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Extremal Density Matrices for the Expectation Value of a Qudit Hamiltonian

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Abstract. An algebraic procedure to find extremal density matrices for the expectation value of a finite Hamiltonian matrix is established. The extremal density matrices for pure states provide a complete description of the system, that is, its corresponding energy spectrum and projectors. For density matrices representing mixed states, one gets the most probable eigenstates that yield extremal mean values of the energy. The procedure uses mainly the stationary solutions of the von Neumann equation of motion, the orbits of the Hamiltonian, and the positivity conditions of the density matrix. The method is illustrated for matrix Hamiltonians of dimensions $d = 2$ and $d = 3$.

1. Introduction

There are mathematical problems emerging in quantum information theory and in finite-dimensional quantum systems which can be studied by an algebraic parametrisation of the density matrix. As examples one can consider Hamiltonian systems characterising symmetric qubits [1], which appear in several branches of physics. The two-site Bose-Hubbard model to study Josephson tunnelling between two-mode Bose-Einstein condensates [2,3]; or Hamiltonians of the Lipkin-Meshkov-Glick type to study many body theories and quantum phase transitions [4,5]. Additionally for symmetric qubits there are entanglement witnesses, i.e., observables that can be measured in a given experimental set-up and thus provide an experimental verification of entanglement [6,7]. There are also many properties in quantum information related with optimisation problems, for instance, in the detection and quantification of entanglement [8]. If we do not have information about an ensemble of systems, by maximizing the entropy the probability of finding the system in any of its possible states is the same. On the contrary having knowledge of the mean value of the energy one can determine the density matrix of a system in thermal equilibrium; or by knowing the mean value of the spin operator the description of the density matrix for the spins in terms of the Pauli matrices and the polarization vector is obtained [9]. The definition of the relative entropy can be used to determine test density matrices associated to a canonical distribution of eigenstates of finite dimensional matrix Hamiltonian, which allows the determination of upper bounds to the exact free energy of Helmholtz to describe stretch vibrations of triatomic molecules [10]. In the studies of indivisible systems the nature of correlations is not obvious. However for these systems, the existence of quantum correlations can be detected by different types of inequalities which are violated for entangled states or by entropic and information inequalities written for the density matrices of systems and subsystems [11].



In finite quantum systems the density matrices can be formulated into a $su(d)$ description [12]. Actually, there are several parametrizations of finite density matrices: generalizations of the Bloch vector [13], the canonical coset decomposition of unitary matrices [14], the recursive procedures to describe $n \times n$ unitary matrices in terms of those of $U(n-1)$ [15], and by defining generalized Euler angles [16]. Recently we have established a procedure to determine the extremal density matrices of a qudit system associated to the expectation value of any observable [17]. These matrices provide an extremal description of the mean values of the energy; and in the case of restricting them to pure states the energy spectrum is recovered. So, apart from being an alternative tool to find the eigen-system, one has information of mixed states which minimize its mean value.

The aim of this work is to compute extremal density matrices in a qudit space by means of an algebraic approach [18] that uses the stationary solutions of the von Neumann equation of motion, the orbits of the Hamiltonian matrix, and the positivity conditions of the density matrix. This approach complement and simplify the variational procedure as we are going to shown. To establish this new method we review in the second section the variational procedure and apply the method to the $d = 2$ dimensional case. In the third section, the algebraic approach is introduced together with the determination of the orbits of the Hamiltonian through the construction of the Gram matrix. An explicit method to get the eigen-system, for the pure case, associated to the Hamiltonian matrices with or without degeneracy is also presented, together with the determination of the density matrices of mixed states corresponding to the extremal mean values of the energy. In section fourth, the Hamiltonian systems of $d = 3$ are studied. Finally a summary and concluding remarks are presented.

2. Variational approach to extremal density matrices

In a previous work [17] we proposed an approach to obtain information of the mean value of a finite dimensional Hamiltonian, in which a general test density matrix is written in terms of the generators $\hat{\lambda}_k$ of a special unitary algebra in d dimensions, $su(d)$, i.e.,

$$\hat{\rho} = \frac{1}{d} \hat{I} + \frac{1}{2} \sum_{k=1}^{d^2-1} \lambda_k \hat{\lambda}_k, \quad (1)$$

with $\lambda_k = \text{Tr}(\hat{\rho} \hat{\lambda}_k)$. The operators $\hat{\lambda}_k$ are completely characterized by means of the commutation and anti-commutation relations [13]

$$[\hat{\lambda}_j, \hat{\lambda}_k] = 2i \sum_{q=1}^{d^2-1} f_{jkq} \hat{\lambda}_q, \quad \{\hat{\lambda}_j, \hat{\lambda}_k\} = \frac{4}{d} \delta_{jk} \hat{I} + 2 \sum_{q=1}^{d^2-1} d_{jkq} \hat{\lambda}_q, \quad (2)$$

where d_{jkq} and f_{jkq} are the symmetric and antisymmetric structure constants given by

$$d_{jkq} = \frac{1}{4} \text{Tr}(\{\hat{\lambda}_j, \hat{\lambda}_k\} \hat{\lambda}_q), \quad f_{jkq} = \frac{1}{4i} \text{Tr}([\hat{\lambda}_j, \hat{\lambda}_k] \hat{\lambda}_q). \quad (3)$$

The density matrix must satisfy the following three properties: (a) It is Hermitian, (b) it has trace one, and (c) all its eigenvalues are positive semidefinite. While for dimension $d = 2$, the condition $\text{Tr}(\hat{\rho}^2) \leq 1$ implies (c), for $d \geq 3$ that is not true. Therefore the positivity conditions of the density matrix are established by the set $\{a_k\}$ of coefficients of its corresponding characteristic polynomial. This set can be obtained by means of the recursive relation known as Newton-Girard formulas [14, 19]

$$a_k = \frac{1}{k} \sum_{j=1}^k (-1)^{j-1} a_{k-j} t_j, \quad (4)$$

with the definitions $a_0 = a_1 = 1$, $a_d = \det \hat{\rho}$, and $t_j = \text{Tr}(\hat{\rho}^j)$, for $j = 1, \dots, d$. Therefore the allowed density matrix must be in the region given by [13, 20, 21]

$$0 \leq a_k \leq \frac{1}{d^k} \binom{d}{k}, \quad (5)$$

where $\binom{d}{k}$ denotes a binomial coefficient. The upper bound defines the most mixed state while the lower bound specifies pure states.

The compatible regions bounding the invariants a_k are obtained through the intersection of the positivity conditions of the density matrix (5) with the respective positivity conditions of the symmetric matrix called Bezoutian [22–24].

In order to consider the mean value of the Hamiltonian together with the $d - 1$ constraints to guarantee the positivity of the density matrix, we define the function

$$f(\lambda_k, \Lambda_j, h_i, c_l) \equiv \text{Tr}(\hat{H} \hat{\rho}) + \sum_{j=2}^d \Lambda_j (a_j - c_j), \quad (6)$$

which depends on $d - 1$ Lagrange multipliers $\{\Lambda_j\}$, $d - 1$ positive real constants $\{c_j\}$ to fix the degree of purity of the density matrix, $d^2 - 1$ independent variables $\{\lambda_k\}$, and d^2 real parameters associated to the expansion

$$\hat{H} = \frac{1}{d} h_0 \hat{I} + \frac{1}{2} \sum_{k=1}^{d^2-1} h_k \hat{\lambda}_k, \quad (7)$$

where $h_0 = \text{Tr}(\hat{H})$ and $h_k = \text{Tr}(\hat{H} \hat{\lambda}_k)$.

The extremal values of (6) one has to take the derivatives of $f(\lambda_k, \Lambda_j, h_i, c_l)$ with respect to the variables $\{\lambda_k\}$ and the Lagrange multipliers $\{\Lambda_j\}$. Their respective derivatives give $d^2 + d - 2$ algebraic equations,

$$\frac{1}{2} h_q + \sum_{j=2}^d \Lambda_j \frac{\partial a_j}{\partial \lambda_q} = 0, \quad q = 1, \dots, d^2 - 1, \quad (8)$$

$$a_p = c_p, \quad p = 2, \dots, d. \quad (9)$$

These sets of algebraic equations determine the critical values of the density matrix, i.e., $\lambda_q = \lambda_q^c$ and $\Lambda_q = \Lambda_q^c$ for which the expectation value of the Hamiltonian takes an extremal value. If we restrict the solutions to pure states $\{c_p = 0\}$, we have shown explicitly that the energy spectrum of the Hamiltonian is recovered for $d = 2$ and 3 [17]. Extremal expressions for the mean value of the Hamiltonian can be obtained with density matrices representing mixed quantum states, which determine also the corresponding mixture of eigenstates of the Hamiltonian.

2.1. $d = 2$

The generators $\{\hat{\lambda}_k\}$ are realised in terms of the Pauli matrices, i.e., $\hat{\lambda}_1 = \hat{\sigma}_1$, $\hat{\lambda}_2 = \hat{\sigma}_2$ and $\hat{\lambda}_3 = \hat{\sigma}_3$. Then the density and Hamiltonian matrices can be written as

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 1 + \lambda_3 & \lambda_1 - i \lambda_2 \\ \lambda_1 + i \lambda_2 & 1 - \lambda_3 \end{pmatrix}, \quad \hat{H} = \frac{1}{2} \begin{pmatrix} h_0 + h_3 & h_1 - i h_2 \\ h_1 + i h_2 & h_0 - h_3 \end{pmatrix}, \quad (10)$$

where $\boldsymbol{\lambda}$ is also called the polarization vector. Substituting the last expressions into the expressions (8) and (9) one obtains the system of equations

$$h_k - 2\Lambda\lambda_k = 0, \quad \frac{1}{4} \left(1 - \lambda_1^2 - \lambda_2^2 - \lambda_3^2 \right) = c_2, \quad (11)$$

with $k = 1, 2$ and 3 . The solutions of the system of equations are $\lambda_k^c = \pm \delta/h h_k$ and $\Lambda^c = \pm h/\delta$. with $h = \sqrt{h_1^2 + h_2^2 + h_3^2}$ and $\delta = \sqrt{1 - 4c_2}$. Thus one gets two density matrices:

$$\hat{\rho}_{\pm}^c = \frac{1}{2} \begin{pmatrix} 1 \pm \delta h_3/h & \pm \delta (h_1 - ih_2)/h \\ \pm \delta (h_1 + ih_2)/h & 1 \mp \delta h_3/h \end{pmatrix}, \quad (12)$$

which yields the extremal mean values of the energy $\langle H \rangle_{\pm}^c = \frac{1}{2} (h_0 \pm \delta h)$. These values depend on the parameter c_2 whose value is bounded, $0 \leq c_2 \leq 1/4$. For $c_2 = 1/4$, one has the maximally mixed state $\hat{\rho}_{\pm}^c = 1/2 \hat{I}_2$, which has maximum entropy. We can distinguish two types of solutions: (a) Pure case (when $c_2 = 0$, that is, $\delta = 1$): The eigenvalues $\epsilon_{\pm} = \frac{1}{2} (h_0 \pm h)$ of the Hamiltonian, and from (12), the corresponding orthogonal projectors. (b) Mixed case (when $0 < c_2 \leq 1/4$): The extremal density matrices for the expectation value of the Hamiltonian are given in terms of the convex sum

$$\hat{\rho}_{\pm}^{\text{mixed}} = \frac{1}{2} (1 + \delta) \hat{\rho}_{\pm}^{\text{pure}} + \frac{1}{2} (1 - \delta) \hat{\rho}_{\mp}^{\text{pure}}, \quad (13)$$

where $p_{\pm} = \frac{1}{2} (1 + \delta)$ indicates the probability of finding the system with eigenvalue ϵ_{+} while $p_{\mp} = \frac{1}{2} (1 - \delta)$ the corresponding probability of finding an energy ϵ_{-} .

3. Algebraic approach

The stationary solutions of the von Neumann equation of motion, which satisfy $[\hat{\rho}, \hat{H}] = 0$, are equivalent to the critical values of the generalised Bloch vector $\boldsymbol{\lambda}$ that make the expectation value of the Hamiltonian an extremal [18]. By replacing Eqs. (1) and (7) into the last expression, using the commutation relations of the generators $\hat{\lambda}_k$, multiplying by $\hat{\lambda}_q$, and tracing over the result; one gets the homogeneous system of equations

$$\sum_j \mathbf{M}_{qj} \lambda_j = 0, \quad q = 1, 2, \dots, d^2 - 1, \quad (14)$$

where we have defined the $d^2 - 1$ -dimensional skew symmetric matrix

$$\mathbf{M}_{i,j} = \sum_{k=1}^{d^2-1} f_{ijk} h_k. \quad (15)$$

The solution through the Gauss-Jordan elimination method of the underdetermined system of equations (14) leads to the critical values for the components of the Bloch vector, $\boldsymbol{\lambda}^c$. Notice that it has n free components, whose number is associated to the dimension of the null space of \mathbf{M} . This implies that maximal mixed states (all the components of the Bloch vector equal to zero) are always critical for any observable because the null space always contains the zero vector.

On the other hand, notice that $\hat{w}_q \equiv i[\hat{H}, \hat{\lambda}_q]$ are hermitian vectors spanning the tangent space of the orbits associated with \hat{H} , with $q = 1, 2, \dots, d^2 - 1$. Then by substituting the Hamiltonian expression (7) one gets

$$\hat{w}_q = \sum_{k,l} f_{qkl} h_k \hat{\lambda}_l. \quad (16)$$

Note that these vectors give the rows of \mathbf{M} , and the number of independent vectors r is determined by the rank of the Gram matrix

$$\mathbf{G}_{q,p} = \text{Tr}(\hat{w}_q \hat{w}_p) = \sum_{k_1, k_2, j} f_{q j k_1} f_{p j k_2} h_{k_1} h_{k_2}. \quad (17)$$

Because the rank \mathbf{G} is an invariant under unitary transformations [25], one has the freedom to calculate the Gram matrix in the diagonal representation of the Hamiltonian, i.e., by means of the diagonal components of the generalised Bloch vector of the Hamiltonian $\mathbf{h} = (h_1, h_2, \dots, h_{d^2-1})$. Thus, if all the eigenvalues of \hat{H} are equal, any density matrix commutes with \hat{H} , implying that $r = 0$. The other extreme is when all the eigenvalues are different [26, 27]; then the dimension of the orbit is associated to the quotient space $U(d)/[U(1) \times \dots \times U(1)]$ and thus one has that $r = d(d-1)$. Thus one has in this case $n = d-1$ free components of the Bloch vector of the critical density matrix. These components can be obtained by establishing the positivity conditions of the density matrices given in expression (9).

3.1. Non degenerate case of \hat{H}

In this case, the rank of the matrix \mathbf{M} is given by $r = d(d-1)$ and the n free variables reach its minimum number, i.e., $n = d-1$. Therefore, $\boldsymbol{\lambda}^c$ is given by

$$\boldsymbol{\lambda}^c = (\lambda_1^c, \dots, \lambda_{d(d-1)}^c, \lambda_{d(d-1)+1}, \dots, \lambda_{d^2-1}), \quad (18)$$

where the $d(d-1)$ components $\{\lambda_q^c\}$ are functions of the parameters of the Hamiltonian, the antisymmetric structure constants and a set of $d-1$ independent free variables.

The substitution of $\boldsymbol{\lambda}^c$ in (1) gives its associated critical density matrix denoted as $\hat{\rho}^c$. Therefore, the determination of the $d-1$ free variables is done by solving the system of $d-1$ polynomial equations (9), which has at most $d!$ different solutions [28, 29]. They satisfy the same polynomial system (9) but give different mean values of \hat{H} . Therefore, the critical density matrices can be written in the form

$$\hat{\rho}_m^c = \frac{1}{d} \hat{I} + \frac{1}{2} \sum_{k=1}^{d^2-1} \lambda_{m,k}^c \hat{\lambda}_k, \quad (19)$$

with m labelling the independent critical solutions. The variables $\{\lambda_{m,k}^c\}$ are function only of the known quantities, i.e., the structure constants, the parameters of the Hamiltonian (h_0, h_k), and $d-1$ constants $\{c_k\}$. The number m of solutions decreases up to d when (19) represent pure states (all $\{c_k = 0\}$) and the extremal density matrices are one-dimensional orthogonal projectors.

In general the expectation value of the Hamiltonian is given by

$$\langle \hat{H} \rangle_m^c \equiv \text{Tr}(\hat{H} \hat{\rho}_m^c), \quad (20)$$

for each critical (or extremal) density matrix $\hat{\rho}_m^c$, with $m = 1, 2, \dots, d!$. For the pure case the expectation values yield the energy spectrum of the system and the extremal density matrices are orthogonal projectors.

3.2. Degenerate case of \hat{H}

In this case the rank of the matrix \mathbf{M} satisfies that $r < d(d-1)$, whose value is associated to the orbits of the Hamiltonian. As the critical Bloch vector $\boldsymbol{\lambda}^c$ has n free variables with $n = d^2 - 1 - r$, one then has that $n > d-1$. Thus, if N denotes the number of variables appearing in the expression for the mean value of the Hamiltonian in the state $\hat{\rho}^c$, there are two cases to consider:

- i) When $1 \leq N \leq d - 1$, one has to select $n - N$ components of the density matrix Bloch vector to have $d - 1$ free variables and then solve the polynomial system of equations (9).
- ii) When $d - 1 < N \leq n$, one has only to pick up $d - 1$ components of the density matrix Bloch vector from the set of N elements, and again to solve the mentioned polynomial equation.

In both cases $d - 1$ free variables are determined by the polynomial system (9). The remaining $n - (d - 1)$ components can be taken equal to zero because they do not affect the commutator of \hat{H} with $\hat{\rho}^c$. Specifically, if we are interested in the eigensystem, i.e., all the set of $\{c_k = 0\}$, one can apply the following method recursively:

- 1) Make zero the $n - (d - 1)$ components, to solve the polynomial system (9), whose solution give at least two extremal density matrices.
- 2) Ask the orthogonality of the first set of solutions $\hat{\rho}_k^c$ with the general density matrix $\hat{\rho}^c$, i.e., $\text{Tr}(\hat{\rho}^c \hat{\rho}_k^c) = 0$, where k labels the number of solutions.
- 3) Substitute the solutions of the linear system, to express the new critical density matrix in terms of the free variables, where $d - 1$ are fixed by means of the positivity conditions (all $\{c_k = 0\}$) and the rest of the components can be taken equal to zero.
- 4) Return to step 1 and repeat the procedure again, until one gets d orthogonal projectors.

Of course, one has in this case several solutions related with the degeneracy of the Hamiltonian in similar form as in the standard diagonalization procedure of a finite Hamiltonian matrix.

4. Case $d=3$.

For the qutrit case, the generators $\hat{\lambda}_k$, with $k = 1, 2, \dots, 8$ can be realized in terms of the Gell-Mann matrices. Thus, an arbitrary density matrix is given by

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} \lambda_7 + \frac{\lambda_8}{\sqrt{3}} + \frac{2}{3} & \lambda_1 - i\lambda_4 & \lambda_2 - i\lambda_5 \\ \lambda_1 + i\lambda_4 & \frac{\lambda_8}{\sqrt{3}} - \lambda_7 + \frac{2}{3} & \lambda_3 - i\lambda_6 \\ \lambda_2 + i\lambda_5 & \lambda_3 + i\lambda_6 & \frac{2}{3} - \frac{2}{\sqrt{3}}\lambda_8 \end{pmatrix}. \quad (21)$$

We will illustrate the procedure taking special cases. For the non-degenerate case we take

$$\hat{H} = \begin{pmatrix} b & \frac{c}{\sqrt{2}} & 0 \\ \frac{c}{\sqrt{2}} & 0 & \frac{c}{\sqrt{2}} \\ 0 & \frac{c}{\sqrt{2}} & b \end{pmatrix}, \quad (22)$$

where b and c are real parameters. The Bloch vector for the Hamiltonian is given by

$$\mathbf{h} = (\sqrt{2}c, 0, \sqrt{2}c, 0, 0, 0, b, -\sqrt{3}b).$$

Substituting the components of \mathbf{h} into (15), one finds that the rank of \mathbf{M} is 6, implying that the Hamiltonian is non degenerate. Solving the system of equations (14) one obtains the extremal Bloch vector for the density matrix

$$\boldsymbol{\lambda} = \left(\frac{c\lambda_2}{\sqrt{2}b} - \frac{\sqrt{6}c\lambda_8}{b}, \lambda_2, \frac{c\lambda_2}{\sqrt{2}b} - \frac{\sqrt{6}c\lambda_8}{b}, 0, 0, 0, -\sqrt{3}\lambda_8, \lambda_8 \right).$$

Thus the associated critical density matrix is found by replacing the components of $\boldsymbol{\lambda}^c$ into (21), which is denoted by $\hat{\rho}^c$. For this case, to guarantee the positivity of the density matrix, one must consider

$$c_2 = \frac{1}{2} (1 - \text{Tr}(\hat{\rho}^c)^2), \quad c_3 = \det \hat{\rho}^c. \quad (23)$$

For the case $d = 3$, the positivity conditions (5) of the density matrix are

$$0 \leq c_2 \leq \frac{1}{3}, \quad 0 \leq c_3 \leq \frac{1}{27}, \quad (24)$$

while the Bezoutian matrix is

$$\mathbf{B}_3 = \begin{pmatrix} 3 & 1 & t_2 \\ 1 & t_2 & t_3 \\ t_2 & t_3 & t_4 \end{pmatrix}.$$

By applying the Cayley-Hamilton theorem and the formula (4) one obtains

$$t_2 = 1 - 2c_2, \quad t_3 = 1 - 3c_2 + 3c_3, \quad t_4 = 1 - 4c_2 + 2c_2^2 + 4c_3. \quad (25)$$

Similarly to the case of $d = 2$, $\det \mathbf{B}_3 \geq 0$ is the only relevant positivity condition of \mathbf{B}_3 . Expressed in terms of $\{c_2, c_3\}$, it gives

$$c_2^2 - 4c_2^3 + 18c_2c_3 - c_3(4 + 27c_3) \geq 0. \quad (26)$$

Thus, the inequalities system formed by (24) and (26) produces the compatible region between c_2 and c_3 . This is shown in Fig. 1(a). The bottom line is associated with one eigenvalue zero (yielding the condition on c_2 for the case $d = 2$), while the other curves imply two equal eigenvalues for the density matrix. The $(c_2, c_3) = (0, 0)$ case is associated to density matrices of pure states and the highest is the maximal mixed state (all the eigenvalues are equal).

Again one has two types of solutions: (a) Pure case (taking $c_2 = c_3 = 0$): Solving the system of equations $c_2 = 0$ and $c_3 = 0$, one arrives to 3 different solutions for λ_2 and λ_8 , denoted by

$$(\lambda_2, \lambda_8)_0 = \left(-1, -\frac{1}{2\sqrt{3}}\right), \quad (\lambda_2, \lambda_8)_\pm = \frac{1}{2} \left(1 \pm \frac{b}{\Delta}, \frac{\sqrt{3}}{6} \mp \frac{\sqrt{3}b}{2\Delta}\right), \quad (27)$$

where we defined $\Delta = \sqrt{b^2 + 4c^2}$, which yield three independent Bloch vectors of the density matrix, namely

$$\lambda_0 = \left(0, -1, 0, 0, 0, 0, \frac{1}{2}, -\frac{1}{2\sqrt{3}}\right), \quad (28)$$

$$\lambda_\pm = \left(\pm \frac{\sqrt{2}c}{\Delta}, \frac{1}{2} \pm \frac{b}{2\Delta}, \pm \frac{\sqrt{2}c}{\Delta}, 0, 0, 0, -\frac{1}{4} \pm \frac{3b}{4\Delta}, \frac{\sqrt{3}}{12} \mp \frac{\sqrt{3}b}{4\Delta}\right), \quad (29)$$

whose norm is equal to $4/3$ and the scalar products between them are equal to $-2/3$. Thus it is straightforward to check that the corresponding extremal density matrices are orthogonal projectors associated to the energy eigenvalues of the Hamiltonian $\epsilon_0 = b$, $\epsilon_\pm = 1/2(b \pm \Delta)$. (b) Mixed case: For any other values for c_2 and c_3 in the region shown in Fig. 1(a), one can solve the polynomial system given by (23). As an example we take $c_2 = 29/100$ and $c_3 = 1/50$. There are 6 different solutions for λ_2 and λ_8 which give rise to 6 Bloch vectors:

$$\begin{aligned} \lambda^{(1)}_\pm &= \left(\pm \frac{\sqrt{2}c}{10\Delta}, \frac{7}{20} \pm \frac{b}{20\Delta}, \pm \frac{\sqrt{2}c}{10\Delta}, 0, 0, 0, -\frac{7}{40} \pm \frac{3b}{40\Delta}, \frac{\sqrt{3}}{120} \mp \frac{\sqrt{3}b}{40\Delta}\right), \\ \lambda^{(2)}_\pm &= \left(\pm \frac{2\sqrt{2}c}{5\Delta}, -\frac{1}{10} \pm \frac{b}{5\Delta}, \pm \frac{2\sqrt{2}c}{5\Delta}, 0, 0, 0, +\frac{1}{20} \pm \frac{3b}{10\Delta}, -\frac{\sqrt{3}}{60} \mp \frac{\sqrt{3}b}{10\Delta}\right), \\ \lambda^{(3)}_\pm &= \left(\pm \frac{3\sqrt{2}c}{10\Delta}, -\frac{1}{4} \pm \frac{3b}{20\Delta}, \pm \frac{3\sqrt{2}c}{10\Delta}, 0, 0, 0, +\frac{1}{8} \pm \frac{9b}{40\Delta}, -\frac{5\sqrt{3}}{120} \mp \frac{9\sqrt{3}b}{120\Delta}\right). \end{aligned} \quad (30)$$

The corresponding extremal expectation values of the Hamiltonian are given by

$$\langle \hat{H} \rangle_\pm^{(1)} = \frac{11b}{20} \pm \frac{\Delta}{20}, \quad \langle \hat{H} \rangle_\pm^{(2)} = \frac{7b}{10} \pm \frac{\Delta}{5}, \quad \langle \hat{H} \rangle_\pm^{(3)} = \frac{3b}{4} \pm \frac{3\Delta}{20}. \quad (31)$$

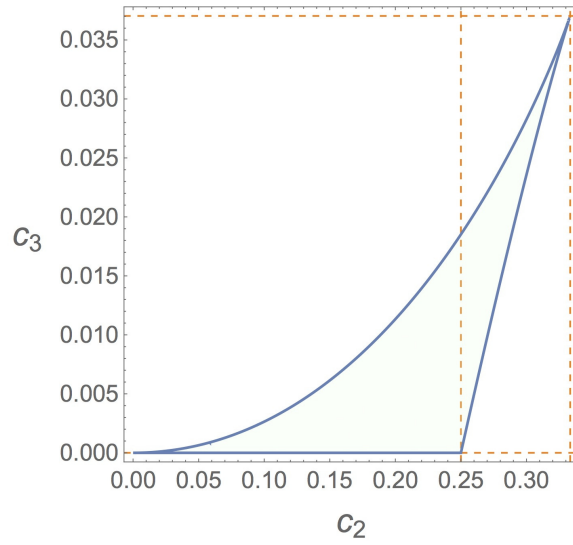


Figure 1. Regions of c_2 , and c_3 , where the positivity conditions of density matrix are satisfied. The horizontal and vertical dashed lines taking the values $c_3 = \{0, 1/27\}$ and $c_2 = \{1/4, 1/3\}$, respectively.

We find the expansion of the extremal density matrices for the mixed case in terms of the pure case described before,

$$\begin{aligned}
 \hat{\rho}_+^{(1)} &= \frac{1}{10} \hat{\rho}_0 + \frac{1}{2} \hat{\rho}_+ + \frac{2}{5} \hat{\rho}_-, & \hat{\rho}_-^{(1)} &= \frac{1}{10} \hat{\rho}_0 + \frac{2}{5} \hat{\rho}_+ + \frac{1}{2} \hat{\rho}_-, \\
 \hat{\rho}_+^{(2)} &= \frac{2}{5} \hat{\rho}_0 + \frac{1}{2} \hat{\rho}_+ + \frac{1}{10} \hat{\rho}_-, & \hat{\rho}_-^{(2)} &= \frac{2}{5} \hat{\rho}_0 + \frac{1}{10} \hat{\rho}_+ + \frac{1}{2} \hat{\rho}_-, \\
 \hat{\rho}_+^{(3)} &= \frac{1}{2} \hat{\rho}_0 + \frac{2}{5} \hat{\rho}_+ + \frac{1}{10} \hat{\rho}_-, & \hat{\rho}_-^{(3)} &= \frac{1}{2} \hat{\rho}_0 + \frac{1}{10} \hat{\rho}_+ + \frac{2}{5} \hat{\rho}_-.
 \end{aligned} \tag{32}$$

Note that the expressions (31) can be checked by calculating the expectation value of the Hamiltonian with the expansions given in the last expression.

4.0.1. Degenerate case. Now we consider the Hamiltonian matrix given by

$$\hat{H} = \begin{pmatrix} 2 & -1+i & -1-\frac{i}{3} \\ -1-i & \frac{13}{3} & 1+i2 \\ -1+\frac{i}{3} & 1-i2 & 3 \end{pmatrix}. \tag{33}$$

In this case the Bloch vector characterising the Hamiltonian is

$$\mathbf{h} = \left(-2, -2, 2, -2, \frac{2}{3}, -4, -\frac{7}{3}, \frac{\sqrt{3}}{9} \right) \tag{34}$$

with $h_0 = \frac{28}{3}$. Replacing this values into the matrix (15), the rank of \mathbf{M} is $r = 4$, which according to [26] exhibits a double degeneracy. Thus, if $\alpha > \beta$ the diagonal representation is $\text{diag}(\alpha, \beta, \beta)$, or in opposite way, if $\beta > \alpha$ then $\text{diag}(\beta, \beta, \alpha)$.

Applying the Gauss-Jordan method to (14), one gets the solutions

$$\begin{aligned}
 \lambda_1^c &= \frac{1}{14} (6\lambda_5 + 8\lambda_6 + \lambda_7 + 7\sqrt{3}\lambda_8), & \lambda_2^c &= \frac{1}{7} (3\lambda_5 - 3\lambda_6 + 11\lambda_7 - 7\sqrt{3}\lambda_8), \\
 \lambda_3^c &= \frac{1}{42} (24\lambda_5 - 24\lambda_6 + 11\lambda_7 - 7\sqrt{3}\lambda_8), & \lambda_4^c &= \frac{1}{42} (-30\lambda_5 + 30\lambda_6 - 19\lambda_7 + 35\sqrt{3}\lambda_8).
 \end{aligned}$$

Hence, the critical Bloch vector is given by $\lambda^c = (\lambda_1^c, \lambda_2^c, \lambda_3^c, \lambda_4^c, \lambda_5, \lambda_6, \lambda_7, \lambda_8)$, with 4 free parameters and its associated critical density matrix is denoted as $\hat{\rho}^c$.

In order to obtain the eigen-system of \hat{H} , we use the procedure established before for the degenerated case:

- We select $\lambda_5 = \lambda_6 = 0$, solve the polynomial condition (23) with $c_2 = c_3 = 0$, and get the following Bloch vectors of the density matrix

$$\lambda^{(1)} = \frac{1}{11} \left(6, 0, 0, 6, 0, 0, 7, 11/\sqrt{3} \right), \quad \lambda^{(2)} = \frac{1}{46} \left(12, 36, 6, 0, 0, 0, 35, 19/\sqrt{3} \right). \quad (35)$$

These yield two density matrices $\hat{\rho}^{(1)}$, and $\hat{\rho}^{(2)}$ which are not independent. Both give an energy eigenvalue $\epsilon = 4/3$.

- We establish the algebraic system of equations,

$$\left\{ \text{Tr} \left(\hat{\rho}^{(1)} \hat{\rho}^c \right), \text{Tr} \left(\hat{\rho}^{(2)} \hat{\rho}^c \right) \right\} = 0, \quad (36)$$

whose solution, together with the positivity condition, gives another independent Bloch vector

$$\lambda^{(3)} = \frac{1}{16} \left(-6, -6, 6, -6, 2, -12, -7, 1/\sqrt{3} \right). \quad (37)$$

Thus we have obtained another extremal density matrix orthogonal to $\hat{\rho}^{(1)}$, and $\hat{\rho}^{(2)}$ and the expectation value of the Hamiltonian yields the eigenvalue $\epsilon_2 = 20/3$. Until now we have obtained 2 independent and orthogonal projectors, namely $\hat{\rho}^{(1)}$ and $\hat{\rho}^{(3)}$.

- We repeat the procedure by establishing the algebraic system of equations

$$\left\{ \text{Tr} \left(\hat{\rho}^{(1)} \hat{\rho}^c \right), \text{Tr} \left(\hat{\rho}^{(3)} \hat{\rho}^c \right) \right\} = 0, \quad (38)$$

whose solution gives the Bloch vector

$$\lambda^{(4)} = \left(-\frac{15}{88}, \frac{3}{8}, -\frac{3}{8}, -\frac{15}{88}, -\frac{1}{8}, \frac{3}{4}, -\frac{35}{176}, -\frac{17}{16\sqrt{3}} \right). \quad (39)$$

One gets then another orthogonal projector $\hat{\rho}^{(4)}$ and the corresponding expectation value of the Hamiltonian is $\epsilon_3 = 4/3$.

We have obtained the complete eigen-system of the degenerated Hamiltonian. For the eigenvalue $\epsilon = 4/3$, we indeed have a family of projectors yielding the same eigenvalue.

5. Summary and Conclusions

The main contribution of our work is to give an algebraic procedure to find extremal density matrices for a given Hamiltonian. Our approach applies to both the degenerate and non degenerate cases of the Hamiltonian. The examples of the procedure are given for dimensions $d = 2, 3$ and show that the Hamiltonian spectrum for the pure case is recovered. For the mixed case, we have verified that the extremal values of the expectation value of the Hamiltonian is a convex sum of the corresponding results for the pure case. We want to enhance that the method can be applied by replacing the Hamiltonian for any observable acting on a qudit space.

We established that an extremal density matrix commutes with the Hamiltonian operator and optimizes its mean value. We demonstrated that at most $d-1$ variables are necessary to find extremal density matrices with appropriate positivity conditions, for the non-degenerated case of the finite matrix Hamiltonian. In the degenerate pure case, one has more free components of the

extremal density matrix which can be selected by asking orthogonality between the projectors, which allow to obtain the energy spectrum.

Finally, for the examples with $d = 2$, and $d = 3$ following the method given in [24], we find also the compatible regions between the coefficients of the characteristic polynomial of the density matrix in terms of the positivity conditions of the Bezoutian matrix in order to provide a self-contained approach.

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