The Gram matrix of a $\mathcal{PT}$-symmetric quantum system *)

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Received 17 October 2003

The eigenstates of a diagonalizable $\mathcal{PT}$-symmetric Hamiltonian satisfy unconventional completeness and orthonormality relations. These relations reflect the properties of a pair of bi-orthonormal bases associated with non-hermitean diagonalizable operators. In a similar vein, such a dual pair of bases is shown to possess, in the presence of $\mathcal{PT}$ symmetry, a Gram matrix of a particular structure: its inverse is obtained by simply swapping the signs of some its matrix elements.

PACS: 03.67.–w
Key words: Gram Matrix, $\mathcal{PT}$ symmetry, bi-orthonormal basis

The spectrum of a non-hermitean Hamiltonian $\hat{H}$ is *real* if the Hamiltonian is invariant under the combined action of self-adjoint parity $\mathcal{P}$ and time reversal $\mathcal{T}$,

$$[\hat{H}, \mathcal{PT}] = 0 \,, \tag{1}$$

and if the energy eigenstates are invariant under the operator $\mathcal{PT}$ [1]. Pairs of *complex conjugate* eigenvalues are also compatible with $\mathcal{PT}$ symmetry but the eigenstates of $\hat{H}$ are no longer invariant under $\mathcal{PT}$. Wigner's representation theory of anti-linear operators [2], when applied to the operator $\mathcal{PT}$ [3], explains these observations in a group-theoretical framework. Alternatively, they follow from the properties of *pseudo-Hermitean* operators [4] satisfying $\eta\hat{H}\eta^{-1} = \hat{H}^\dagger$ equivalent to Eq. (1) if $\eta = \mathcal{P}$.

Consider a (diagonalizable) *non-Hermitean* Hamiltonian $\hat{H}$ with a discrete spectrum [5]. The operators $\hat{H}$ and and its adjoint $\hat{H}^\dagger$ have complete sets of eigenstates:

$$\hat{H}|E_n\rangle = E_n|E_n\rangle \,, \quad \hat{H}^\dagger|E^n\rangle = E^n|E^n\rangle \,, \quad n = 1, 2, \dots \,, \tag{2}$$

with, in general, complex conjugate eigenvalues, $E^n = E_n^*$. The eigenstates constitute *bi-orthonormal* bases in $\mathcal{H}$ with two resolutions of unity,

$$\sum_n |E^n\rangle\langle E_n| = \sum_n |E_n\rangle\langle E^n| = \hat{I} \,, \tag{3}$$

and as dual bases, they satisfy orthonormality relations,

$$\langle E^n|E_m\rangle = \langle E_m|E^n\rangle = \delta_{nm} \,, \quad m, n = 1, 2, \dots \tag{4}$$

*) Presented at the 1st International Workshop "Pseudo-Hermitian Hamiltonians in Quantum Physics", Prague, Czech Republic, June 16–17, 2003

It has been shown [6] that $\mathcal{PT}$ symmetry of the Hamiltonian (2) implies the existence of a simple relation between the state $|E_n\rangle$ and its dual partner $|E^n\rangle$,

$$|E^n\rangle = s_n \mathcal{P} |E_n\rangle = \mathcal{P}\mathcal{C}_s |E_n\rangle \,, \quad s_n = \pm 1 \,, \tag{5}$$

where the *signature* $s = (s_1, s_2, \ldots)$ depends on the actual Hamiltonian, and the operator $\mathcal{C}_s$ is given by

$$\mathcal{C}_s = \sum_m s_m |E_m\rangle\langle E^m| \neq \sum_m s_m |E^m\rangle\langle E_m| = \mathcal{C}_s^\dagger \,. \tag{6}$$

The unconventional completeness and orthogonality relations which are characteristic for $\mathcal{PT}$-symmetric systems having real eigenvalues only are a direct consequence of Eq. (5). Numerical work suggests [7] that there is a completeness relation of the form

$$\sum_n s_n \phi_n(x) \phi_n(y) = \delta(x-y) \,, \tag{7}$$

which is a consequence of the completeness relations (3),

$$\sum_n |E_n\rangle\langle E^n| = \sum_n s_n |E_n\rangle\langle E_n| \mathcal{P} = \hat{I} \,, \tag{8}$$

when rewritten (in the position representation) by means of Eq. (5).

Similarly, the orthonormality condition for dual states turns into a relation which has been interpreted [8] as the existence of a non-positive scalar product among the eigenstates of $\hat{H}$. To see this, write the scalar product (4) in the position representation, using again (5) and $\mathcal{PT}$-invariance,

$$\langle E^n | E_m\rangle = s_n \langle E_n | \mathcal{P} | E_m\rangle = s_n \int \mathrm{d}x \, \phi_n(x) \phi_m(x) = \delta_{nm} \,, \tag{9}$$

or $(\phi_n, \phi_m) = s_n \delta_{nm}$, in the notation of [7].

Let us now turn to the properties of the *Gram* matrix G of a $\mathcal{PT}$-symmetric quantum system. For a general bi-orthonormal pair of bases one defines the Gram matrix by

$$\mathsf{G}_{mn} = \langle E_m | E_n \rangle \,; \tag{10}$$

its inverse G^{-1} exists since the states $\{|E_m\rangle\}$ are linearly independent, and its matrix elements are given by

$$\left(\mathsf{G}^{-1}\right)_{mn} = \langle E^m | E^n\rangle \equiv \mathsf{G}^{mn} \,. \tag{11}$$

Given the states $\{|E_m\rangle\}$ and hence G, one finds the *dual* states $\{|E^n\rangle\}$ through the inversion of G:

$$|E^n\rangle = \sum_m |E_m\rangle\langle E^m | E^n\rangle = \sum_m \mathsf{G}^{mn} |E_m\rangle \equiv \sum_m \left(\mathsf{G}^{-1}\right)_{mn} |E_m\rangle \,. \tag{12}$$

Equation (5) establishes a simple link between each state $|E_m\rangle$ and its partner $|E^m\rangle$. It will be shown now to imply a simple relation between G and its inverse,

$$\mathsf{G}^{-1} = \mathsf{SGS}\,, \qquad \text{where} \quad \mathsf{S} = \mathrm{diag}(s_1, s_2, \ldots)\,, \tag{13}$$

with S a real diagonal matrix, being determined entirely by the signature s of the system studied. To derive this relation, multiply the resolutions of unity given in (3) with each other,

$$\hat{I} = \left(\sum_m |E^m\rangle\langle E_m|\right)\left(\sum_n |E_n\rangle\langle E^n|\right) = \sum_{m,n} \mathsf{G}_{mn}|E^m\rangle\langle E^n|\,, \tag{14}$$

and use Eq. (5) giving

$$\hat{I} = \sum_{m,n} \mathsf{G}_{mn} s_m \mathcal{P}|E_m\rangle\langle E_n|\mathcal{P} s_n\,. \tag{15}$$

Finally, multiply this equation with $\langle E^k|\mathcal{P}$ from the left and with $\mathcal{P}|E^l\rangle$ from the right to find

$$\mathsf{G}^{kl} \equiv \left(\mathsf{G}^{-1}\right)_{kl} = \sum_{m,n} \mathsf{G}_{mn} s_m \delta_{km} s_n \delta_{nl} = s_k \mathsf{G}_{kl} s_l\,, \tag{16}$$

which is the matrix version of Eq. (13).

As a result, the inverse G^{-1} of the Gram matrix G is obtained by multiplying each of the matrix elements G_{mn} by the product $s_m s_n$ which takes the values ± 1 only. Due to $s_m^2 = 1$, the diagonal elements of the Gram matrix and those of its inverse are necessarily equal. Furthermore, having determined the eigenstates $|E_m\rangle$ of a $\mathcal{PT}$-symmetric Hamiltonian operator $\hat{H}$ and hence its Gram matrix via $\langle E_m|E_n\rangle$, the dual states are given by

$$|E^n\rangle = \sum_m s_m s_n \mathsf{G}_{mn}|E_m\rangle\,, \tag{17}$$

thus considerably simplifying Eq. (12): the usually cumbersome inversion of G can be avoided.

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