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On operator inequalities as tools in quantum theory

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Summary. A brief survey of the use of operator inequalities in the modern quantum theory of matter is given. In particular the Rayleigh–Ritz variation principle is formulated in terms of operator inequalities, and the properties of outer and inner projections of self-adjoint operators and especially the molecular Hamiltonian and its resolvent are discussed in some detail.

Key words: Operator inequalities – Quantum theory – Rayleigh–Ritz variation principle

1. Introduction

In her work on molecular quantum mechanics, quantum biochemistry, quantum biology, etc., Professor Alberte Pullman has made some of the most important and interesting applications of the new quantum theory of matter during the last few decades. In these practical treatments of many-electron systems in frameworks of atomic nuclei, she has often needed intricate theoretical methods, and – in those cases when such tools were not available – she and her collaborators have created the necessary methodology. This paper on the importance of operator inequalities in modern quantum theory is dedicated to Professor Alberte Pullman in view of her outstanding contributions also to the development of new methods in the study of large molecules. The author would also like to take this opportunity to thank Professor Alberte Pullman for her lectures on Quantum Biochemistry at the Florida Winter Institute in Quantum Chemistry and Solid-State Theory in the 1960's and for her many excellent contributions to the yearly Sanibel Symposia over more than three decades and which are still going on.

2. Definition of operator inequalities

In this paper we will consider linear operators T defined on a Hilbert space $\mathscr{H} = \{x\}$ having a positive definite binary product $\langle x|y\rangle$ with the property

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$\langle x|x\rangle \geqslant 0$ and with $\langle x|x\rangle = 0$ only for the zero-element $x = \varnothing$. The operator T is said to have the domain $D(T)$, if both x and Tx belong to the space $\mathscr{H}$ when x is in $D(T)$. In addition to T, we will consider its adjoint operator $T^\dagger$ defined through the relation $\langle Tx|y\rangle = \langle x|T^\dagger y\rangle$.

Since the time of von Neumann [1], operator inequalities have played an important rule in the formulation of quantum theory. They apply particularly to the *self-adjoint operators* A having the property $A^\dagger = A$, for which the expectation values $\langle A\rangle = \langle x|Ax\rangle/\langle x|x\rangle = \langle x|A|x\rangle/\langle x|x\rangle$ are by definition *real* quantities. Such an operator is said to be *positive definite*, if and only if $\langle x|A|x\rangle > 0$ for all x in the domain $D(A)$ of A. For such an operator, one uses the notation $A > 0$, where the symbol 0 represents the zero-operator, which relation is known as an operator inequality.

More generally, if $\langle x|A|x\rangle > \langle x|B|x\rangle$ for all x in the intersection between the domains $D(A)$ and $D(B)$, then one uses the notation $A > B$, which means that *the operator A is larger than the operator B*. Putting $x = Ty$, one gets also $\langle y|T^\dagger AT|y\rangle > \langle y|T^\dagger BT|y\rangle$ for all y for which this relation has a meaning, i.e. $T^\dagger AT > T^\dagger BT$. From the inequality $A > B$, one can hence derive the inequality $T^\dagger AB > T^\dagger BT$:

$$A > B, \quad \rightarrow T^\dagger AT > T^\dagger BT. \tag{1}$$

This theorem has some interesting corollaries.

If $A > 0$, and one chooses $T = A^{-1}$, one gets immediately $A^{-1} > 0$. On the other hand, if $A > 1$, where 1 represents the identity operator, and one chooses $T = A^{-1/2}$ (the positive square root), one gets directly $1 > A^{-1}$. If $A > 1$, and one chooses $T = A^{1/2}$, one gets $A^2 > A$. On the other hand, if $0 < A < 1$, and one chooses $T = A^{1/2}$, one gets $0 < A^2 < A$. In summary, one obtains:

$$A > 0, \quad \rightarrow A^{-1} > 0, \tag{2a}$$

$$A > 1, \quad \rightarrow A^{-1} < 1, \tag{2b}$$

$$A > 1, \quad \rightarrow A^2 > A, \tag{2c}$$

$$0 < A < 1, \qquad 0 < A^2 < A, \tag{2d}$$

Let us now consider some more complicated relations. If $A > B > 0$, and one chooses $T = B^{-1/2}$ (the positive square root), one gets immediately $B^{-1/2}AB^{-1/2} > 1$, and (2b) gives then $(B^{-1/2}AB^{-1/2})^{-1} < 1$, i.e. $B^{+1/2}A^{-1}B^{+1/2} < 1$, or $A^{-1} < B^{-1}$. In the special case when B has no inverse, one has to proceed somewhat differently. Starting out from the relation $A > B \geqslant 0$, and choosing $T = A^{-1/2}$, one gets $1 > A^{-1/2}BA^{-1/2} \geqslant 0$, and Eq. (2d) gives then:

$$0 \leqslant A^{-1/2}BA^{-1/2} \cdot A^{-1/2}BA^{-1/2} < A^{-1/2}BA^{-1/2}, \tag{3}$$

or

$$0 \leqslant BA^{-1}B < B. \tag{4}$$

In summary one hence has:

$$A > B > 0, \quad \rightarrow 0 < A^{-1} < B^{-1}, \tag{5a}$$

$$A > B \geqslant 0, \quad \rightarrow 0 \leqslant BA^{-1}B < B, \tag{5b}$$

where Eq. (5a) follows from Eq. (5b) whenever the operator B has an inverse.

3. Projection operators

A self-adjoint operator O is said to be a *projector*, if it is idempotent so that $O^2 = O$. In such a case, one has also $O = O^\dagger O$, which means that $\langle x|O|x\rangle = \langle x|O^\dagger O|x\rangle = \langle Ox|Ox\rangle \geqslant 0$, or that $O \geqslant 0$. The operator $P = 1 - O$ is also a self-adjoint projector, which gives the inequality $P = 1 - O \geqslant 0$, and hence one has the fundamental theorem that:

$$0 \leqslant O \leqslant 1. \tag{6}$$

If $A > 0$, and one chooses $T = A^{1/2}$ (the positive square root) and applies Eq. (1), one obtains the inequality:

$$0 \leqslant A^{1/2} O A^{1/2} \leqslant A, \tag{7}$$

where the operator:

$$A' = A^{1/2} O A^{1/2} \tag{8}$$

will be referred to as the *inner projection* of A with respect to the projector O. Another operator of essential importance in the theory has the form

$$\bar{A} = OAO, \tag{9}$$

and it will be referred to as the *outer projection* of A with respect to the projector O. The properties of the inner and outer projections will be studied in greater detail below.

Dirac [2] considered the bracket $\langle x|y\rangle$ as the product of a bra-vector $\langle x|$ and a ket-vector $|y\rangle$, and he also introduced the dyadic product in the form of a *ket-bra operator* $R = |b\rangle\langle a|$ defined through the relation $Rx = b\langle a|x\rangle$ and having the properties $R^\dagger = |a\rangle\langle b|$, $R^2 = \langle a|b\rangle R$, $Tr\, R = \langle a|b\rangle$. We note in particular that, if $\langle x|x\rangle \neq 0$, then the operator $R = |x\rangle\langle x|x\rangle^{-1}\langle x|$ is a one-dimensional projector.

It is easily shown that, if a linear manifold M_f of order p is spanned by the linearly independent set $\boldsymbol{f} = \{f_1, f_2, f_3, \ldots, f_p\}$, the orthogonal projector Q on this manifold is given by the formula [3]:

$$Q = |\boldsymbol{f}\rangle\langle \boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle \boldsymbol{f}|. \tag{10}$$

We will here and in the following let bold-face symbols denote rectangular matrices including row vectors, column vectors, and quadratic matrices with the understanding that the elements of the bold-face product $\boldsymbol{C} = \boldsymbol{A} \cdot \boldsymbol{B}$ are defined by the relation $C_{kl} = \sum_\alpha A_{k\alpha} B_{\alpha l}$, i.e. one multiplies the columns of the first factor with the rows of the second factor. Since the set $\boldsymbol{f}$ is linearly independent, the matrix $\boldsymbol{\Delta}_f = \langle \boldsymbol{f}|\boldsymbol{f}\rangle$ has an inverse $\boldsymbol{d} = \langle \boldsymbol{f}|\boldsymbol{f}\rangle^{-1}$, and Eq. (10) has hence the explicit meaning:

$$Q = \sum_{kl} |f_k\rangle d_{kl} \langle f_l|, \tag{11}$$

i.e. a double sum containing p^2 terms. It is then easily shown that the operator Q satisfies the three fundamental relations:

$$Q^2 = Q, \qquad Q^\dagger = Q, \qquad Tr\, Q = p. \tag{12}$$

If one puts $p = 1, 2, 3, \ldots$, it is clear that one has the operator inequalities:

$$O \leqslant Q_1 \leqslant Q_2 \leqslant Q_3 \leqslant \cdots \leqslant Q_p \leqslant Q_{p+1} \leqslant \cdots \leqslant 1. \tag{13}$$

If $\boldsymbol{\varphi} = \{\varphi_k\}$ is an orthonormal set which spans the entire Hilbert space $\mathscr{H}$, the associated projector is the identity operator 1, and one gets the relation:

$$1 = |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}| = \sum_k |\varphi_k\rangle\langle\varphi_k|, \tag{14}$$

which represents a *resolution of the identity*. We note that the sum in the right-hand member is convergent in the *operator sense* [4]. For a linear operator T in general, one gets then:

$$T\boldsymbol{\varphi} = 1 \cdot T\boldsymbol{\varphi} = |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}| \cdot T\boldsymbol{\varphi} = \boldsymbol{\varphi}\langle\boldsymbol{\varphi}|T|\boldsymbol{\varphi}\rangle = \boldsymbol{\varphi}\boldsymbol{T}, \tag{15}$$

where $\boldsymbol{T} = \langle\boldsymbol{\varphi}|T|\boldsymbol{\varphi}\rangle$ is the *matrix representation* of the operator T having the elements $T_{kl} = \langle\varphi_k|T|\varphi_l\rangle$. For the operator T itself, one gets further:

$$\begin{aligned} T &= 1 \cdot T \cdot 1 = |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}| \cdot T \cdot |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}| = |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}|T|\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}| = |\boldsymbol{\varphi}\rangle\boldsymbol{T}\langle\boldsymbol{\varphi}| \\ &= \sum_{kl} |\varphi_k\rangle T_{kl}\langle\varphi_l| = \sum_{kl} T_{kl}P_{lk}, \end{aligned} \tag{16}$$

which is the expansion of the operator T in terms of the fundamental units $P_{lk} = |\varphi_k\rangle\langle\varphi_l|$, which apparently span the operator space [5].

If a self-adjoint operator A has a discrete spectrum $\{a_k\}$ associated with the normalized eigenfunctions u_k, so that $Au_k = a_k u_k$, then one has:

$$A = 1 \cdot A \cdot 1 = \sum_{kl} |u_k\rangle A_{kl}\langle u_l| = \sum_k |u_k\rangle a_k \langle u_k| = \sum_k a_k P_{kk}, \tag{17}$$

where $P_{kk} = |u_k\rangle\langle u_k|$ is a one-dimensional projector satisfying the inequality $0 \leqslant P_{kk} \leqslant 1$. Equation (17) is the *spectral resolution* of the operator A, and we note particularly that, if A has a lowest eigenvalue a_0, so that $a_k \geqslant a_0$ for all k, then $a_k P_{kk} \geqslant a_0 P_{kk}$, and one gets:

$$A = \sum_k a_k P_{kk} \geqslant a_0 \sum_k P_{kk} = a_0 \cdot 1. \tag{18}$$

In such a case, the operator A is always larger than its lowest eigenvalue multiplied by the identity operator. This theorem may also be generalized to the case when the operator A has a spectrum which is fully or partly continuous.

4. The general variation principle

Of essential importance in both the theoretical development and the applications of modern quantum theory is the general *variation principle*, which says that the Schrödinger equation $H\Psi = E\Psi$ for eigenfunctions Ψ in $\mathscr{H}$ is equivalent with the relation $\delta\langle H\rangle = 0$, where $\langle H\rangle = \langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ is the expectation value of the self-adjoint Hamiltonian operator H. For any quotient $E = A/B$, one has $\delta E = (B\,\delta A - A\,\delta B)/B^2 = (\delta A - E\,\delta B)/B$, i.e.

$$\delta\langle H\rangle = \{\langle\delta\Psi|H - E \cdot 1|\Psi\rangle + \langle\delta\Psi|H - E \cdot 1|\Psi\rangle^*\}/\langle\Psi|\Psi\rangle, \tag{19}$$

for arbitrary variations $\delta\Psi$, which relation immediately proves the theorem without any further restrictions on the Hamiltonian H. In the application of this principle, one looks for stationary points in general: maxima, minima, and saddle points. It should be observed that this variation principle may hence be applied also to Dirac's relativistic Hamiltonian.

5. Operators bounded from below

Some of the self-adjoint operators studied in quantum theory may be bounded over the entire Hilbert space, others may be bounded from below, others may be bounded from above, whereas others may be completely unbounded. In this section, we will devote our interest to operators A which are *bounded from below* in the sense that its expectation values fulfill the inequality $\langle A \rangle \geqslant \alpha$, which relation is equivalent with the operator inequality $A \geqslant \alpha \cdot 1$. It is interesting to observe that this property is characteristic for the non-relativistic molecular Hamiltonian defined by the relation:

$$H = \sum_k \boldsymbol{p}_k^2/2m_k + \sum_{k<l} e_k e_l / r_{kl}$$

$$= e^2 \sum_{g<h} Z_g Z_h / R_{gh} + \sum_g \boldsymbol{p}_g^2/2M_g + \sum_i \left(\boldsymbol{p}_i^2/2m - e^2 \sum_g Z_g / r_i \right) + e^2 \sum_{i<j} 1/r_{ij}, \quad (20)$$

where the indices k and l run over all particles involved, whereas the indices g and h run over the atomic nuclei considered as point charges and the indices i and j over the electrons. Many molecular theoreticians would take this property for granted on physical grounds, but it should be observed that it is a strict mathematical property. From the exact solution of the hydrogen-atom problem and Eq. (18), one has the inequality:

$$\boldsymbol{p}_i^2/2m - e^2 Z_g / r_{ig} \geqslant (-me^4 Z_g^2/2\hbar^2) \cdot 1. \quad (21)$$

If A is the numer of atomic nuclei and N the number of electrons, one gets the following rough estimate of the third term in the Hamiltonian of Eq. (20):

$$\sum_i \left(\boldsymbol{p}_i^2/2m - e^2 \sum_g Z_g / r_i \right) = \sum_i \sum_g (1/A) \left(\boldsymbol{p}_i^2/2m - e^2 \sum_g A Z_g / r_i \right)$$

$$\geqslant \sum_i \sum_g (1/A)(-me^4 A^2 Z_g^2/2\hbar^2) \cdot 1 = (-me^4 AN/2\hbar^2) \cdot 1 \sum_g Z_g^2. \quad (22)$$

All the other terms in the Hamiltonian of Eq. (20) are positive definite, and this means that the total Hamiltonian is *bounded from below*. At the same time, this Hamiltonian is an excellent example of the complications which may occur in the elementary molecular theory.

Since the molecular Hamiltonian of Eq. (20) is invariant under translations and rotations of the three-dimensional space coordinate system, the total momentum and the total angular momentum are immediately constants of motion. The first statement implies that one may separate the motion of the center of mass $\boldsymbol{\xi}$ defined through the relation:

$$\boldsymbol{\xi} = \sum_k m_k \boldsymbol{r}_k \Big/ \sum_k m_k, \qquad M = \sum_k m_k, \quad (23)$$

from the remaining part of the Hamiltonian, so that:

$$H = \boldsymbol{p}_\xi^2/2M + H', \quad (24)$$

where H' depends only on the relative coordinates $\boldsymbol{r}'_k = \boldsymbol{r}_k - \boldsymbol{r}_0$, with respect to a reference point r_0 moving with the system. In such a case, one may write the total wave function in the product form $\Psi = \varphi(\xi)\Psi'$ and the energy as a sum $E = E_\xi + E'$. Since E_ξ has a continuous spectrum which goes from 0 to $+\infty$, and

which is superimposed on the spectrum of E', it is clear that the bottom of the spectrum of E has continuous character.

The Coulombic Hamiltonian H', which has the center of mass motion removed, is of essential interest both in molecular physics and in mathematics, and a great deal of work has been carried out by the mathematicians during the last few decades as to the spectral properties of this operator with the results reported to the quantum chemists particularly by Professor Barry Simon at California Institute of Technology.

The relation $H'\Psi' = E'\Psi'$ as a differential equation has, of course, solutions Ψ' for every real or complex value of E'. It becomes an eigenvalue problem, if one requires that the solutions Ψ' should satisfy certain *boundary conditions*, and the possible eigenvalues E' corresponding to such solutions give then the spectrum $\{E'\}$ associated with the boundary conditions. The boundary conditions usually introduced into the quantum theory of matter are of two types:

(1) If an eigenfunction Ψ' is quadratically integrable, i.e. if it belongs to the L^2 Hilbert space, then the associated eigenvalue E' is *discrete*, and the associated eigenstate is *closed* and correspond to the existence of an atom or a molecule.

(2) If an eigenfunction Ψ' does not belong to L^2 but remains *finite* even at infinity, then the associated eigenvalue E' belongs to a *continuous* part of the spectrum, and the associated state is a *scattering state* corresponding to a molecular collision or a chemical reaction.

It is obvious that the nature of a particular eigenvalue E' is of fundamental importance for the physical and chemical interpretations of the theory, and we will temporarily refer to it as the *key problem* in spectral theory. At this point, it is somewhat disturbing that the condition (2) is not more explicitly related to the L^2 Hilbert space, and we will come back to this problem below.

One is, of course, particularly interested in the nature of the lowest eigenvalue E_0 of the spectrum of H', and an answer is provided by the WHVZ-theorem named after Weyl, Hunzinger, van Winter, and Zhislin [6], which says that, if one can find a quadratically integrable trial function Φ such that its expectation value $\langle H' \rangle$ is lower than the energy of all separated clusters, then the lowest eigenvalue E_0 of the system is necessarily *discrete* and corresponds to the existence of a closed state, i.e. to the existence of an atom or a molecule. It is interesting to observe that the quantum chemists have used this theorem intuitively since the start of computational molecular physics, and that this conjecture has now an exact mathematical basis. For the sake of simplicity, we will in the following assume that we consider only Hamiltonians with the center of mass motion removed, and we will then drop the prime on H'.

6. Variation principle for operators bounded from below

In addition to the general variation principle mentioned above, one has in the quantum theory of matter used a special Rayleigh–Ritz variation principle [7] which is valid only for operators bounded from below, and which has many interesting properties. Even if it is studied in great detail in many quantum-mechanical textbooks, we will here look at it from the point of view of operator inequalities. For this purpose, we will consider a self-adjoint Hamiltonian H, which is bounded from below so that $\langle H \rangle > \alpha$, or which is the same $H > \alpha \cdot 1$,

where 1 is the identity operator. We will denote the best lower bound by E_0, and the key problem is now whether one has $H > E_0$ or $H \geqslant E_0$. In the former case, the bound E_0 is not attained by any trial function, and this case will occur if E_0 belongs to the continuum. In the second case, there exists a wave function Ψ_0, for which the minimum E_0 is attained, so that $\langle \Psi_0 | H | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle = E_0$, or:

$$\langle \Psi_0 | H - E_0 \cdot 1 | \Psi_0 \rangle = 0. \tag{25}$$

At this point, it is convenient to use a lemma which says that, if Ω is a semi-positive operator with the property $\Omega \geqslant 0$, and $\langle \varphi | \Omega | \varphi \rangle = 0$, then one has $\Omega \varphi = 0$. For the proof, one puts $\phi = \psi + \lambda \varphi$, where λ is a real parameter, which gives $\langle \phi | \Omega | \phi \rangle = \langle \psi | \Omega | \psi \rangle + 2\lambda \operatorname{Re}\{\langle \psi | \Omega | \varphi \rangle \geqslant 0$ and leads to a contradiction unless $\langle \psi | \Omega | \varphi \rangle = 0$ for all ψ, which proves the theorem. Putting $\Omega = H - E_0 \cdot 1$ and using (25), one obtains:

$$(H - E_0 \cdot 1)\Psi_0 = 0, \tag{26}$$

which means that the lower bound E_0 is a discrete eigenvalue associated with the wave function Ψ_0 corresponding to a closed ground state.

A well-known theorem says that the eigenfunctions to H associated with different discrete eigenvalues are orthogonal to each other, or – for a degenerate eigenvalue – may be chosen in that way. In the next step, it is hence natural to consider the lowest bound for the expectation value $\langle H \rangle$, when the trial wave function Φ is assumed to be *orthogonal* to the normalized eigenfunction Ψ_0. Denoting the best lower bound by E_1, one has either $\langle H \rangle > E_1$ or $\langle H \rangle \geqslant E_1$. If $O_0 = |\Psi_0\rangle\langle\Psi_0|$ is the projector associated with the eigenfunction, then $P_0 = 1 - O_0$ is the projector for its orthogonal complement, and the trial function Φ may then be written in the form $\Phi = P_0 \Psi$, where Ψ is an arbitrary element of L^2. One gets directly $\langle \Phi | \Psi_0 \rangle = \langle P_0 \Psi | \Psi_0 \rangle = \langle \Psi | P_0 \Psi_0 \rangle = 0$, which is the property desired. We note further that one has $HO_0 = E_0 O_0 = O_0 H$, i.e. that O_0 commutes with H, and the same is then true also for P_0. From the relation:

$$\begin{aligned} \langle H \rangle &= \langle \Phi | H | \Phi \rangle / \langle \Phi | \Phi \rangle = \langle P_0 \Psi | H | P_0 \Psi \rangle / \langle P_0 \Psi | P_0 \Psi \rangle \\ &= \langle \Psi | P_0 H P_0 | \Psi \rangle / \langle \Psi | P_0 P_0 | \Psi \rangle = \langle \Psi | H P_0 | \Psi \rangle / \langle \Psi P_0 | \Psi \rangle > E_1, \end{aligned} \tag{27}$$

one gets immediately the operator inequality:

$$(H - E_1 \cdot 1) P_0 > 0, \tag{28}$$

which we will now study in greater detail. One observes that one has the relation $HP_0 = H - E_0 O_0 = H - E_0(1 - P_0) = (H - E_0) - E_0 P_0$, and Eq. (27) gives then the operator inequality:

$$1 - O_0 = P_0(\langle H \rangle - E_0)/(E_1 - E_0). \tag{29}$$

It is easily shown that this inequality is equivalent with the well-known *Eckart's criterion* [8] for the accuracy or a trial wave function Φ approximating the ground state. Assuming that Φ is normalized to unity and the phase chosen so that the binary product $\langle \Phi | \Psi_0 \rangle$ is positive, so that $0 < \langle \Phi | \Psi_0 \rangle < 1$, one has $\| \Phi - \Psi_0 \| = 2(1 - \langle \Phi | \Psi_0 \rangle)$ and further from (29):

$$1 - \langle \Phi | \Psi_0 \rangle^2 < (\langle H \rangle - E_0)/(E_1 - E_0), \tag{30}$$

which relation says that if $\langle H \rangle$ converges towards E_0, then $\langle \Phi | \Psi_0 \rangle$ converges towards 1, the quantity $\| \Phi - \Psi_0 \|$ converges towards zero, and the trial function Φ towards the exact eigenfunction Ψ_0 for the ground state.

If, on the other hand, the lowest bound E_1 is attained for the wave function Ψ_1, then one has the inequality $\langle H\rangle \geqslant E_1$, which means that $\langle\Psi_1|H|\Psi_1\rangle/\langle\Psi_1|\Psi_1\rangle \geqslant E_1$, or:

$$\langle\Psi_1|H - E_1 \cdot 1|\Psi_1\rangle \geqslant 0. \tag{31}$$

Since $\Omega = H - E_1 \cdot 1 \geqslant 0$, the previously used lemma will now give the result:

$$(H - E_1 \cdot 1)\Psi_1 = 0, \tag{32}$$

which means that Ψ_1 is the eigenfunction associated with the eigenvalue E_1, which is now the next lowest eigenvalue. From now on, we will assume that Ψ_1 is normalized to unity and that it has the projector $O_1 = |\Psi_1\rangle\langle\Psi_1|$.

In order to proceed, we will then consider the expectation value $\langle H\rangle$ for all trial wave functions Φ which are orthogonal to both Ψ_0 and Ψ_1, and which hence have the general form $\Phi = P_1\Psi$, where $P_1 = 1 - O_0 - O_1$. We note that the projectors O_0 and O_1 are mutually exclusive, so that $O_0O_1 = 0$, and that O_0 and O_1 as well as P_1 commute with H. We will denote the best lower bound to $\langle H\rangle$ by E_2, which gives:

$$\langle\Phi|H|\Phi\rangle/\langle\Phi|\Phi\rangle = \langle\Psi|HP_1|\Psi\rangle/\langle\Psi|P_1|\Psi\rangle \geqslant E_2, \tag{33}$$

or

$$\langle\Psi|(H - E_2 \cdot 1)P_1|\Psi\rangle \geqslant 0, \tag{34}$$

which gives the operator inequality:

$$(H - E_2 \cdot 1)P_1 \geqslant 0, \tag{35}$$

which is easily generalized and ultimately gives an inequality connecting the spectral resolution of H and the resolution of the identity. We note that if the equal sign is attained for the wave function Ψ_2, the previously used lemma shows that one has the relation:

$$(H - E_2 \cdot 1)\Psi_2 = 0, \tag{36}$$

which shows that the function Ψ_2 is an eigenfunction to H associated with the next-next lowest eigenvalue E_2. One then proceeds by considering all trial wave function Φ orthogonal to the exact eigenfunctions Ψ_0, Ψ_1, Ψ_2, etc. We note that the Rayleigh–Ritz variation principle gives *upper bounds* to the true eigenvalues in order from below. It is sometimes claimed that this principle is not useable for determining the properties of the low-lying excited states, since it requires the knowledge of the exact eigenfunctions Ψ_0, Ψ_1, Ψ_2, ... for the lower states, but fortunately there exists a well-known generalization of this principle to which we will return below. The Rayleigh–Ritz variation principle is in fact the basis for many quantum-mechanical applications: the Hartree–Fock (HF) method, the method of superposition of configurations often referred to as the configurational interaction (CI) method, etc., and it is certainly the foundation for an essential part of the large-scale computational efforts.

7. Some properties of outer projections

In this subsection, we will study the properties of the outer projection of an operator as defined by Eq. (9). For this purpose, we will consider a self-adjoint Hamiltonian H which is bounded from below, so that $H > \alpha \cdot 1$, and a self-

adjoint projector P satisfying the relation $P^2 = P$ of order $p = Tr\, P$, which may even be infinite. The outer projection is then defined by the relation:

$$\bar{H} = PHP, \tag{37}$$

and we note that even this operator is bounded from below, since one has $\bar{H} > \alpha \cdot P$, where $\alpha \cdot P \geqslant 0$ if α is positive, and $\alpha \cdot P \geqslant a$ if α is negative. Next we will consider the eigenvalue problem:

$$\bar{H}\bar{\Psi} = \bar{E}\bar{\Psi}. \tag{38}$$

Multiplying this relation to the left by P, one obtains $P\bar{E}\bar{\Psi} = \bar{E}\bar{\Psi}$, which means that, for $\bar{E} \neq 0$, one has $P\bar{\Psi} = \bar{\Psi}$, i.e.:

$$P\bar{\Psi} = \bar{\Psi}, \tag{39}$$

and, for $\bar{E} \neq 0$, all the eigenfunctions of $\bar{H}$ are hence situated in the subspace of P. All functions in the subspace of $(1 - P)$ are, of course, trivial eigenfunctions to $\bar{H}$ associated with the special eigenvalue $\bar{E} = 0$, but there may also exist non-trivial eigenfunctions in the subspace of P associated with the eigenvalue $\bar{E} = 0$. From now on, we will concentrate our interest to eigenfunctions $\bar{\Psi}$ in the subspace of P satisfying Eq. (39). For such functions, one has the identity:

$$\langle \bar{\Psi} | H | \bar{\Psi} \rangle = \langle P\bar{\Psi} | H | P\bar{\Psi} \rangle = \langle \bar{\Psi} | PHP | \bar{\Psi} \rangle = \langle \bar{\Psi} | \bar{H} | \bar{\Psi} \rangle, \tag{40}$$

which we will now use to compare the eigenvalues of $\bar{H}$ and H, and prove the general theorem that the eigenvalues to $\bar{H}$ are upper bounds to the eigenvalues of H in order from below:

$$\bar{E}_k > E_k, \tag{41}$$

provided that the spectra of $\bar{H}$ and H both start with a series of discrete eigenvalues. If $\bar{\Psi}_0$ is the normalized eigenfunction to $\bar{H}$ associated with the eigenvalue $\bar{E}_0$ then the Rayleigh–Ritz variation principle applied to H gives the inequality:

$$E_0 \leqslant \langle \bar{\Psi}_0 | H | \bar{\Psi}_0 \rangle = \langle \bar{\Psi}_0 | \bar{H} | \bar{\Psi}_0 \rangle = \bar{E}_0. \tag{42}$$

In order to proceed, one considers the auxiliary function $\bar{u}_1 = \bar{\Psi}_0 \alpha_{01} + \bar{\Psi}_1 \alpha_{11}$, which is normalized to unity due to the condition $|\alpha_{01}|^2 + |\alpha_{11}|^2 = 1$, and which is further chosen orthogonal to the function Ψ_0, so that $\langle \Psi_0 | \bar{u}_1 \rangle = \langle \Psi_0 | \bar{\Psi}_0 \rangle \alpha_{01} + \langle \Psi_0 | \bar{\Psi}_1 \rangle \alpha_{11} = 0$. Applying the Rayleigh–Ritz principle once more, one gets:

$$\begin{aligned} E_1 \leqslant \langle \bar{u}_1 | H | \bar{u}_1 \rangle &= \langle \bar{u}_1 | \bar{H} | \bar{u}_1 \rangle \\ &= \langle \bar{\Psi}_0 \alpha_{01} + \bar{\Psi}_1 \alpha_{11} | \bar{H} | \bar{\Psi}_0 \alpha_{01} + \bar{\Psi}_1 \alpha_{11} \rangle \\ &= \bar{E}_0 |\alpha_{01}|^2 + \bar{E}_1 |\alpha_{11}|^2 \\ &< \bar{E}_1 \end{aligned} \tag{43}$$

In order to proceed, one considers the auxiliary function:

$$\bar{u}_2 = \bar{\Psi}_0 \alpha_{02} + \bar{\Psi}_1 \alpha_{12} + \bar{\Psi}_2 \alpha_{22}, \tag{44}$$

and by normalizing it to unity and chosing it orthogonal to Ψ_0 and Ψ_1, one proves further that:

$$E_2 \leqslant \bar{E}_0 |\alpha_{01}|^2 + \bar{E}_1 |\alpha_{11}|^2 + \bar{E}_2 |\alpha_{21}|^2 \leqslant \bar{E}_2, \tag{45}$$

etc. As we will see below, the outer projections play a fundamental role in quantum theory: in the discussion of the expansion methods, in perturbation theory, in studying the properties of resolvents, etc.

8. Expansion methods

A characteristic feature of the abstract Hilbert space $\mathscr{H}$ is that it is *separable*, i.e. that there exists an enumerable set $\mathscr{H}' = \{g_1, g_2, g_3, \ldots\}$ which is everywhere dense in the space [1]. Applying Schmidt's successive orthonormalization procedure to this set, one obtains an orthonormal set $\boldsymbol{\varphi} = \{\varphi_1, \varphi_2, \varphi_3, \ldots\}$ which is *complete*, and it is then easily shown that for every element Ψ one has an expansion theorem:

$$\Psi = \boldsymbol{\varphi}\boldsymbol{a} = \sum_k \varphi_k a_k, \tag{46}$$

where the infinite sum is convergent in the norm. In the computational applications, it is of course not possible to handle an infinite basis, and one has to be satisfied by using a *finite basis* $\boldsymbol{f} = \{f_1, f_2, f_3, \ldots, f_p\}$ of order p consisting of n linearly independent but not necessarily orthonormal functions f_k, and the best approximation in terms of this basis, $\Psi \approx \sum_k f_k c_k$, is then derived by using the Rayleigh–Ritz variation principle, which leads to the conventional secular equation.

We will here approach this problem in a slightly different way, by considering the outer projection of the Hamiltonian H with respect to the projector Q defined by Eq. (10):

$$\bar{H} = QHQ, \qquad Q = |\boldsymbol{f}\rangle\langle\boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle\boldsymbol{f}|, \tag{47}$$

where $\boldsymbol{\Delta} = \langle\boldsymbol{f}|\boldsymbol{f}\rangle$ is the metric matrix of order $p \times p$, and its eigenvalue problem:

$$\bar{H}\bar{\Psi} = \bar{E}\bar{\Psi}. \tag{48}$$

Since $\bar{\Psi}$ is in the subspace of Q and satisfies Eq. (39), it is possible to expand $\bar{\Psi}$ exactly in terms of this basis:

$$\bar{\Psi} = Q\bar{\Psi} = |\boldsymbol{f}\rangle\langle\boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle\boldsymbol{f}|\bar{\Psi} = \boldsymbol{f}\langle\boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle\boldsymbol{f}|\Psi\rangle = \boldsymbol{f}\boldsymbol{c}, \tag{49}$$

where

$$\boldsymbol{c} = \langle\boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle\boldsymbol{f}|\bar{\Psi}\rangle. \tag{50}$$

For the outer projection $\bar{H}$, one has further:

$$\bar{H} = QHQ = |\boldsymbol{f}\rangle\langle\boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle\boldsymbol{f}|H|\boldsymbol{f}\rangle\langle\boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle\boldsymbol{f}|, \tag{51}$$

and this means that the eigenvalue Eq. (48) takes the form:

$$|\boldsymbol{f}\rangle\langle\boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle\boldsymbol{f}|H|\boldsymbol{f}\rangle\boldsymbol{c} = \bar{E}\boldsymbol{f}\boldsymbol{c}, \tag{52}$$

where one may compare the coefficients for $\boldsymbol{f}$ on both sides. Multiplying Eq. (52) to the left by $\langle\boldsymbol{f}|$, one gets also:

$$\langle\boldsymbol{f}|H|\boldsymbol{f}\rangle\boldsymbol{c} = \bar{E}\langle\boldsymbol{f}|\boldsymbol{f}\rangle\boldsymbol{c}, \tag{53}$$

or

$$\langle\boldsymbol{f}|H - \bar{E}\cdot|\boldsymbol{f}\rangle\boldsymbol{c} = \boldsymbol{0}, \tag{54}$$

which is a system of p linear equations with the secular equations:

$$|\langle f|H - \bar{E} \cdot 1|f\rangle| = 0, \tag{55}$$

having p roots $\bar{E}_1, \bar{E}_2, \bar{E}_3, \ldots, \bar{E}_p$, which are all upper bounds to the true eigenvalues $E_1, E_2, E_3, \ldots, E_p$ to the Hamiltonian H according to the general theorem for outer projections. In this approach, there are no approximations involved, and all the eigenfunctions $\bar{\Psi}_k$ belong to the L^2 Hilbert space. If one increases the number p of basis functions, it is remarkable that some of the eigenvalues of $\bar{H}$ decrease very slowly, whereas others seem to be less stable, and the standard interpretation is that the former approximate discrete eigenvalues of H, whereas the latter in some way may be connected with the continuum.

One may wonder how the continuum eigenfunctions, which are not quadratically integrable, may in any way be connected with a method which renders eigenfunctions in L^2. The answer is that, the continuum eigenfunctions which are usually defined by boundary conditions of the type (2) treated above, may also be defined through the relation [10]:

$$\Psi(E) = d\Phi(E)/dE, \tag{56}$$

where $\Phi(E)$ should be an element of L^2. That this definition is meaningful is illustrated by the simple example of a plane wave $\psi(k) = \exp(ikx)$ with the principal function (with respect to k):

$$\Phi(k) = \{\exp(ikx) - 1\}/ix, \tag{57}$$

which belongs to L^2. Equation (56) implies that one has a limiting procedure of the form:

$$\Psi(X, E) = \lim_{n\to\infty} \{\Phi(X, E + 1/n) - \Phi(X, E)\}/n = \lim_{n\to\infty} \Psi_n(X), \tag{58}$$

which means that there exists a series of elements $\Psi_1, \Psi_2, \Psi_3, \ldots$ in L^2 which *converges* towards the eigenfunction Ψ in the continuum. It is obvious from the definition that this cannot be a convergence in the norm, and that Eq. (58) implies a *point-by-point convergence*, i.e. that:

$$|\Psi(X, E) - \Psi_n(X)| \leqslant \epsilon, \quad \text{whenever } n > N(X, n), \tag{59}$$

and that this convergence, of course, cannot be uniform. Many computational practitioners have found out that this is an excellent way to obtain wave functions in the continuum, and there is no question that this approach deserves a more detailed investigation – particularly since many quantum chemists working with the Coulombic Hamiltonian of Eq. (20) have found it impractical to separate the center of mass motion, since this is usually mixing up the electronic and nuclear coordinates in a complicated way.

Let us now consider a sequence of outer projections $\bar{H}_1, \bar{H}_2, \ldots, \bar{H}_p$, defined by the relation:

$$\bar{H}_k = Q_k H Q_k. \tag{60}$$

Since each $\bar{H}_k$ is an outer projection of the next member $\bar{H}_{k+1}$ of the sequence, it is evident that the eigenvalues of $\bar{H}_k$ are upper bounds to the eigenvalues of $\bar{H}_{k+1}$ in order from below, which is the content of the well-known Hylleraas–Undheim *separation theorem* [9].

9. Eigenvalue properties derived from operator inequalities

If a self-adjoint operator A is positive definite, so that $A > 0$, it is clear that all its eigenvalues a_k must be positive, and – reversely – if all the eigenvalues of an operator are positive, it follows from its spectral resolution that the operator must be positive definite. In general, however, it is somewhat more difficult to derive eigenvalue properties from the existence of an operator inequality, and it is hence worthwhile to note the existence of the following fundamental theorem:

If A and B are two self-adjoint operators bounded from below having the properties that $A > B$ and $D(A)$ belongs to $D(B)$, the eigenvalues have the property that $a_k > b_k$ in order from below. For the proof, we will denote that eigenfunctions of A and B by the symbols u_k and v_k, respectively, so that:

$$Au_k = a_k u_k, \qquad Bv_k = b_k v_k. \tag{61}$$

Applying the Rayleigh–Ritz variation principle to the operator B, one has immediately:

$$b_0 \leqslant \langle u_0 | B | u_0 \rangle < \langle u_0 | A | u_0 \rangle = a_0. \tag{62}$$

One observes that all the eigenfunctions u_k of A belong to $D(B)$. In order to proceed, one considers the auxiliary function $\varphi_1 = u_0\alpha_{01} + u_1\alpha_{11}$, which is normalized to unity and chosen orthogonal to the function v_1. The Rayleigh–Ritz variation principle gives in this case:

$$b_1 \leqslant \langle \varphi_1 | B | \varphi_1 \rangle < \langle \varphi_1 | A | \varphi_1 \rangle = \langle u_0\alpha_{01} + u_1\alpha_{11} | A | u_0\alpha_{01} + u_1\alpha_{11} \rangle$$

$$= a_0 |\alpha_{01}|^2 + a_1 |\alpha_{11}|^2 \leqslant a_1. \tag{63a}$$

The next auxiliary function has the form $\varphi_2 = u_0\alpha_{02} + u_1\alpha_{12} + u_2\alpha_{22}$, and this function is supposed to be normalized to unity and to be chosen orthogonal with respect to both v_0 and v_1, which gives:

$$b_2 \leqslant \langle \varphi_2 | B | \varphi_2 \rangle < \langle \varphi_2 | A | \varphi_2 \rangle = \langle u_0\alpha_{02} + u_1\alpha_{12} + u_{22}\alpha_{22} | A | u_0\alpha_{02} + u_1\alpha_{12} + u_2\alpha_{22} \rangle$$

$$= a_0 |\alpha_{02}|^2 + a_1 |\alpha_{12}|^2 + a_2 |\alpha_{22}|^2 \leqslant a_2, \tag{63b}$$

etc. We note that the auxiliary functions in the proof are chosen in essentially the same way as the auxiliary functions occurring in the treatment of the outer projections given above. This theorem has become of essential importance in many quantum-mechanical applications.

10. Lower bounds to energy eigenvalues

Since the Rayleigh–Ritz method provides upper bounds to the energy eigenvalues, it is important to find some methods which would provide also *lower bounds* to these eigenvalues. The elementary methods available [11] were not particularly useful, and this field was almost dormant until Alexander Weinstein and his group at the University of Maryland started a completely new approach based on operator inequalitites and the fundamental theorem mentioned above [12]. In

the case, when the total Hamiltonian had the form $H = H_0 + V$, where the perturbation V is positive definite, they replaced V by a lower bound V' given by Aronszajn [13], which in our notations would take the form:

$$V' = V|\boldsymbol{g}\rangle\langle\boldsymbol{g}|V|\boldsymbol{g}\rangle^{-1}\langle\boldsymbol{g}|V, \tag{64}$$

where $\boldsymbol{g} = \{g_1, g_2, g_3, \ldots, g_p\}$ is a set of p linearly independent basis functions and $V' \to V$, when the set becomes complete. The so-called *intermediate Hamiltonian* $H' = H_0 + V'$ would then be a lower bound to the original Hamiltonian H, and the inequality $H' < H$ would then give $E'_k < E_k$ for the eigenvalues in order from below. The eigenvalue problem $H'\Psi' = E'\Psi'$ was usually solved by a modified form of localized perturbation theory [14], and this approach would only run into difficulties if part of the spectrum of the unperturbed Hamiltonian H_0 would be a continuum.

Inspired by the work of the Weinstein school and particularly by a series of lectures by David Fox and Norman Bazley at the Uppsala Summer Institutes in the early 1960's, the Uppsala and Florida projects tried to attack this problem from a slightly different point of view. If A is positive definite, $A > 0$, Eq. (7) shows that the *inner projection* A' with respect to the self-adjoint projector O defined by Eq. (8):

$$A' = A^{1/2}OA^{1/2}, \tag{65}$$

provides a lower bound to the operator A. If one replaces the projector O by the projector Q defined by Eq. (10), one obtains the special expression:

$$A' = A^{1/2}QA^{1/2} = A^{1/2}|\boldsymbol{f}\rangle\langle\boldsymbol{f}|\boldsymbol{f}\rangle^{-1}\langle\boldsymbol{f}|A^{1/2}, \tag{66}$$

and making the substitution $\boldsymbol{h} = A^{1/2}|\boldsymbol{f}\rangle$, one obtains finally

$$A' = |\boldsymbol{h}\rangle\langle\boldsymbol{h}|A^{-1}|\boldsymbol{h}\rangle^{-1}\langle\boldsymbol{h}|, \tag{67}$$

which is the form of the inner projection we are going to use. Here $\boldsymbol{h} = \{h_1, h_2, h_3, \ldots, h_p\}$ is any linearly independent set of p basis functions in the space under consideration. We note that, for any linear operator A having an inverse A^{-1}, the inner projection A' converges towards A when $p \to \infty$, and the set $\boldsymbol{h}$ becomes complete and that the convergence is from below whenever A is positive definite or has a finite negative part [15].

The primary goal was to try to find a formal exact solution to the Schrödinger equation $H\Psi = E\Psi$ by means of *partitioning technique* [16], and then to derive lower bounds to the eigenvalues by using inner projections. For this purpose, one introduces a normalized *reference function* φ and a boundary condition in the form of the intermediate normalization $\langle\varphi|\Psi\rangle = 1$, which gives a spectrum $\{E\}_\varphi$. It is easily shown that, if one introduces a complex variable z and considers the inhomogeneous Schrödinger:

$$(H - z \cdot 1)\Psi_z = a\varphi, \tag{68}$$

where the parameter a is determined by the boundary condition $\langle\varphi|\Psi_z\rangle = 1$, and further the projection $P = 1 - |\varphi\rangle\langle\varphi|$ having the property $P\Psi_z = \Psi_z - \varphi$, then one has $P(H - z \cdot 1)\Psi_z = 0$, and the explicit solution:

$$\Psi_z = (1 - PH/z)^{-1}\varphi = W\varphi, \tag{69}$$

where

$$W = (1 - PH/z)^{-1}, \tag{70}$$

is often referred to as the *wave operator*, which transforms the reference function φ into the exact solution Ψ_z. Using the identities $(A-B)^{-1} = A^{-1} + (A-B)^{-1}BA^{-1}$ and $(1-RS)^{-1}R = R(1-SR)^{-1}$, one obtains the transformation:

$$W = 1 + TH, \tag{71}$$

with

$$T = (z \cdot 1 - PH)^{-1}P = P(z \cdot 1 - HP)^{-1} = P(z \cdot 1 - PHP)^{-1}P, \tag{72}$$

where the operator T is often referred as the *reduced resolvent*. It should be observed that it contains the outer projection $\bar{H} = PHP$ of the Hamiltonian and that it becomes singular for $z = \bar{E}_k$ but not for the ordinary eigenvalues. Multiplying Eq. (68) to the left by $\langle\varphi|$, one obtains $a = \langle\varphi|H - z \cdot 1|\Psi_z\rangle - \langle\varphi|H|\Psi_z\rangle - z = f(z) - z$, where $f(z) = \langle\varphi|H|\Psi_z\rangle = \langle\varphi|HW|\varphi\rangle = \langle\varphi|H + HTH|\varphi\rangle$ becomes a key function in the theory. It is easily shown that, if z is chosen on the real axis, then there is always a true eigenvalue E situated between z and $z_1 = f(z)$, and the function $f(z)$ is hence often referred to as the *bracketing function*. Since the inhomogeneous Eq. (68) goes over into the Schrödinger equation for $a(z) = 0$, one may find the eigenvalues $z = E$ by solving the "algebraic" equation:

$$a(z) = f(z) - z = 0, \tag{73}$$

which actually corresponds to the reduced characteristic equation for the problem. If it is solved by the Newton–Raphson method, the result corresponds to the use of the quantum mechanical variation principle. For more details, the reader is referred elsewhere [16]. If the total Hamiltonian has the form $H = H_0 + V$, one finds that – in addition to the wave operator – the key operator in the theory is the *reaction operator* t defined by the relation:

$$t = (1 - VT_0)^{-1}V, \qquad t^{-1} = V^{-1} - T_0, \tag{74}$$

where $T_0 = (z \cdot 1 - PH_0)^{-1}P = P(z \cdot 1 - PH_0P)^{-1}P$. In the simplest case, the reference function φ may be chosen as the normalized eigenfunction φ_0 of H_0 associated with the eigenvalue E_0, and then the total energy E may be written in the form:

$$E = E_0 + \langle\varphi_0|t|\varphi_0\rangle, \tag{75}$$

and one can then find a lower bound by using the inner projection t' of the reaction operator t according to (67):

$$t' = |\boldsymbol{h}\rangle\langle\boldsymbol{h}|t^{-1}|\boldsymbol{h}\rangle^{-1}\langle\boldsymbol{h}| = |\boldsymbol{h}\rangle\langle\boldsymbol{h}|V^{-1} - T_0|\boldsymbol{h}\rangle^{-1}\langle\boldsymbol{h}|. \tag{76}$$

Using this approach combined with the properties of the bracketing function $f(z)$, lower bounds for the eigenvalues of quite a few simple systems have been calculated [17] even in the case when H_0 has a partly continuous spectrum. It should be pointed out, however, that – in spite of this good start – there is still no good theory for the lower bounds of many-electron systems, and that this important field is still waiting to be developed.

11. Some properties of the resolvent; connection between inner and outer projections

In the studies of eigenvalue problems of the type $(H - E \cdot 1)\Psi = 0$, one of the key operators in mathematics is the *resolvent*.

$$R(z) = (z \cdot 1 - H)^{-1}, \tag{77}$$

where z is a complex variable. The eigenfunctions Ψ are the same, but the eigenvalues r are transformed according to the relation $r = (z - E)^{-1}$. The importance of the resolvent is stressed by the fact that, even if the Hamiltonian is unbounded in one way or another, the resolvent is always *bounded* as long as $|z - E| > \varrho$, and one has the relation $\| R\Phi \| < (1/\varrho) \| \Phi \|$. The resolvent has its name from the fact that it immediately renders a solution to the inhomogeneous Eq. (68) in the form:

$$\Psi_z = -aR(z)\varphi = R(z)\varphi / \langle \varphi | R(z) | \varphi \rangle, \tag{78}$$

where, in the last member the value of the parameter a is chosen so that the intermediate normalization $\langle \varphi | \Psi_z \rangle = 1$ is automatically satisfied. In this approach, the eigenvalues $z = E$ are found by looking for the simple poles of the denominator $W(z) = \langle \varphi | R(z) | \varphi \rangle$, which has become known as the *Weinstein function*. It is evident that, for $z = E$, the right-hand member takes the form ∞/∞, but one can avoid the rather cumbersome limiting procedure by instead using the *resolvent identity* [18]:

$$R(z)\varphi / \langle \varphi | R(z) | \varphi \rangle = (1 - PH/z)^{-1}\varphi, \tag{79}$$

where $P = 1 - |\varphi\rangle\langle\varphi|$ is the projector used above. We note that this identity connects the resolvent method with the partitioning technique.

Resolvents are used in many parts of theoretical physics, particularly in connection with the so-called propagator methods, and we will now try to approximate them in terms of inner projections. According to Eq. (67), one has:

$$R'(z) = |\boldsymbol{h}\rangle\langle\boldsymbol{h}|R^{-1}|\boldsymbol{h}\rangle^{-1}\langle\boldsymbol{h}| = |\boldsymbol{h}\rangle\langle\boldsymbol{h}|z \cdot 1 - H|\boldsymbol{h}\rangle^{-1}\langle\boldsymbol{h}|, \tag{80}$$

and we will now look for its singular points, which obviously occur for the zero-points of the determinant $|\langle \boldsymbol{h}|z \cdot 1 - H|\boldsymbol{h}\rangle|$. However, in connection with Eq. (55), we have already shown that, if $Q = |\boldsymbol{h}\rangle\langle\boldsymbol{h}|\boldsymbol{h}\rangle^{-1}\langle\boldsymbol{h}|$ is the projector associated with the subspace of order p spanned by the elements $\boldsymbol{h} = \{h_1, h_2, h_3, \ldots, h_p\}$, then the zero-points of the determinant $|\langle \boldsymbol{h}|z \cdot 1 - H|\boldsymbol{h}\rangle|$ correspond to the exact eigenvalues of the outer projection $\bar{H} = QHQ$. Hence one has the general theorem that the singularities of the *inner projection of the resolvent* are identical with the eigenvalues of the *outer projection of the Hamiltonian* with respect to the same linear manifold, or – which is the same – that the eigenvalues of R' are given by the formula $r'_k = (z - \bar{E}_k)^{-1}$.

This statement has an important corollary. If H is a Hamiltonian bounded from below, so that $H > \alpha \cdot 1$, then for real values of z one has $H - z \cdot 1 > \alpha \cdot 1 - z \cdot 1 > 0$, provided that $z < \alpha$. According to Eq. (5a), one obtains $0 < (H - z \cdot 1)^{-1} < (\alpha \cdot 1 - z \cdot 1)^{-1}$, which means that the operator $-R(z)$

is positive definite for $z < \alpha$. In such a case, the operator inequality:

$$0 < -R'(z) < -R(z), \tag{81}$$

gives for the associated eigenvalues in order from below:

$$0 < -(z - \bar{E}_k)^{-1} < -(z - E_k)^{-1}, \tag{82}$$

or $-(z - \bar{E}_k) > -(z - E_k) > 0$, i.e. $\bar{E}_k - z > E_k - z > 0$ for $z < \alpha$, or simply:

$$\bar{E}_k > E_k. \tag{83}$$

The fact that the eigenvalues $\bar{E}_k$ of the outer projection $\bar{H} = QHQ$ are upper bounds to the true eigenvalues E_k may hence be associated with the operator inequality of Eq. (81).

12. Concluding remarks

We have here concentrated our interest on the importance of operator inequalities as tools in the quantum theory of matter, but they are of course of great importance also in other fields. As an example, we may take Eq. (5b) which in econometrics is known as Becker's lemma [19]. In the case when the equality sign is valid, one observes that the operator $A^{-1/2}BA^{-1/2}$ is a projector, and Kalman [20] has used this fact for a new construction of the least square method. In general, linear algebra, operator inequalities, and the projection operator formalism are of essential importance in the search for linear relations in the natural sciences [21].

In conclusion, one can certainly say that operator inequalities are a strong mathematical tool which has so far been used only to a small extent in the quantum theory of matter, and for which one can hence expect an important development in the future. In this field it would probably be good, if – following the example of Professor Alberte Pullman – one would concentrate more on the development of the theoretical methods before one starts large-scale calculations, since this would certainly lead to a richer development of our entire field. In this connection Professor Alberte Pullman has been a great pioneer.

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