1000  | \{-0.90039, -0.64018, -0.14531, 1.06785, 1.61803\} |
|       | 3000  | \{-0.90932, -0.48701, 0.00000, 0.46853, 1.92780\} |
|       | 3000  | \{-0.94658, -0.51690, -0.18438, 0.93842, 1.70944\} |
|       | 600   | \{-1.00000, -0.61803, 0.00000, 1.00000, 1.61803\} |
|       | 25    | \{-1.00000, -1.00000, 1.00000, 1.00000, 1.00000\} |

**TABLE IV: Extremal values for DWF**

| \( d \) | \( W_{\text{max}} \) | \( W_{\text{min}} \) |
|-------|------------------|------------------|
| 2     | \( \frac{1}{2}(1 + \sqrt{3}) \approx 0.683 \) | \( \frac{1}{2}(1 - \sqrt{3}) \approx -0.183 \) |
| 3     | \( \frac{1}{2}(1 + \sqrt{5}) \approx 0.539 \) | \( -\frac{1}{2} \) |
| 4     | 0.4665           | -0.2242          |
| 5     | 0.411            | -\frac{1}{2}    |
| 7     | 0.3454           | -\frac{1}{2}    |
| 8     | 0.3186           | -0.1247          |

The same reasoning can be used to obtain the maxima of the DWF, using the largest eigenvalue of any of the \( A_\alpha \). Using the spectra tabulated in section \( IV \) we obtained the extremal values of the DWF for small dimensions \( d \), listed in Table \( IV \). The results support Wootters’ conjecture for odd-prime \( d \).

**VI. AN APPLICATION: QUANTUM RANDOM ACCESS CODES**

In this section we review the quantum information protocol known as quantum random access codes, and present a code construction that relies on states maximizing the discrete Wigner function. Let us start by recalling what these codes are using a simple example.

Imagine a situation in which Alice encodes \( m \) classical bits into \( n \) bits (\( m > n \)), which she sends to Bob, who will need to know that value of a single bit (out of the \( m \) possible ones) with a probability of at least \( p \). We may represent such an encoding/decoding scheme by the notation: \( m \to n \).

Prior to sending the \( n \)-bit message, however, Alice does not know which of the \( m \) bits Bob will need to read out. To maximise the least probability of success \( p \), Alice and Bob need to agree on the use of a particular, efficient \( m \to n \) encoding.

We can consider the quantum generalization of this situation, in which Alice can send Bob \( n \) qubits of communication, instead of \( n \) bits. The idea behind these so-called quantum random access codes (QRACs) is very old by quantum information standards; it appeared in a paper written circa 1970 and published in 1983 by Stephen Wiesner. \[19\].

These codes were re-discovered in \[20\], where the explicit comparison with classical codes was made.

**A. Example: \( 3 \to 1 \) QRAC with a qubit**

Let us illustrate the idea with a \( 3 \to 1 \) quantum random access code (QRAC) that encodes three bits into a single qubit. This QRAC was attributed to Isaac Chuang in ref. \[20\].
Instead of concerning ourselves with the least decoding probability of success $p$, we will use as figure of merit the average probability of success $p_\text{avg}$. With three bits, Alice has $2^3 = 8$ possible bit-strings $b_0 b_1 b_2$. For each possibility she will prepare one particular state from the set depicted in Figure 1. These states lie on the vertices of a cube inscribed within the Bloch sphere, which is the representation of one-qubit pure states using spherical-coordinate angles $\theta, \phi$:

$$|\psi(\theta, \phi)\rangle = \cos(\theta/2) |0\rangle + \exp(i\phi) \sin(\theta/2) |1\rangle. \quad (18)$$

If Bob wants to read out bit $b_0$ he measures along the $x$-axis and associates a positive result with $b_0 = 0$. To read bits $b_1 [b_2]$ he measures along the $y$-axis [z-axis] and again associates a positive result with $b_1 = 0 [b_2 = 0]$. It is easy to see that Bob’s average probability of success is given by $p_\text{avg} = \cos^2(\theta/2) = 1/2 + \sqrt{3}/6 \approx 0.79$, where the angle $\theta$ is given in the caption to Figure 1. The optimal classical $3 \rightarrow 1$ random access code succeeds only with average probability $p_c = 0.75$, as can be checked easily through a search over all deterministic protocols.

Note that the QRAC just presented uses decoding measurements which are projections onto the canonical set of MUB for a qubit, that is, the $X, Y$ and $Z$ bases. The encoding states are found by optimizing the probability of correctly decoding each coding state.

![FIG. 1: Encoding states for the $3 \rightarrow 1$ QRAC using a single qubit. Alice prepares one out of eight states on the vertices of a cube inscribed within the Bloch sphere, depending on her three-bit string. The angle $\theta$ is such that $\cos^2(\theta/2) = 1/2 + \sqrt{3}/6 \approx 0.79$, which is the probability of Bob correctly decoding a single bit out of the three.](image)

B. A QRAC construction from $A_5$

The full set of $d^{d+1}$ phase-space point operators $A_\alpha$ can be used to build a particularly symmetric set of quantum random access codes. The encoding states will be those maximizing each $\langle A_\alpha \rangle$. Our results from section V showed that those are the largest-eigenvalue eigenstates of each $A_\alpha$.

Our goal is to construct a QRAC that encodes $(d + 1)$ messages with $d$ possible values each, using a single quantum $d$-level system that will be sent by Alice and measured by Bob. As in the case with qubits, our strategy will be for Bob to decode by performing projective measurements onto one out of the $(d + 1)$ MUB that exist for this $d$-dimensional system (for power-of-prime $d$). Alice has to find $d^{d+1}$ different encoding states, each of which will decode correctly with the highest possible probability.

As we have shown in section V the pure quantum state $|\psi_\alpha\rangle$ that maximizes $\langle A_\alpha \rangle$ is the eigenvector with largest eigenvalue $\lambda_\alpha^{\text{max}}$ of $(A_\alpha)$. Bob’s decoding procedure involves measuring the encoding state $|\psi_\alpha\rangle$ onto one of the $(d + 1)$ MUB’s. His average probability of successfully decoding will be the average $1/d + 1$ of $\langle A_\alpha \rangle$ onto one of the $(d + 1)$ MUB’s. To maximize this decoding probability for encoding state $|\psi_\alpha\rangle$, we need to minimize

$$\max \left( \frac{1}{d + 1} \sum_{\lambda \geq \alpha} \langle Q_\lambda \rangle \right) \quad \text{max} \left( \langle A_\alpha \rangle + 1 \right) \quad (19)$$

$$= \frac{1}{d + 1} (\lambda^{\text{max}}_\alpha + 1). \quad (20)$$

The average performance of this QRAC protocol can be found by averaging the probability of success of the $d^{d+1}$ encoding states, each corresponding to one phase-space point operator $A_\alpha$:

$$p_q = \frac{1}{d^{d+1}} \frac{1}{d + 1} \sum_{\alpha} (\lambda^{\text{max}}_\alpha + 1). \quad (21)$$

We see that the protocol’s average success rate $p_q$ depends on the value of the sum of the largest eigenvalues of each of the $d^{d+1}$ possible phase-space point operators $A_\alpha$.

Using the MUB constructions described in section III and the point operator spectra calculated in section IV we were able to compute $p_q$ for a $(d + 1) \rightarrow d$ QRAC using systems of dimension $d = 2, 3, 4, 5, 7$ and 8. The results are summarized in Table V. The construction recovers the known success rate of the $3 \rightarrow 1$ QRAC with a qubit.

It is clear that this construction can be extended to higher-dimensional systems, provided a DWF can be defined for them. This will be the case for power-of-prime dimensions $d$, using for example the finite-field construction given in [2].

It would be interesting to investigate how these protocols fare against the optimal classical protocols. This would require evaluating the optimal probability of success for a $(d + 1) \rightarrow d$ $d$-level classical random access code,
TABLE V: QRAC success rate $p_q$

| Dimension $d$ | Success rate $p_q$ |
|---------------|-------------------|
| $d = 2$       | $\pm\sqrt{3} \approx 0.789$ |
| $d = 3$       | $\frac{1}{2} + \frac{\sqrt{3}}{2} \approx 0.637$ |
| $d = 4$       | 0.5424            |
| $d = 5$       | 0.4700            |
| $d = 7$       | 0.3720            |
| $d = 8$       | 0.3372            |

something that to our knowledge has not been done for $d > 2$. In [20] some asymptotic results were obtained for large $d$, indicating that while there may be an advantage of quantum over classical for small dimensions $d$, this advantage practically disappears in the asymptotic regime.

VII. CONCLUSION

We have reviewed the definition of discrete Wigner functions given in [2] used to describe quantum systems in a discrete phase-space. We calculated the spectra of phase-space point operators for small dimensions, and used them to obtain the extrema of the discrete Wigner function for systems in Hilbert-space dimensions $d = 2, 3, 4, 5, 7$ and $8$. We then described the protocol known as quantum random access codes (QRAC), and used the phase-space point operators to find encoding states and to obtain the efficiency of a QRAC construction whose encoding states maximize the discrete Wigner function at each phase-space point.

APPENDIX

Let $\rho$ be a density matrix, hence positive semi-definite, Hermitian and with unit trace. Let $|\psi\rangle$ be a pure state. In this Appendix we prove that the extrema of

$$\langle \phi | \rho | \phi \rangle$$

are obtained when $|\phi\rangle$ is an eigenstate corresponding to extremal eigenvalues of $\rho$.

We start by showing that the state that maximizes this expression is the eigenstate $|\lambda_{\text{max}}\rangle$ corresponding to the largest eigenvalue $\lambda_{\text{max}}$ of $\rho$. It is easy to evaluate eq. (A.1) for $|\phi\rangle = |\lambda_{\text{max}}\rangle$:

$$\langle \lambda_{\text{max}} | \rho | \lambda_{\text{max}} \rangle = \lambda_{\text{max}} \langle \lambda_{\text{max}} | \lambda_{\text{max}} \rangle = \lambda_{\text{max}}. \quad (A.2)$$

Let us now consider the expansion of a general state $|\phi\rangle = \sum_i d_i |i\rangle$ in the basis that diagonalizes $\rho$. For $|\phi\rangle$, the expression we are trying to maximize takes the value:

$$\langle \phi | \rho | \phi \rangle = \sum_i \lambda_i |d_i|^2 = \lambda_{\text{max}} (1 - \Delta) + \sum_{j \neq \lambda_{\text{max}}} \lambda_i |d_i|^2, \quad (A.3)$$

where $\lambda_i$ are the eigenvalues of $\rho$. We have rewritten the sum to single out the term corresponding to $\lambda_{\text{max}}$, and defined $\Delta > 0$ such that $(1 - \Delta) = |d_{\text{max}}|^2$. Now, because all $\lambda_i \leq \lambda_{\text{max}}$ (by definition of $\lambda_{\text{max}}$), we have

$$\langle \phi | \rho | \phi \rangle = \lambda_{\text{max}} (1 - \Delta) + \sum_{j \neq \lambda_{\text{max}}} \lambda_i |d_i|^2 \leq \lambda_{\text{max}}. \quad (A.4)$$

So we have proven that any set of coefficients different from those of $|\lambda_{\text{max}}\rangle$ leads to a smaller expectation value for $\rho$, and so $|\lambda_{\text{max}}\rangle$ maximizes this expectation value. A similar argument can be made to prove that the state which minimizes $\langle \phi | \rho | \phi \rangle$ is the eigenstate corresponding to the smallest eigenvalue of $\rho$.

The claim following eq. (16) is justified by applying the result above to $\rho = \sum_{\lambda \geq \alpha} Q_{\lambda}$.

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