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Real eigenvalues of non-hermitian operators*

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ABSTRACT

A basic fact, having fundamental significance in quantum mechanics, is that hermitian (or self-adjoint) operators have only real eigenvalues. However, in certain applications in molecular physics, one deals with non-hermitian operators. We discuss a condition for non-hermitian operators to have real eigenvalues, proving that it is the case if and only if it can be decomposed as a product of two, generally non-commuting hermitian operators, one of which is positive definite. The theorem is illustrated on the example of non-hermitian effective Hamiltonians occurring in the non-perturbative form of the Bloch equation.

$$\begin{aligned}\hat{P}\hat{H}^{\mathrm{eff}} &= \sum_{ik} |\Phi_i\rangle\ \hat{H}^{\mathrm{eff}}\ \langle\Phi_k|. \\ &= \sum_j E_j \underbrace{\left|\sum_i T_{ij}\ \Phi_i\right\rangle}_{|\psi_j\rangle} \underbrace{\left\langle \sum_k T^{-1}_{jk}\ \Phi_k\right|}_{\langle\phi_j|} \\ &= \sum_j E_j\ |\psi_j\rangle\langle\phi_j|\end{aligned}$$

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1. Introduction

Standard self-consistent-field (SCF) equations

$$\boldsymbol{F}C_i = \varepsilon_i \boldsymbol{S} C_i \tag{1}$$

with the Fock matrix $\boldsymbol{F}$, molecular orbital (MO) coefficients C_i and MO energies ε_i emerge from the matrix representation of the eigenvalue equation of the Fock operator in the non-orthogonal basis set of atomic orbitals characterised by the metric (overlap) matrix $\boldsymbol{S}$. The Fock operator being hermitian, its eigenvalues are real numbers, so are the MO energies ε_i in a finite basis. Equation (1) is usually solved by some efficient technique, e.g. the Cholesky-decomposition of the metric matrix. However, multiplying by $\boldsymbol{S^{-1}}$, Equation (1) can be rewritten as

$$\boldsymbol{G}C_i = \varepsilon_i C_i \tag{2}$$

where

$$\boldsymbol{G} = \boldsymbol{S^{-1}F} \tag{3}$$

is a non-hermitian matrix, whose eigenvalues are nevertheless real.

In matrix theory, there is a theorem which precisely formulates a condition under which a non-hermitian matrix has only real eigenvalues. The statement is:

Theorem: *A non-hermitian matrix* $\boldsymbol{G}$ *has real eigenvalues if and only if it can be decomposed as a product of a positive definite hermitian and another hermitian matrix.*

Evidently, the (inverse) metric matrix being positive definite, Equation (3) exactly exhibits this structure.

In this paper, after recapitulating the proof of the above theorem for matrices in Section 2, we formulate the question whether an analogous statement holds for non-hermitian operators. An affirmative answer is provided in Section 3.

In molecular physics, one often deals with non-hermitian model Hamiltonians, despite the basic fact that physical quantities are described by self-adjoint

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operators. Some important examples are:

(1) The similarity-transformed Hamiltonian in coupled-cluster (CC) theory [1–3],

$$\hat{\bar{H}} = e^{-\hat{T}} \hat{H} e^{\hat{T}}, \tag{4}$$

where $\hat{T}$ is the cluster operator
(2) Transcorrelated Hamiltonians [4–9]
(3) The effective Hamiltonian in the Bloch equation [10–14], or the effective Hamiltonian in Mukherjee's energy-independent partitioning technique [15]
(4) The original, non-hermitian formulation of Mayer's chemical Hamiltonian approach [16–18]
(5) Application of non-hermitian (complex) potentials in the theory of resonances and scattering problems [19]

Non-hermitian Hamiltonians have been widely studied in theoretical physics [20–24], out of the realm of molecular physics, resulting in several alternatives of the above theorem [22, 25].

Equation (4) is not of present interest, since (i) it exhibits a similarity transformation, thus the eigenvalues of $\hat{H}$ and $\hat{\bar{H}}$ coincide; and (ii) in CC theory, one does not diagonalise $\hat{\bar{H}}$, but solves momentum-like equations instead. Transcorrelated Hamiltonians are also examples for similarity transformations. An application of the present result to item (3) will be presented in Section 4. Items (4) and (5) are more special examples, these are not discussed in this paper.

2. The proof for matrices

Proof of the theorem for matrices has to be elaborated in both directions:

(1) If $\boldsymbol{G} = \boldsymbol{AB}$, with $\boldsymbol{A}$ and $\boldsymbol{B}$ hermitian and $\boldsymbol{A}$ positive definite, then the eigenvalues of $\boldsymbol{G}$ are real
(2) If $\boldsymbol{G}$ is diagonalisable and has real eigenvalues, then it can be decomposed as $\boldsymbol{G} = \boldsymbol{AB}$ with the mentioned properties.

The theorem is well known in linear algebra. Here we present a simple proof for completeness.

2.1. Direction (1)

Suppose we have two hermitian matrices, $\boldsymbol{A}$ and $\boldsymbol{B}$, with $\boldsymbol{A}$ positive definite, the matrices $\boldsymbol{A^{1/2}}$, and $\boldsymbol{A^{-1/2}}$ are therefore well defined. (By $\boldsymbol{A^{1/2}}$, we mean the positive definite square root of $\boldsymbol{A}$ which is obviously invertible.) Then, let us construct the product matrix

$$\boldsymbol{G = AB} \equiv \underbrace{\boldsymbol{A^{1/2}}}_{\boldsymbol{A}} \overbrace{\boldsymbol{A^{1/2}}}^{\boldsymbol{C}} \boldsymbol{B} \underbrace{\boldsymbol{A^{1/2}}}_{\boldsymbol{I}} \boldsymbol{A^{-1/2}} \tag{5}$$

where the unit matrix $\boldsymbol{I}$ was introduced. Since $\boldsymbol{A}$ and $\boldsymbol{B}$ are hermitian, so is $\boldsymbol{C} = \boldsymbol{A^{1/2} B A^{1/2}}$, thus we have

$$\boldsymbol{G = A^{1/2} C A^{-1/2}}, \tag{6}$$

which is a similarity transformation of the hermitian $\boldsymbol{C}$. Since the latter has real eigenvalues, those of $\boldsymbol{G}$ must also be real, q.e.d.

2.2. Direction (2)

If $\boldsymbol{G}$ is diagonalisable, then

$$\boldsymbol{G = L D L^{-1}} \tag{7}$$

where $\boldsymbol{D}$ is a diagonal matrix, with some invertible matrix $\boldsymbol{L}$, which is, owing to the non-hermiticity of $\boldsymbol{G}$, not unitary. We assume that all diagonal elements of $\boldsymbol{D}$ are real. Then, consider the construction augmenting Equation (7) with a unit matrix $\boldsymbol{I} = \boldsymbol{L^\dagger L^{\dagger\,-1}}$ in between $\boldsymbol{L}$ and $\boldsymbol{D}$:

$$\boldsymbol{G} = \underbrace{\boldsymbol{L L^\dagger}}_{\boldsymbol{A}} \underbrace{\boldsymbol{L^{\dagger\,-1} D L^{-1}}}_{\boldsymbol{B}}. \tag{8}$$

Here $\boldsymbol{B} = \boldsymbol{L^{\dagger\,-1} D L^{-1}}$ is hermitian for real $\boldsymbol{D}$, while $\boldsymbol{A} = \boldsymbol{L L^\dagger}$ is positive definite and hermitian, by which the proof for matrices is completed.

Note that the proof in this direction remains valid for any decomposition of $\boldsymbol{G}$ as $\boldsymbol{L' D' L'^{-1}}$, where $\boldsymbol{D'}$ is hermitian but nondiagonal, thus the decomposition $\boldsymbol{G} = \boldsymbol{AB}$ is not unique.

3. The proof for operators

For linear operators, the theorem can be stated as follows.

Theorem: *A non-hermitian operator $\hat{G}$ has real eigenvalues if and only if it can be decomposed as a product of two hermitian operators one of which is positive definite.*

The implications, again, have to be shown in both directions. However, direction (1) emerges as a trivial transcript of Equations (5)–(6) which were written for the case of matrices: If operators $\hat{A}$ and $\hat{B}$ are hermitian and $\hat{A}$ is positive definite, then operator $\hat{G} = \hat{A}\hat{B}$ has real eigenvalues, albeit it is not hermitian. (We must not suppose

that $\hat{A}$ and $\hat{B}$ commute.) This statement follows from the construction, analogous to (5)

$$\hat{G} = \hat{A}\hat{B} \equiv \underbrace{\hat{A}^{1/2}}_{\hat{A}} \overbrace{\hat{A}^{1/2}\,\hat{B}\,\underbrace{\hat{A}^{1/2}}_{\hat{I}}}^{\hat{C}}\,\hat{A}^{-1/2} \tag{9}$$

with $\hat{I}$ standing for the unity operator. Operator $\hat{C}$ is hermitian by construction, and $\hat{G}$ is obtained as its similarity transformation, the eigenvalues of $\hat{G}$ are real.

The reverse direction requires some care, as, to remain general, one does not want to turn to a matrix representation in which a 'diagonal operator' $\hat{D}$ could be defined. Instead, let us formulate the reverse statement using the concept of spectral decomposition. Consider a non-hermitian operator $\hat{G}$ having right eigenvectors ψ_i

$$\hat{G}|\psi_i\rangle = \epsilon_i|\psi_i\rangle \tag{10}$$

with real eigenvalues ϵ_i, and left eigenvectors ϕ_i

$$\langle\phi_i|\hat{G} = \langle\phi_i|\epsilon_i. \tag{11}$$

For simplicity, the case of a discrete spectrum is discussed.

Non-hermiticity of $\hat{G}$ is manifested in that the two sets of eigenvectors are not the same. However, they form a biorthogonal set:

$$\langle\phi_i|\psi_k\rangle = \delta_{ik}, \tag{12}$$

assuming suitable normalisation $\langle\phi_i|\psi_i\rangle = 1$. This biorthogonal property for non-hermitian operators is well known in operator calculus, but, for completeness, we recapitulate a proof in the Appendix.

With these two sets of eigenvectors, the spectral decomposition of the non-hermitian operator $\hat{G}$ with real eigenvalues ϵ_j can be written as

$$\hat{G} = \sum_j \epsilon_j|\psi_j\rangle\langle\phi_j|, \tag{13}$$

as it can be verified by simple substitution of Equation (13) into Equations (10) and (11) and using biorthogonality, Equation (12) of the eigenvectors.

Let us develop a constructive proof. Define two hermitian auxiliary operators

$$\hat{A} = \sum_i s_i|\psi_i\rangle\langle\psi_i| \tag{14}$$

with the right eigenvectors of $\hat{G}$ and scalars $s_i > 0$, and

$$\hat{B} = \sum_j \frac{\epsilon_j}{s_j}|\phi_j\rangle\langle\phi_j| \tag{15}$$

with the real eigenvalues ϵ_j of $\hat{G}$ and the left eigenvectors of the latter, Equation (11). Constructions of Equations (14) and (15) are not to be considered as spectral decompositions, since neither of the sets $\{\psi_i\}$ or $\{\phi_j\}$ are orthonormal. Since both s_i and ϵ_j are real, both operators $\hat{A}$ and $\hat{B}$ are hermitian by construction. Moreover, $\hat{A}$ is positive definite with s_i positive. Evaluating the product one obtains:

$$\begin{aligned}\hat{A}\hat{B} &= \sum_i \sum_j s_i \frac{\epsilon_j}{s_j}|\psi_i\rangle \underbrace{\langle\psi_i|\phi_j\rangle}_{\delta_{ij}}\langle\phi_j| \\ &= \sum_i \epsilon_i|\psi_i\rangle\langle\phi_i| = \hat{G}.\end{aligned} \tag{16}$$

That is, the non-hermitian operator $\hat{G}$ having real eigenvalues has been decomposed as a product of two hermitian operators $\hat{A}\hat{B}$, of which $\hat{A}$ is positive definite. This completes the proof in the reverse direction.

Since in the above construction the real positive parameters in $\hat{A}$, s_i, are arbitrary, this decomposition is not unique, just like the similar decomposition of matrices in the preceding section. Note finally that the adjoint of $\hat{G}$ is

$$\hat{G}^\dagger = \hat{B}\hat{A}.$$

For $\hat{G}$ to be non-hermitian, $\hat{A}$ and $\hat{B}$ must not commute. Further,

$$\left[G, G^\dagger\right] = \hat{A}\hat{B}^2\hat{A} - \hat{B}\hat{A}^2\hat{B} \neq 0,$$

thus this $\hat{G}$ is not a normal operator, either. We can, therefore, formulate the following

Corollary: *If a normal operator $\hat{N}$ is not hermitian, it must have at least one complex eigenvalue.*

4. Application to the theory of effective Hamiltonians

Effective Hamiltonians have long been dealt with in molecular physics, starting from Löwdin's partitioning technique [26, 27], Mukherjee's energy-independent partitioning technique [15], the effective Hamiltonian in ' perturb-then-diagonalise' versions of multi-reference (MR) perturbation theory (PT) [28–32], and the field of the Bloch equation [10, 11]. Wave operators and effective Hamiltonians have also been used in the field of the ro-vibrational molecular Schrödinger equation [33–35], an area on which Attila Császár, to whom this Volume is dedicated to, has been extensively working. Here we present an application to the non-perturbative formal Bloch equation.

Consider a set of exact eigenfunctions of a Hamiltonian $\hat{H}$,

$$\Psi_1, \Psi_2, \ldots \Psi_p.$$

They satisfy the eigenvalue equations

$$\hat{H}\Psi_i = E_i\Psi_i, \quad i = 1, 2, \ldots p,$$

and, owing to the hermiticity of $\hat{H}$, form an orthonormal basis in the p-dimensional eigensubspace.

Consider now a set, formed by the same number of model functions:

$$\{\Phi_i\}, \quad i = 1, 2, \ldots p,$$

which are chosen to be orthonormal, $\langle\Phi_i|\Phi_j\rangle = \delta_{ij}$, spanning a p-dimensional model space. The interrelation matrix between the two sets is

$$T_{ik} = \langle\Phi_i|\Psi_k\rangle$$

For the set $\{\Phi_i\}$, we only assume that they represent an approximation to Ψ_i which is not singularly wrong, i.e. the diagonal overlaps

$$T_{ii} = \langle\Phi_i|\Psi_i\rangle \neq 0$$

are nonzero for all i. We also assume that matrix $\boldsymbol{T}$ is nonsingular.

The next step is to define a formal wave operator $\hat{\Omega}$ by

$$\hat{\Omega} = \sum_{ik} |\Psi_i\rangle T^{-1}_{ik} \langle\Phi_k| \tag{17}$$

where T^{-1}_{ik} is a shorthand for the elements of the inverse of matrix $\boldsymbol{T}$. This wave operator obviously maps the model space to the exact eigensubspace, and has the following properties:

(1) It is idempotent:

$$\hat{\Omega}^2 = \hat{\Omega}$$

which results from simple substitution of Equation (17)

(2) It is obviously not hermitian: $\hat{\Omega}^\dagger \neq \hat{\Omega}$

(3) $\mathrm{Tr}\,\hat{\Omega} = p$

(4) It satisfies the non-perturbative form of the Bloch equation

$$\hat{H}\hat{\Omega} = \hat{\Omega}\hat{H}\hat{\Omega}, \tag{18}$$

which, again, follows easily from simple substitution.

This form of the wave operator is a skew projector from the mathematical point of view, owing to the properties of items (1) and (2).

The above construction makes clear that this wave operator corresponds to a MR theory. The single-reference version of (18), where $p = 1$ and the definition $\Omega = |\Psi\rangle\langle\Phi|$ is used for the wave operator, was termed the nonlinear Schrödinger equation by Löwdin [11] (see also ref. [36]).

Note that Equation (18) can also be obtained from the requirement that Ω commutes with the Hamiltonian, multiplying the commutator with Ω and using the idempotency of the wave operator.

The Bloch Equation (18) is not easy to solve, partly because it has many solutions. An equation of the same structure can be written down in a one-electron theory for the density matrix $\mathbf{P}$ and the Fockian $\boldsymbol{F}$ [37–39]:

$$\boldsymbol{FP} = \boldsymbol{PFP}.$$

Iterative solution of the above equation, albeit slow, is possible [37–39], and it provides the density matrix without explicit diagonalisation of $\boldsymbol{F}$.

We now proceed with constructing the decomposition of the effective Hamiltonian, formulated in the field of the Bloch equation as

$$\hat{H}^{\mathrm{eff}} = \hat{H}\hat{\Omega}. \tag{19}$$

Matrix elements of $\hat{H}^{\mathrm{eff}}$ in the model space read

$$H^{\mathrm{eff}}_{ab} = \langle\Phi_a|\hat{H}\hat{\Omega}|\Phi_b\rangle. \tag{20}$$

This is a $p \times p$ dimensional non-hermitian effective Hamiltonian matrix, that is diagonalisable, and has p exact eigenvalues. This can be simply verified:

$$\begin{aligned}\left(H^{\mathrm{eff}}T\right)_{ij} &= \sum_b \langle\Phi_i|\hat{H}\hat{\Omega}|\Phi_b\rangle T_{bj} \\ &= \sum_{bkl} \langle\Phi_i| \underbrace{\hat{H}|\Psi_k\rangle}_{E_k\Psi_k} T^{-1}_{kl} \underbrace{\langle\Phi_l|\Phi_b\rangle}_{\delta_{lb}} T_{bj} \\ &= E_j T_{ij}, \end{aligned} \tag{21}$$

where the definition of the wave operator was substituted, and the orthonormality of the model space functions was utilised. The result can simply be written as

$$\left(T^{-1}H^{\mathrm{eff}}T\right)_{ij} = E_j\delta_{ij} \tag{22}$$

indicating that the interrelation matrix diagonalises the non-hermitian Hamiltonian in the model space with all of its eigenvalues remaining real. Therefore, in accord with the theorem under discussion, the effective Hamiltonian of Equation (19) must feature a decomposed form

as the product of a positive definite and a hermitian operator. Rearranging Equation (20) as

$$H^{\text{eff}}_{ik} = \sum_j E_j T_{ij} T^{-1}_{jk} \tag{23}$$

allows one to express the model space projection of $\hat{H}^{\text{eff}}$ as

$$\hat{P}\hat{H}^{\text{eff}} = \sum_{ik} |\Phi_i\rangle \hat{H}^{\text{eff}} \langle\Phi_k|. \tag{24a}$$

$$= \sum_j E_j \underbrace{\left| \sum_i T_{ij}\, \Phi_i \right\rangle}_{|\psi_j\rangle} \underbrace{\left\langle \sum_k T^{-1}_{jk}\ \ \Phi_k \right|}_{\langle\phi_j|} \tag{24b}$$

$$= \sum_j E_j\ |\psi_j\rangle\langle\phi_j| \tag{24c}$$

for real matrix elements of $\boldsymbol{T}$. Here, the model space projector

$$\hat{P} = \sum_i |\Phi_i\rangle\langle\Phi_i|$$

was used, and the form Equation (23) was substituted for $\hat{H}^{\text{eff}}$ to get (24b). The form (24c) perfectly matches the structure of Equation (13) in Section 2.2: it is a spectral resolution of a non-hermitian Hamiltonian, with real eigenvalues E_j. Therefore, the construction used in Section 2.2 applies. First, it is evident that the sets $\{\psi\}$ and $\{\phi\}$ are biorthogonal:

$$\langle\phi_j|\psi_l\rangle = \sum_{ik} T^{-1}_{jk} \underbrace{\langle\Phi_k|\Phi_i\rangle}_{\delta_{ki}} T_{il} = \delta_{jl}.$$

Next, one defines, following Equations (14) and (15),

$$\hat{A} = \sum_i s_i |\psi_i\rangle\langle\psi_i|$$

with arbitrary but positive parameters s_i, and

$$\hat{B} = \sum_j \frac{E_j}{s_j} |\phi_j\rangle\langle\phi_j|.$$

Both $\hat{A}$ and $\hat{B}$ are hermitian and $\hat{A}$ is positive definite, and their product gives the effective Hamiltonian (24c). This illustrates the theorem.

5. Conclusion

Inspired by the Hartree-Fock-Roothaan equation (the eigenvalue problem of the Fockian represented in an overlapping basis set), we recapitulated a theorem of matrix theory stating that the spectrum of a nonhermitian matrix is real if and only if it appears as a product of two non-commuting hermitian matrices, one of which is positive definite. We presented a formal constructive proof for the analogous statement for operators, using the formalism of spectral decompositions for nonhermitian operators. The proof makes it evident that the decomposition is not unique. The non-perturbative form of the Bloch equation results in a nonhermitian effective Hamiltonian, and the formal theorem is illustrated on this example.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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Appendix

Here we recapitulate that Equation (12) is correct. Assume that $\hat{M} \neq \hat{M}^\dagger$ is a non-hermitian operator, its eigenvalue equation reading

$$\hat{M}|\psi_i\rangle = a_i|\psi_i\rangle. \tag{A1}$$

The eigenvalue problem of the adjoint operator reads

$$\hat{M}^\dagger|\phi_j\rangle = b_j|\phi_j\rangle. \tag{A2}$$

Taking the adjoint of Equation (A2) one gets:

$$\langle\phi_j|\hat{M} = b_j^*\langle\phi_j|, \tag{A3}$$

with right and left eigenvectors (ψ and ϕ) and eigenvalues (a and b^*) of $\hat{M}$, respectively. Multiplying Equation (A1) by $\langle\phi_j|$ from the left and Equation (A3) by $|\psi_i\rangle$ from the right, one obtains:

$$\langle\phi_j|\hat{M}|\psi_i\rangle = a_i\langle\phi_j|\psi_i\rangle \tag{A4}$$

and

$$\langle\phi_j|\hat{M}|\psi_i\rangle = b_j^*\langle\phi_j|\psi_i\rangle. \tag{A5}$$

Taking their differences:

$$0 = \left(a_i - b_j^*\right)\ \langle\phi_j|\psi_i\rangle. \tag{A6}$$

Assuming $\langle\phi_i|\psi_i\rangle$ is nonzero, this leads to

$$a_i = b_i^*.$$

That is, the left- and right eigenvalues are the complex conjugates of each other. (In the discussion of the present paper, a_i are real, thus they are equal.) In this case, one usually applies the normalisation condition:

$$\langle\phi_i|\psi_i\rangle = 1.$$

If, however, $i \neq j$, the eigenvalue differences are nonzero in general (the case of degeneracy may be separately discussed). Then, we obtain:

$$\langle\phi_i|\psi_j\rangle = 0.$$

Combining the last two equations one arrives at the biorthogonality property Equation (12).