On the Eigenvalue Problem in Multipartite Quantum Systems

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Abstract. We show that the Hamiltonian of a multiqudit system can be diagonalized through a sequence of unitary transformations written in terms of Hubbard operators. As an application this formalism is applied to particular cases of two and three-qubit systems.

1. Introduction

The eigenvalue problem plays a relevant role in quantum mechanics. Indeed, the set of eigenvalues of a linear operator $A$ yields the numerical results that one would obtain when the observable represented by $A$ is measured \cite{1}. In the case where the system of study is integrated by several parts some algebraic subtleties should be taken into account. For instance, consider a system of $n$ subsystems with $d$ levels each, the pure states are represented by vectors in the Hilbert space $\mathcal{H}_d^\otimes n$, here $\otimes$ denotes the Kronecker (tensor or direct) product \cite{2, 3}, and $\mathcal{H}_d$ stands for the Hilbert space of a single $d$-level system (qudit). An operator $A_k$ acting on the $k$-th subsystem is promoted to act on the entire space in the following way

$$A_k \leftrightarrow I_d \otimes I_d \otimes \cdots \otimes I_d \otimes A_k \otimes I_d \otimes \cdots \otimes I_d \quad (k-1)\text{-times}$$

$$\quad \otimes \quad \otimes \quad \otimes \quad (n-k)\text{-times}$$

where $I_d$ is the identity operator in $\mathcal{H}_d$. It is not difficult to realize that the matrix representation of (1) has at most $d^{n+1} < d^{2n}$ entries different from zero. This fact suggests to look for a convenient framework to handle with the involved cumbersome calculations. To approach the tensor product algebra in a more convenient way we proposed the use of Hubbard operators \cite{2–4}. Indeed, these are also referred as X-operators and satisfy the following properties

i) $X^{i,j}X^{k,m} = \delta_{jk}X^{i,m}$ (multiplication rule)

ii) $\sum_k X^{k,k} = 1$ (completeness)

iii) $(X^{i,j})^\dagger = X^{j,i}$ (non-hermiticity)

Because of property ii) any linear operator $A$ acting on the whole system can be expressed in terms of the X-operators. For instance, the Hamiltonian of the system in this representation

$$A_k \leftrightarrow I_d \otimes I_d \otimes \cdots \otimes I_d \otimes A_k \otimes I_d \otimes \cdots \otimes I_d \quad (k-1)\text{-times}$$

$$\quad \otimes \quad \otimes \quad \otimes \quad (n-k)\text{-times}$$

would have at most $d^{n+1} < d^{2n}$ non-zero matrix elements.
reads
\[ H = \sum_{i_{n-1}, \ldots, i_0} h_{i_{n-1}, \ldots, i_0} X^{i_{n-1}j_{n-1}} \otimes \cdots \otimes X^{i_1j_1} \otimes X^{i_0j_0}, \]  
\tag{2}

Of particular interest is the diagonalization of Hamiltonians with nearest-neighbour spin interaction. Among them are the bipartite three dimensional anisotropic Ising model [5], the XY Heisenberg model for spin-1/2, which can be exactly diagonalized using the Jordan-Wigner transformation [6], etc. For higher spins the diagonalization of some Heisenberg models have been accomplished numerically [7]. In the present work we use the tensor product properties of the Hubbard operators to diagonalize some spin interacting Hamiltonians. Indeed, it has been shown in [2,4] that the tensor products in equation (2) can be written as an X-operator depending on just two indices. Such a representation allows us to generalize the Unitary Transformation Method (UTM) introduced by Ovchinnikov [8] to diagonalize a Hermitian operator in an easy manner.

This contribution is organized as follows. In Section 2 we present a short review of the UTM for a single \( d \)-level system. The formalism of Hubbard operators for systems of several qudits is discussed in Section 3. It is shown that cumbersome calculations of the tensor product can be turned into simple relations of indices. Moreover, we generalize the UTM for hermitian operators acting on a multiqubit space. In Sec. 4 this formalism is applied to specific cases of two and three-qubit Hamiltonians. Finally, some remarks are given in Sec. 5.

2. A review of the unitary transformation method

Let \( B = \{ |p\rangle : p = 0, 1, \ldots, d - 1 \} \) be an orthonormal basis of \( \mathcal{H}_d \). Thus, a vector \( |\psi\rangle \in \mathcal{H} \) can be written as a normalized linear combination of the basis elements

\[ |\psi\rangle = \sum_{p=0}^{d-1} c_p |p\rangle, \quad c_p \in \mathbb{C}, \quad \sum_{p=0}^{d-1} |c_p|^2 = 1. \tag{3} \]

On the other hand, the simplest representation of Hubbard operators acting on \( \mathcal{H}_d \) is constructed as the following outer products

\[ X^{p,q}_d := |p\rangle \langle q|, \quad p, q = 0, 1, \ldots, d - 1, \tag{4} \]

where the sub-index \( d \) makes reference to the dimension of the space. It is not difficult to prove that the operator so defined fulfill the properties i) – iii). Furthermore, the matrix representation of (4) has 1 in the entry \( (i+1, j+1) \) and zero elsewhere. The action of the operator \( X^{p,q}_d \) on any basis vector follows immediately

\[ X^{p,q}_d |r\rangle = \delta_{q,r} |p\rangle. \tag{5} \]

Thus, the Hamiltonian \( H \) of the system can be written as a linear combination of Hubbard operators

\[ H = \sum_{p=0}^{d-1} \epsilon_p X^{p,p}_d + \sum_{p \neq q}^{d-1} V_{p,q} X^{p,q}_d, \quad \epsilon_d \in \mathbb{R}, \quad V_{p,q} \in \mathbb{C}, \quad V_{q,p} = V_{p,q}^*, \tag{6} \]

the conditions on the coefficients follow from the fact \( H^\dagger = H \). We restrict ourselves to the case where all coefficients are real, hence \( V_{q,p} = V_{p,q} \). In order to solve the eigenvalue equation

\[ H |E_p\rangle = E_p |E_p\rangle, \quad p = 0, 1, \ldots, d - 1, \tag{7} \]
we look for an unitary operator $U$ so that the transformed Hamiltonian

$$H' = UHU^\dagger = \sum_{p=0}^{d-1} E_p X_d^{p,p}. \tag{8}$$

is indeed diagonal. Note that in this representation the states $|p\rangle$ are eigenstates of (8) with eigenvalue $E_p$. Remark that degeneracy is not been taking into account. Moreover, the states fulfilling (7) are obtained as eigenvalue $E|\alpha_k,\ell\rangle = \exp[\alpha_k,\ell(X^k,\ell - X^{d,\ell})]$, $k < \ell$, $\alpha_k,\ell \in \mathbb{R}$. \tag{9}

For fixed indices $k$ and $\ell$ and using the Baker-Campell-Hausdorff formula it is easy to show that the operator (9) changes $H$ to

$$H^{(1)} = U_{k,\ell}(\alpha_k,\ell)HU_{k,\ell}^\dagger(\alpha_k,\ell) = \sum_{p=0}^{d-1} \epsilon_p^{(1)} X_n^{p,p} + \sum_{p\neq q} V_{p,q}^{(1)} X_n^{p,q}, \tag{10}$$

where

$$\begin{align*}
\epsilon_k^{(1)} &= \frac{1}{2}(\epsilon_k + \epsilon_\ell) + \frac{1}{2}(\epsilon_k - \epsilon_\ell) \cos 2\alpha_k,\ell + V_{k,\ell} \sin 2\alpha_k,\ell, \\
\epsilon_\ell^{(1)} &= \frac{1}{2}(\epsilon_k + \epsilon_\ell) - \frac{1}{2}(\epsilon_k - \epsilon_\ell) \cos 2\alpha_k,\ell - V_{k,\ell} \sin 2\alpha_k,\ell, \\
V_{k,\ell} &= -\frac{1}{2}(\epsilon_k - \epsilon_\ell) \sin 2\alpha_k,\ell + V_{k,\ell} \cos 2\alpha_k,\ell, \\
V_{k,p}^{(1)} &= V_{k,p} \cos \alpha_k,\ell + V_{\ell,p} \sin \alpha_k,\ell, \\
V_{p,\ell}^{(1)} &= V_{p,\ell} \cos \alpha_k,\ell - V_{p,k} \sin \alpha_k,\ell, \\
\epsilon_p^{(1)} &= \epsilon_p, \\
V_{p,q}^{(1)} &= V_{p,q}, \quad p \neq k, \ell.
\end{align*} \tag{11}$$

The former procedure can be repeated iteratively to get $H^{(r)} = VHV^\dagger$ where the transformation $V = V(\alpha_k,\ell, \ldots, \alpha_{k_1,\ell_1}) = U_{k_1,\ell_1} \cdots U_{k_r,\ell_r}$, with $r \leq n(n - 1)/2$. To erase the off-diagonal elements we require $V_{k_1,\ell_1}^{(r)} = V_{k_2,\ell_2}^{(r)} = \ldots = V_{k_r,\ell_r}^{(r)} = 0$. These conditions constitute a system of $r$ non-linear equations in the parameters $\alpha_{k_1,\ell_1}, \ldots, \alpha_{k_r,\ell_r}$, whose solution allows to find the operator $V$. Clearly, the eigenvalues of both $H^{(r)}$ and $H$ are the numbers $\epsilon^{(r)}$. Moreover, the eigenvectors of $H$ are computed as $|E_p\rangle = V^\dagger|p\rangle$. According to Ovchinnikov \cite{8} we should solve $d(d - 1)/2$ non-linear equations, however it will be shown that in some cases the number of equations and parameters can be reduced.

3. Multiqudit systems

The Hilbert space $\mathcal{H}_d^{\otimes n}$ of a system of $n$ qudits is constructed as follows

$$\mathcal{H}_d^{\otimes n} = \text{Span}\{ |i_{n-1}\rangle \otimes \cdots \otimes |i_1\rangle \otimes |i_0\rangle, \quad i_\ell = 0, 1, \ldots, d - 1\}. \tag{12}$$

According to Ref. \cite{4} the basis elements can be labeled using a single-index notation identifying $|i_{n-1}\rangle \otimes \cdots \otimes |i_1\rangle \otimes |i_0\rangle \equiv |i_{n-1} \cdots i_1 \cdots i_0\rangle$, where $i = (i_{n-1} \cdots i_0)_d$. The last expression indicates that the numbers $i_\ell$ are the coefficients of the expansion of $i$ in base $d$ and they are related with the physical state of the $(n - \ell)$-th subsystem. Moreover, any vector $|\psi\rangle \in \mathcal{H}_d^{\otimes n}$ is a linear combination of the form

$$|\psi\rangle = \sum_{i=0}^{d^n-1} c_i |i\rangle = \sum_{i=0}^{d^n-1} c_i |i_{n-1} \cdots i_0\rangle, \quad i = (i_{n-1} \cdots i_0)_d. \tag{13}$$
On the other hand, it was shown in [4] that any linear operator $A$ acting on the Hilbert space of a multipartite system can be written in terms of Hubbard operators using a single-index for both rows and columns, for instance the Hamiltonian (2) reads

$$H = \sum_{i,j=0}^{d^n-1} h_{i_{n-1}, \ldots, i_0; j_{n-1}, \ldots, j_0} X^{i,j}_{d^n}, \quad i = (i_{n-1} \cdots i_0)_d, \quad j = (j_{n-1} \cdots j_0)_d. \quad (14)$$

This representation is convenient to deal with some algebraic calculations. For instance, the action of $H$ on a linear combination (13) follows immediately from equation (5). Note that if a $n$-qudit Hamiltonian is written in this form then can be diagonalized by the UTM. This observation generalizes the method for multiqudit systems. In the following Section two particular cases are studied.

4. Applications
An operator defined as follows

$$H_2 = \epsilon_n X_{d,n}^2 + \epsilon_m X_{d,m}^m + V_{n,m}\{X_{d,n}^{n,m} + X_{d,m}^{m,n}\}, \quad m > n, \quad \epsilon_m \geq \epsilon_n. \quad (15)$$

is known as a two-level form. In particular, when $d = 2$ the well-known two-level Hamiltonian is recovered. We now consider the transformation (10) on $H_2$ with $k = n$ and $\ell = m$. To take the operator (15) to a diagonal form we require $V_{n,m}^{(1)} = 0$, which yields the condition

$$(\epsilon_n - \epsilon_m) \sin(2 \alpha_{n,m}) = 2 V_{n,m} \cos(2 \alpha_{n,m}), \quad (16)$$

hence it is obtained

$$\sin(2 \alpha_{n,m}) = \frac{-2 V_{n,m}}{[(\epsilon_n - \epsilon_m)^2 + 4(V_{n,m})^2]^{1/2}}, \quad \cos(2 \alpha_{n,m}) = \frac{\epsilon_m - \epsilon_n}{[(\epsilon_n - \epsilon_m)^2 + 4(V_{n,m})^2]^{1/2}}. \quad (17)$$

Substituting the last equations in the expressions for $\epsilon_n^{(1)}$ and $\epsilon_m^{(1)}$ in (11) the two eigenvalues of $H_2$ are immediately computed

$$E_n = \epsilon_n^{(1)} = \frac{1}{2}(\epsilon_n + \epsilon_m) - \frac{1}{2} \left[(\epsilon_n - \epsilon_m)^2 + 4(V_{n,m})^2]\right]^{1/2},$$
$$E_m = \epsilon_m^{(1)} = \frac{1}{2}(\epsilon_n + \epsilon_m) + \frac{1}{2} \left[(\epsilon_n - \epsilon_m)^2 + 4(V_{n,m})^2]\right]^{1/2}. \quad (18)$$

The eigenvectors are calculated as $|E_p\rangle = U_{n,m}^{\dagger}(\alpha_{n,m})|p\rangle$, for $p = n, m$. Hence, we obtain

$$|E_n\rangle = \cos \alpha_{n,m}|n\rangle + \sin \alpha_{n,m}|m\rangle, \quad |E_m\rangle = \cos \alpha_{n,m}|n\rangle - \sin \alpha_{n,m}|m\rangle, \quad (19)$$

where

$$\cos \alpha_{n,m} = \left[ \frac{E_m - \epsilon_n}{E_m - E_n} \right]^{1/2}. \quad (20)$$

As an example consider the Hamiltonian for the two-qubit anisotropic Ising model proposed by Delgado [5]

$$H_2 = -\sum_{i=1}^{2} \lambda_i \sigma_i \otimes \sigma_i + b_3 (1 \otimes \sigma_3) + c_3 (\sigma_3 \otimes 1), \quad (21)$$
where $\sigma_i$ are the Pauli matrices and $\lambda_i, b_3$ and $c_3$ are real parameters. Using equation (14) and identifying $\lambda_1 = \lambda, \lambda_2 = \chi$ and $\lambda_3 = \beta$ this operator can be written as $H_2 = h_1 + h_2$, where

\begin{align*}
h_1 &= (\chi - \lambda) (X_4^{0,3} + X_4^{3,0}) + (b_3 + c_3 - \beta)X_4^{0,0} - (b_3 + c_3 + \beta)X_4^{3,3} \\
h_2 &= (\chi + \lambda) (X_4^{1,2} + X_4^{2,1}) + (-b_3 + c_3 + \beta)X_4^{2,1} - (b_3 - c_3 + \beta)X_4^{2,2}.
\end{align*}

(22)

are two-level forms. In order to diagonalize $H_2$ we apply a sequence of two transformations (9) as follows $H_2^{(2)} = U_{1.2}U_{0.3}H_2U_{1.2}^\dagger$. Note that the action of $U_{0.3} (U_{1.2})$ leaves $h_2(h_1)$ invariant. So, the conditions $V_{0.3}^{(2)} = V_{1.2}^{(2)} = 0$ yield the parameters $\alpha_{0,3}$ and $\alpha_{1,2}$. Moreover, the eigenvalues are computed using equations (19)

\begin{align*}
E_0 &= -\beta - [(b_3 + c_3)^2 + (\chi - \lambda)^2]^{1/2}, & E_1 &= \beta - [(b_3 - c_3)^2 + (\chi + \lambda)^2]^{1/2}, \\
E_2 &= \beta + [(b_3 - c_3)^2 + (\chi + \lambda)^2]^{1/2}, & E_3 &= -\beta + [(b_3 + c_3)^2 + (\chi - \lambda)^2]^{1/2}.
\end{align*}

(23)

The corresponding eigenvectors in the single-index and computational basis read

\begin{align*}
|E_0\rangle &= \cos \alpha_{0,3} |0\rangle + \sin \alpha_{0,3} |3\rangle = \cos \alpha_{0,3} |00\rangle + \sin \alpha_{0,3} |11\rangle, \\
|E_1\rangle &= \cos \alpha_{1,2} |1\rangle + \sin \alpha_{1,2} |2\rangle = \cos \alpha_{1,2} |01\rangle + \sin \alpha_{1,2} |10\rangle, \\
|E_2\rangle &= \cos \alpha_{1,2} |1\rangle - \sin \alpha_{1,2} |2\rangle = \cos \alpha_{1,2} |01\rangle - \sin \alpha_{1,2} |10\rangle, \\
|E_3\rangle &= \cos \alpha_{0,3} |0\rangle - \sin \alpha_{0,3} |3\rangle = \cos \alpha_{0,3} |00\rangle - \sin \alpha_{0,3} |11\rangle,
\end{align*}

(24)

where

\[
\cos \alpha_{0,3} = \sqrt{\frac{E_3 - \epsilon_0}{E_3 - E_0}}, \quad \text{and} \quad \cos \alpha_{1,2} = \sqrt{\frac{E_2 - \epsilon_1}{E_2 - E_1}}.
\]

(25)

We now consider a particular case of a four-level form given by

\[
H_4 = \epsilon_p X_d^{p,p} + \epsilon_q (X_d^{q,q} + X_d^{p,r} + X_d^{s,s}) + \gamma (X_d^{p,s} + X_d^{r,r} + X_d^{q,s} + X_d^{r,s}) + h.c., \quad \gamma, \delta \in \mathbb{R}.
\]

(26)

In order to diagonalize $H_4$ we take a sequence of transformations (9). The entries of the transformed operator $H_4^{(1)} = U_{q,s}H_4U_{q,s}^\dagger$ read

\[
\begin{align*}
\epsilon_q^{(1)} &= \epsilon_q + \delta \sin(2\alpha_{q,s}), & \epsilon_s^{(1)} &= \epsilon_s - \delta \sin(2\alpha_{q,s}), & V_{q,s}^{(1)} &= \delta \cos(2\alpha_{q,s}), \\
V_{p,q}^{(1)} &= \gamma \cos \alpha_{q,s} + \gamma \sin \alpha_{q,s}, & V_{q,r}^{(1)} &= \delta \cos \alpha_{q,s} + \delta \sin \alpha_{q,s}, \\
V_{p,s}^{(1)} &= \gamma \cos \alpha_{q,s} - \gamma \sin \alpha_{q,s}, & V_{r,s}^{(1)} &= \delta \cos \alpha_{q,s} - \delta \sin \alpha_{q,s}.
\end{align*}
\]

(27)

Remark that $V_{\ell,k}^{(1)} = V_{k,\ell}^{(1)}$ and the other entries remain the same. As a second step we make the transformation $H_4^{(2)} = U_{q,r}H_4^{(1)}U_{q,r}^\dagger$, where

\[
\begin{align*}
\epsilon_q^{(2)} &= \frac{1}{2} (\epsilon_q^{(1)} + \epsilon_r^{(1)}) + \frac{1}{2} (\epsilon_q^{(1)} - \epsilon_r^{(1)}) \cos(2\alpha_{q,r}) + V_{q,r}^{(1)} \sin(2\alpha_{q,r}), \\
\epsilon_r^{(2)} &= \frac{1}{2} (\epsilon_q^{(1)} + \epsilon_r^{(1)}) - \frac{1}{2} (\epsilon_q^{(1)} - \epsilon_r^{(1)}) \cos(2\alpha_{q,r}) - V_{q,r}^{(1)} \sin(2\alpha_{q,r}), \\
V_{q,r}^{(2)} &= -\frac{1}{2} (\epsilon_q^{(1)} - \epsilon_r^{(1)}) \sin(2\alpha_{q,r}) + V_{q,r}^{(1)} \cos(2\alpha_{q,r}), \\
V_{q,s}^{(2)} &= V_{q,s}^{(1)} \cos \alpha_{q,r} + V_{r,s}^{(1)} \sin \alpha_{q,r}, & V_{q,p}^{(2)} &= V_{q,p}^{(1)} \cos \alpha_{q,r} + V_{r,p}^{(1)} \sin \alpha_{r,p}, \\
V_{p,r}^{(2)} &= V_{p,r}^{(1)} \cos \alpha_{q,r} - V_{p,q}^{(1)} \sin \alpha_{q,r}, & V_{s,r}^{(2)} &= V_{s,r}^{(1)} \cos \alpha_{q,r} - V_{s,q}^{(1)} \sin \alpha_{r,p}.
\end{align*}
\]

(28)
To erase the off-diagonal elements we require $V_{q,s}^{(2)} = V_{r,t}^{(2)} = 0$. The first condition fulfills if $V_{q,s}^{(1)} = V_{r,t}^{(1)} = 0$ and hence $\alpha_{q,s} = \pi/4$, the latter yields $\cos^2(\alpha_{q,r}) = 1/9$ and $H_4^{(2)}$ reduces to a two-form

$$H_4^{(2)} = \epsilon_p X_{d}^{p,p} + (\epsilon_q + 2\delta)X_{d}^{q,q} + (\epsilon_q - \delta)(X_{d}^{r,r} + X_{d}^{s,s}) + \sqrt{3}\gamma\{X_{d}^{p,q} + X_{d}^{q,p}\}.$$  \hfill (29)

This can be diagonalized using the previous method. The eigenvalues of $H_4$ read

$$E_p = \frac{1}{2}(\epsilon_p + \epsilon_q + 2\delta) - \frac{1}{2} \left[(\epsilon_p - \epsilon_q - 2\delta)^2 + 12\gamma^2\right]^{1/2},$$

$$E_q = \frac{1}{2}(\epsilon_p + \epsilon_q + 2\delta) - \frac{1}{2} \left[(\epsilon_p - \epsilon_q - 2\delta)^2 + 12\gamma^2\right]^{1/2}, \quad E_r = E_s = \epsilon_q - \delta.$$  \hfill (30)

The normalized eigenvectors are obtained as $|E_k\rangle = U_{q,s}^{\dagger}U_{q,s}^{\dagger}U_{p,q}^{\dagger}|k\rangle$, for $k = p, q, r, s$. We find

$$|E_p\rangle = \cos \alpha_{p,q}|p\rangle + \frac{1}{\sqrt{3}} \sin \alpha_{p,q} (|q\rangle + |r\rangle + |s\rangle),$$

$$|E_q\rangle = - \sin \alpha_{p,q}|p\rangle + \frac{1}{\sqrt{3}} \cos \alpha_{p,q} (|q\rangle + |r\rangle + |s\rangle),$$

$$|E_r\rangle = - \frac{1}{\sqrt{6}}|q\rangle + \frac{2}{3}\sqrt{2}|r\rangle + \frac{1}{\sqrt{6}}|s\rangle,$$

$$|E_s\rangle = \frac{1}{\sqrt{2}}(|s\rangle - |q\rangle), \quad \text{where } \cos \alpha_{p,q} = \left[\frac{E_q - \epsilon_p}{E_q - E_p}\right]^{1/2}.$$  \hfill (31)

The four-level form (26) is useful in the study of a three-qubit system with pairwise interaction given by (21). In such a case it can be shown that the corresponding Hamiltonian is written as the sum of two four-forms (26) with $d = 2^3$, and its eigenvalues and eigenvectors are obtained using the method formerly presented [9]. More general problems can be approached using this formalism. For instance, one can consider the eigenvalue problem of the hierarchy of $n$-qubit Hamiltonians studied in [10, 11]. In the case of higher spin, the Hamiltonian (21) can be generalized by changing $\sigma_i \rightarrow J_i$, where $J_i$ is the $i$-th generator of $SU(2)$ with arbitrary $j$. In such a case the corresponding eigenvalues and eigenvectors can be found by diagonalizing two $2^{2j}$-level forms. These results will be reported elsewhere.

5. Conclusions

The unitary transformation method was originally proposed to diagonalize a single $d$-level system Hamiltonian. However, we have shown that the method can be extended to the case of $n$ qudits by means of the tensor product algebra of Hubbard operators. The developed formalism was applied to particular cases with $d = 2$ and $n = 2, 3$, still the general case can be treated once the Hamiltonian is written as a sum of appropriate $k$-level forms.

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