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Some remarks on propagators and resolvents

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Summary. The background of the propagator methods introduced into quantum chemistry by Linderberg and Öhrn is briefly reviewed. Emphasis is put on its connection with the superresolvent associated with the Liouvillians superoperator as shown by Goscinski *et al.* The paper stresses the importance of the effectiveness of the resolvent approach in general, and points out that, for the ordinary Hamiltonian, this method is not only conceptually important as the basis for infinite-order perturbation theory and rational approximations but also as the foundation for a large-scale computational effort still to come. Even if it may be premature to ask for a similar effort related to the superoperator, it would certainly be of value to carry out some test calculations based on the Hilbert–Schmidt binary product, in which the Liouvillian superoperator is automatically self-adjoint, and to compare the results with those obtained from the more conventional propagator methods. The importance of the use of approximations based on "inner projections" in both these approaches is also mentioned.

Key words: Propagators – Resolvents – Liouvillians

1 Introduction

A fundamental problem in quantum theory is to solve the Schrödinger equation:

$$H\Psi = E\Psi, \tag{1.1}$$

where H is the Hamiltonian operator, which is self-adjoint and bounded from below, and the eigenfunction Ψ is subject to some specific boundary condition. In this paper we will use the following concepts and terminology: The linear space (Ψ) consisting of all wave functions Ψ in the L^2 Hilbert space will be referred as the *wave function space*, and the space $\{T\}$ of all linear mappings T defined on this space will be called the *operator space*, whereas the space $\{\hat{M}\}$ of all mappings

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$\hat{M}$ defined on the operator space will be referred to as the *superoperator space*. In the wave function space, we will introduce the standard binary product in terms of Dirac's bracket notation $\langle a|b\rangle$, and this notation $T = |b\rangle\langle a|$ for the dyadic (ket–bra) operator defined by the relation $T\Psi = b\langle a|\Psi\rangle$. We note that the operator T has a single non-vanishing eigenvalue $\lambda = \langle a|b\rangle$, and that it satisfies the relations $T^{\dagger} = |a\rangle\langle b|$ and $\mathrm{Tr}\, T = \langle a|b\rangle$.

In many parts of quantum theory, there has been a desire to try to calculate energy differences $\nu = E_{\mathrm{f}} - E_{\mathrm{i}}$ directly without first solving the Schrödinger equation for the initial state Ψ_{I} and final state Ψ_{f} associated with the Hamiltonian H. For this purpose, it is convenient to introduce a Liouvillian superoperator $\hat{L}$, which is defined on an operator space $\{T\}$ through the relation:

$$\hat{L}T \equiv HT - TH. \tag{1.2}$$

If one considers the ket–bra operator $C = |\Psi_{\mathrm{f}}\rangle\langle\Psi_{\mathrm{i}}|$, it is obvious that C is an eigenoperator to the Liouvillian having the property

$$\hat{L}C = (E_{\mathrm{f}} - E_{\mathrm{i}})C, \tag{1.3}$$

i.e. the energy differences ν are the eigenvalues of the Liouvillian. However, if one takes the ordinary harmonic oscillator as an example, it is clear that all its eigenvalues ν are going to be infinitely degenerate, and that it is not possible to attack the eigenvalue problem in the conventional way. During the 1950's, there were special methods developed in field theory and nuclear physics, which became known as *propagator methods*, and – around 1965 – Linderberg and Öhrn [1] successfully introduced such methods into quantum chemistry. A *propagator* of two linear operators, A and B, and a complex variable z is a binary form $\langle\langle A;B\rangle\rangle_z$ which is usually defined implicitly through a so-called propagator relation. By means of the proper spectral resolutions and various decoupling schemes, Linderberg and Öhrn turned the propagator methods into powerful tools for calculating energy differences, ionization potentials, and electron affinities for atoms and molecules, which has led to many important applications [2]. The propagator methods in quantum chemistry have later been further developed by several authors [3]. If one iterates the fundamental propagator relation, one gets a geometric expansion in terms of the quantity $z^{-1}\hat{L}$ with the sum $(\hat{1} - z^{-1}\hat{L})^{-1}$, where $\hat{1}$ is the identity mapping in the superoperator space, and in this way Goscinski et al. [4] could give an explicit expression for the propagator $\langle\langle A;B\rangle\rangle_z$ involving the *superresolvent*:

$$\hat{R}(z) = (z\cdot\hat{1} - \hat{L})^{-1}. \tag{1.4}$$

The close connection between the propagators and the resolvents has been studied in greater detail elsewhere [5]. However, the author feels that neither the propagator methods nor the resolvent techniques have so far been given enough attention by the computational quantum chemists, and has taken this opportunity to emphasize their importance once more.

2. The resolvent method for the Hamiltonian

Let us start by considering the eigenvalue problem (1.1) for the ordinary Hamiltonian H, subject to the boundary condition $\langle\varphi|\Psi\rangle = 1$, where φ is a normalized reference function in the L^2 Hilbert space. The relation $\langle\varphi|\Psi\rangle = 1$ is often referred to as the "intermediate normalization", and we note that it may be used for the discrete states Ψ as well as the scattering states Ψ in the continuum. However, instead of the original eigenvalue problem

$$H\Psi = E\Psi, \quad \langle\varphi|\Psi\rangle = 1, \tag{2.1}$$

we will now consider the inhomogeneous equation

$$(H - z\cdot 1)\Psi_z = a\varphi, \quad \langle\varphi|\Psi_z\rangle = 1, \tag{2.2}$$

where the coefficient a has to be adapted to the boundary condition $\langle\varphi|\Psi_z\rangle = 1$. Multiplying the first relation (2.2) by $\langle\varphi|$, one gets immediately the explicit expression

$$a = \langle\varphi|(H - z\cdot 1)\Psi_z\rangle = \langle\varphi|H|\Psi_z\rangle - z \equiv a(z), \tag{2.3}$$

i.e. the coefficient a is a function of the complex variable z. In order to solve the inhomogeneous equation, one introduces the operator

$$R(z) = (z\cdot 1 - H)^{-1}, \tag{2.4}$$

which is called the *resolvent* associated with the Hamiltonian H, and which gives the solution in the form

$$\Psi_z = -aR(z)\varphi. \tag{2.5}$$

The properties of the resolvent have been studied by the mathematicians since the end of the last century. Whenever $|z - E| > \rho$, the resolvent is a *bounded* operator, which in terms of the norm $\|x\| = \langle x|x\rangle^{1/2}$. satisfies the inequality $\|R(z)\Phi\| \leq \|\Phi\|$. From the identity

$$R(z) = z^{-1} + z^{-1}HR(z), \tag{2.6}$$

one may further – if desired – derive many relations of propagator type. From the boundary condition $\langle\varphi|\Psi_z\rangle = 1$, one gets further a different expression for the coefficient a:

$$a = -1/\langle\varphi|R(z)|\varphi\rangle. \tag{2.7}$$

Substituting this expression into Eq. (2.5), one gets the explicit solution

$$\Psi_z = \frac{R(z)\varphi}{\langle\varphi|R(z)|\varphi\rangle}, \tag{2.8}$$

which takes the indefinite form ∞/∞ whenever z approaches an eigenvalue $z = E$. In order to proceed, it is convenient to introduce the projector $O = |\varphi\rangle\langle\varphi|$ for the reference space as well as the projector for its orthogonal complement $P = 1 - O$. From the identity $(z\cdot 1 - H)R(z) \equiv 1$, one gets immediately a series of identities

$$\begin{gathered}
(z\cdot 1 - H)R \equiv 1,\\
(z\cdot 1 - H)R\varphi \equiv \varphi, \quad \langle\varphi|(z\cdot 1 - H)R\varphi\rangle = 1,\\
(z\cdot 1 - H)R\varphi \equiv \varphi\langle\varphi|(z\cdot 1 - H)R\varphi\rangle,\\
(z\cdot 1 - H)R\varphi \equiv z\varphi\langle\varphi|R\varphi\rangle - OHR\varphi,\\
(z\cdot 1 - PH)R\varphi \equiv z\varphi\langle\varphi|R\varphi\rangle,\\
R\varphi/\langle\varphi|R|\varphi\rangle \equiv (1 - PH/z)^{-1}\varphi.
\end{gathered} \tag{2.9}$$

which are valid for all values of z and all normalized reference functions φ. Hence one has the simple formula

$$\Psi_z = (1 - PH/z)^{-1}\varphi, \tag{2.10}$$

which remains finite even for $z = E$, and which gives the connection between the resolvent technique and the partitioning technique [6]. It is evident that the function $a = a(z)$ is the key quantity, and that the z-values for which $a(z) = 0$ should correspond to the eigenvalues $z = E$, since the homogeneous equation (2.2) is then reduced to the homogeneous Schrödinger equation (2.1). It should be observed, however, that the equation $a(z) = 0$ is not identical to the characteristic equation but to the *reduced characteristic equation* having even multiple eigenvalues represented by single roots. The reason for this is the following.

Let us first observe that the resolvent $R(z)$ is not self-adjoint but is complex-hermitean, so that $\{R(z)\}^\dagger = R(z^*)$, where z^* denotes the complex conjugate value of z. Since the resolvent has the derivative $\mathrm{d}R/\mathrm{d}z = -R^2$, the fundamental function $a(z) = -\langle\varphi|R(z)|\varphi\rangle^{-1}$ has the derivative

$$\begin{aligned}\mathrm{d}a(z)/\mathrm{d}z &= \langle\varphi|R(z)|\varphi\rangle^{-2}\langle\varphi|\mathrm{d}R(z)/\mathrm{d}z|\varphi\rangle\\ &= -\langle\varphi|R(z)|\varphi\rangle^{-2}\langle\varphi|R^2|\varphi\rangle\\ &= -\langle\varphi|R(z)|\varphi\rangle^{-2}\langle R^\dagger\varphi|R\varphi\rangle\\ &= -\langle\Psi_{z^*}|\Psi_z\rangle. \end{aligned}\tag{2.11}$$

This means that, for real values of z, the derivative $\mathrm{d}a/\mathrm{d}z$ is always *negative* and never zero, and this implies that the equation $a(z) = 0$ can never have multiple roots. As a consequence, the function $\langle\varphi|R(z)|\varphi\rangle$ has only single poles, which reflects an important property of the resolvent.

Since the function $a = a(z)$ has such a simple derivative, it seems convenient to solve the equation $a(z) = 0$ by means of the Newton–Raphson method, which gives the second-order iteration formula

$$z_{\mathrm{NR}} = z - a(z)/a'(z)\tag{2.12}$$

Using the relations (2.2) and particularly the fact that $\langle\varphi|\Psi_z\rangle = 1 = \langle\Psi_{z^*}|\varphi\rangle$, one obtains

$$\begin{aligned}z_{\mathrm{NR}} &= z - a(z)/a'(z) = z - a(z)\langle\Psi_{z^*}|\varphi\rangle/a'(z)\\ &= z - \langle\Psi_{z^*}|a(z)\varphi\rangle/a'(z)\\ &= z + \langle\Psi_{z^*}|H - z\cdot 1|\Psi_z\rangle/\langle\Psi_{z^*}||\Psi_z\rangle\\ &= \frac{\langle\Psi_{z^*}|H|\Psi_z\rangle}{\langle\Psi_{z^*}|\Psi_z\rangle},\end{aligned}\tag{2.13}$$

where the last expression is the *bi-variational* formula, i.e. the ordinary variational formula modified to take into account the fact that z is now a complex variable [7].

Substituting formula (2.10) into Eq. (2.3), one gets an alternative expression for the function $a(z)$:

$$a(z) = \langle\varphi|H|\Psi_z\rangle - z = \langle\varphi|H(1 - PH/z)^{-1}|\varphi\rangle - z = f(z) - z,\tag{2.14}$$

where

$$f(z) \equiv \langle\varphi|H(1 - PH/z)^{-1}|\varphi\rangle\tag{2.15}$$

is the so-called *bracketing function*, which for real z has the important property that between z and $f(z)$ there is always a true eigenvalue E. For the *wave operator* $W = (1 - PH/z)^{-1}$, one may use the expansion

$$W = (1 - PH/z)^{-1} = 1 + (z\cdot 1 - PH)^{-1}PH = 1 + TH,\tag{2.16}$$

where the operator T defined by the first of the relations

$$T = (z \cdot 1 - PH)^{-1}P = P(z \cdot 1 - HP)^{-1} = P(z \cdot 1 - PHP)^{-1}P \tag{2.17}$$

is usually referred to as the *reduced resolvent* associated with the auxiliary Hamiltonian $\bar{H} = PHP$. Since the Hamiltonian H is bounded from below, it is easily shown that the eigenvalues $\bar{E}_k$ of its "outer projection" $\bar{H} = PHP$ are always upper bounds (in order) to the true eigenvalues E_k, so that

$$\bar{E}_k > E_k. \tag{2.18}$$

So far, this approach is mathematically exact, and we note that this depends on the fact that the operator $P = 1 - |\varphi\rangle\langle\varphi|$ for the orthogonal complement to $O = |\varphi\rangle\langle\varphi|$ is defined on the entire infinite Hilbert space.

In many cases, however, it is convenient to use approximations based on the introduction of a finite basis set of order p defined by p linearly independent – but not necessarily orthonormal-functions – functions $\boldsymbol{h} = (h_1, h_2, h_3, \ldots, h_p)$. If A is an arbitrary linear operator having an inverse A^{-1}, the operator may be approximated by a so-called *inner projection* [8]:

$$A' = |\boldsymbol{h}\rangle\langle\boldsymbol{h}|A^{-1}|\boldsymbol{h}\rangle^{-1}\langle\boldsymbol{h}|. \tag{2.19}$$

It is easily shown that, if $p \to \infty$ and the set $\boldsymbol{h}$ becomes complete, then A' converges towards A. If further the operator A is positive definite or has only a finite number of negative eigenvalues, then – if the set $\boldsymbol{h}$ is sufficiently large – A' converges towards A *from below*. This is a remarkable property, since in computational quantum chemistry one is otherwise accustomed to the fact that the use of a truncated basis set always leads to approximations providing upper bounds as reflected e.g. in relation (2.26). If one applies the inner projection to the resolvent operator $R(z) = (z \cdot 1 - H)^{-1}$, one gets for instance

$$R'(z) = |\boldsymbol{h}\rangle\langle\boldsymbol{h}|z \cdot 1 - H|\boldsymbol{h}\rangle^{-1}\langle\boldsymbol{h}|. \tag{2.20}$$

which expression becomes singular for the eigenvalues of the matrix $\langle\boldsymbol{h}|H|\boldsymbol{h}\rangle$. In some of the propagator methods, it has turned out to be very useful to utilize this expression to estimate the remainder in any propagator formula based on repeated use of the relation (2.6). It should be observed, however, that there are also many other uses of the inner projections in the theory developed above.

If $H = H_0 + \lambda V$, one may use this formalism to derive various types of *perturbation theory*, and to get exact expressions for the wave and reaction operators associated with infinite-order perturbation theory [9]. However, since each (k, l) element of the inverse of the matrix $\Delta = \langle\boldsymbol{h}|A^{-1}|\boldsymbol{h}\rangle$ in relation (2.27) may be expressed as the quotient between the cofactor of Δ_{lk} and the full determinant $|\Delta|$, one may use the inner projections to derive *rational approximations* in terms of the parameter λ [10]. The applications carried out so far show that this may be a very powerful approach to many problems in quantum chemistry.

In many parts of computational quantum chemistry, the main trend so far has been to use CI-methods based on GUGA and similar schemes and enormous number crunchers to get the results desired for small and intermediate size molecules. However, it is evident that, even with a further development of the supercomputers, this type of ab initio methods will never be applicable to molecules over a certain size, and that this may provide a severe limitation. In the opinion of the author, time has hence come to pay more attention to the various forms of the resolvent methods for the ordinary molecular Hamiltonian H, and try to develop the software necessary for the application of these methods to quantum chemistry. Even if this may require a very large programming effort, it may turn out to be exceedingly efficient and worthwhile for the future development of our field.

3. The resolvent and propagator methods for the Liouvillian

It is evident that, if the eigenvalue problem $H\Psi = E\Psi$ for the ordinary Hamiltonian H represents a formidable problem in operator space, then the eigenvalue problem $\hat{L}C = \nu C$ in the superoperator space ought to be at least one-order of magnitude more difficult. As mentioned in the introduction, it was Linderberg and Öhrn who should be given the credit for attacking this difficult problem in molecular physics by means of the propagator methods. It was also pointed out that the propagator methods are connected with the superresolvent

$$\hat{R}(z) = (z\hat{1} - \hat{L})^{-1}, \tag{3.1}$$

and its expansions

$$\hat{R}(z) = z^{-1} + z^{-2}\hat{L}\hat{R}(z) = z^{-1} + z^{-2}\hat{L} + z^{3} \qquad \hat{L}^{2}\hat{R}(z) = \cdots \tag{3.2}$$

When the propagator methods were developed in field theory and nuclear physics in the 1950's, the computational tools were very limited, and in order to solve the problems one had to introduce further simplifications and approximations, which from a more modern point of view may seem questionable. This approach led also to the introduction of a binary product in the operator space which has many undesirable properties – among other things the Liouvillian was not self-adjoint in this particular metric. With the development of the modern supercomputers, we are today in a somewhat different situation, and the author feels that perhaps time has come to try to put the theory of the Liouvillian and its superresolvent on a more sound mathematical basis.

Let us first of all introduce a complete orthonormal basis $\boldsymbol{\varphi} = \{\varphi_1, \varphi_2, \dots, \varphi_k, \dots\}$ in the wave function space having the properties

$$\langle \varphi_k | \varphi_1 \rangle = \delta_{kl}, \quad 1 = |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}| = \sum_k |\varphi_k\rangle\langle\varphi_k|. \tag{3.3}$$

Every linear operator T has then a matrix representation $\boldsymbol{T} = \{T_{kl}\}$, where $T_{kl} = \langle \varphi_k | T | \varphi_1 \rangle$. Of particular interest are such operators for which the sum of all absolute squares $|T_{kl}|^2$ is finite:

$$\sum_{kl} |\boldsymbol{T}_{kl}|^2 < \infty, \tag{3.4}$$

and in mathematics, they are known as the *Hilbert–Schmidt* operators. If one introduces the binary operator product

$$\{T_1 | T_2\} = \operatorname{Tr} T_1^\dagger T_2 = \sum_{kl} (T_1)_{kl}^*(T_2)_{kl}, \tag{3.5}$$

it may be shown that the Hilbert Schmidt operators $\{T\}$ form a linear space, which is another realization of the abstract Hilbert space introduced by von Neumann [11]. This binary product has further the convenient property that the Liouvillian remains a *self-adjoint* superoperator:

$$\{T_1 | \hat{L}T_2\} = \{\hat{L}T_1 | T_2\}, \tag{3.6}$$

which is of fundamental importance in studying its spectra properties. It should further be observed that the operators $P_{lk} = |\varphi_k\rangle\langle\varphi_l|$ form an orthonormal basis for the operator space $\{T\}$, and that one has now the expansion theorem

$$T = 1\cdot T\cdot 1 = |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}|T|\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}| = \sum_{kl} |\varphi_k\rangle\langle\varphi_k|T|\varphi_1\rangle\langle\varphi_l|$$
$$= \sum_{kl} T_{kl}P_{lk}, \tag{3.7}$$

which proves this statement.

Since the Liouvillian $\hat{L}$ now works on the Hilbert space $\{T\}$ formed by the Hilbert–Schmidt operators T, the remaining part of the treatment follows the same scheme as developed for the Hamiltonian working on the Hilbert space $\{\Psi\}$ and we can be very brief. Instead of the eigenvalue problem $\hat{L}C = \nu C$, we will consider the inhomogeneous equation

$$(\hat{L} - z\cdot\hat{1})C_z = aF, \tag{3.8}$$

where F is a normalized reference operator. For the sake of simplicity, we will choose $F = |\varphi\rangle\langle\varphi|$, where φ is our previous reference function. We will solve the eigenvalue problem and the inhomogeneous equation subject to the intermediate normalization

$$\{F\,|\,C_z\} = 1, \tag{3.9}$$

i.e.

$$\{F\,|\,C_z\} = \mathrm{Tr}\,|\varphi\rangle\langle\varphi|C_z = \langle\varphi|C_z|\varphi\rangle = 1. \tag{3.10}$$

Using the superresolvent (3.1), one gets immediately the solution

$$C_z = -a\hat{R}(z)F = \hat{R}(z)F/\{F\,|\hat{R}(z)|\,F\}, \tag{3.11}$$

where $\{F\,|\hat{R}(z)F\} = \langle\varphi\,|\hat{R}(z)F|\,\varphi\rangle$. It is evident that the quantity

$$a(z) = -1/\{\mathrm{F}\,|\hat{R}(z)|F\} \tag{3.12}$$

is again going to be the key quantity of the theory. In analogy with Eq. (2.19), one gets directly

$$\mathrm{d}a(z)/\mathrm{d}z = -\{C_{z^*}\,|\,C_z\}, \tag{3.13}$$

and, since $a'(z)$ is always negative and never zero, the equation $a(z) = 0$ can only have single roots and the function $W(z) = \{F\,|\hat{R}(z)|F\}$ only have single poles. This result implies that every eigenvalue ν can appear only once, which is a particularly important feature in this connection, since the Liouvillian itself may easily have infinitely degenerate eigenvalues as shown by the example of the harmonic oscillator. One may now solve Eq. $a(z) = 0$ by iteratively using the Newton–Raphson formula according to Eq. (2.20), and in analogy with Eq. (2.21), one can then derive the formula

$$z_{\mathrm{NR}} = \frac{\{C_{z^*}|\hat{L}|C_z\}}{\{C_{z^*}|C_z\}}, \tag{3.14}$$

which shows the connection with the bi-variational principle. At this point, one should observe that, whereas the Hamiltonian H is bounded from below, the superoperator $\hat{L}$ is not bounded at all.

In analogy with Eq. (2.9), one can now derive an identity which leads to the explicit formula for the solution

$$C_z = \hat{R}(z)F/\{F|\hat{R}(z)|F\} \equiv (\hat{I} - \hat{P}\hat{L}/z)^{-1}F, \tag{3.15}$$

and from then on the development goes in parallel with the theory developed for the Hamiltonian. We note particularly that, if $\boldsymbol{H} = (H_1, H_2, H_3, \ldots, H_p)$ is a set of linearly independent operators in the operator space, then every superoperator $\hat{M}$ having an inverse $\hat{M}^{-1}$ may be approximated by an inner projection:

$$\hat{M}'(z) = |\boldsymbol{H}\}\{\boldsymbol{H}|\hat{M}^{-1}|\boldsymbol{H}\}^{-1}\{\boldsymbol{H}|, \tag{3.16}$$

which for the superresolvent takes the special form

$$\hat{R}'(Z) = |\boldsymbol{H}\}\{\boldsymbol{H}|z \cdot \hat{I} - \hat{L}|\boldsymbol{H}\}^{-1}\{\boldsymbol{H}|; \tag{3.17}$$

we note that this expression converges but no longer from below. In connection with the propagator methods and expansions of the type (3.2), the inner projection has already turned out to be a valuable approximation. In the work by Linderberg and Öhrn, there is a consistent improvement of the propagator approach connecting the time-dependent Hartree–Fock method with the random-phase approximation (RPA) and the Tamm-Dancoff Scheme (TDS) leading to the antisymmetrized-geminal-power (AGP) method, which gives important aspects on the connection between molecular physics and the solid-state theory of superconductivity, and similar phenomena.

Since we do not yet have any large-scale computational scheme developed for the resolvent method of the ordinary Hamiltonian, it would certainly be premature to ask for such a scheme for the resolvent method of the Liouvillian. However, it would certainly be interesting to have some simple test case studied using the concept of the Hilbert–Schmidt space as a foundation, and to compare the results with those obtained from the conventional propagator schemes. Perhaps it would not be improper to ask for such a test study in connection with the important anniversary now celebrated by the prominent leaders in this field, Linderberg and Öhrn.

Dedication. This paper is dedicated to Professor Jan Linderberg, Aarhus University, Denmark, and to Professor Yngve Öhrn, University of Florida, in connection with their 60th birthdays in 1994 in view of their important contributions to quantum chemistry and particularly to the propagator methods. Jan Linderberg was the first student, who got his PhD in the new field of "quantum chemistry" at Uppsala University, and – since this volume is specially dedicated to him – I would like to add that as a research leader I was particularly impressed by his independence and originality already as a student, and his ability to go to the literature to pick up new trends and to create new ideas of his own. This is how he and his collaborator found the propagator methods. Jan Linderberg and Yngve Öhrn are to be congratulated for their successful scientific carriers at the international level, and I wish them both many happy years to come.

References

1. Linderberg J, Öhrn Y (1965) Proc Roy Soc London Ser A285:445; Öhrn Y, Linderberg J (1965) Phys Rev 139:A1063; Linderberg J, Öhrn Y (1967) Chem Phys Lett 1:295; Linderberg J, Öhrn Y (1968) J Chem Phys 49:716; Linderberg J, Öhrn Y (1973) Propagators in quantum chemistry. Academic Press, New York; Öhrn Y (1976) In: Parr RG, Pullman B (eds) Proc 2nd Int Cong Quantum Chem. Reidel, Dordrecht; Linderberg J, Öhrn Y (1977) Int J Quantum Chem 12:161; Linderberg J, Öhrn Y, Linderberg J (1979) Int J Quantum Chem 15: 343; Öhrn Y, Born G (1981) Adv quantum chem 13:1; Öhrn Y (1989) in Mukherjee D (ed) Lecture notes in chemistry, Vol 50 Springer, New York

2. Jørgensen P, Öhrn Y (1973) Chem Phys Letters 18:261; (1973) Phys Rev 8A:112; Purvis GD, Öhrn Y (1974) J Chem Phys 60:4063; ibid (1975) 62:2045; (1975) Chem Phys Letters 33:396; Tyner Redmon L, Purvis GD, Öhrn Y (1975) J Chem Phys 63:5011; Nehrkorn C, Purvis GD, Öhrn Y (1976) J Chem Phys 64: 1752; Purvis GD, Öhrn Y (1976) J Chem Phys 65:917; Kurtz H, Purvis GD, Öhrn Y (1976) Int J Quantum Chem Symp 10:311; ibid (1977) Symp 11:359; Born G, Kurtz H, Öhrn Y (1978) J Chem Phys 68:74; Kurtz H, Öhrn Y (1978) J Chem Phys 69:1162; Öhrn Y (1978) in: Excited states in quantum chemistry. Reidel Dordrecht, p 317; Born G, Öhrn Y (1978) Int J Quantum Chem Symp 12:143; Born G, Öhrn Y (1979) Chem Phys Letters 61:307; (1980) Physica Scripta 21:378; Mishra M, Öhrn Y (1980) Chem Phys Letters 71:549; Ortiz B JV, Öhrn Y (1980) J Chem Phys 72:5744; Mishra M, Öhrn Y (1980) Int J Quantum Chem Symp 14:335; Ortiz B JV, Öhrn Y (1981) J Chem Phys 77:548; Mishra M, Froelich P, Öhrn Y (1981) Chem Phys Letters 81:339; Ortiz B JV, Basu R, Öhrn Y (1983) Chem Phys Letters 103:29; Weiner B, Jensen HJ Aa, Öhrn Y (1984) J Chem Phys 80:2009; Weiner B, Öhrn Y (1984) J Chem Phys 80:5866; ibid (1987) 91:563; Sangfelt E, Roychowdhury R, Weiner B, Öhrn Y (1987) J Chem Phys 86:4523
3. See e.g. the following survey papers, which also contain extensive bibliographies: Jørgensen P (1975) Ann Rev Phys Chem 26:359; Oddershede J (1978) Adv Quantum Chem 11:275; Öhrn Y, Born G (1981) Adv Quantum Chem 13:1
4. Goscinski O, Lukman B (1970) Chem Phys Letters 6:37; ibid (1970) 7:573; Goscinski O (1971) Phys Letters 9:293; Pickup BJ, Goscinski O (1973) Mol Phys 26:1013; Simons J (1976) J Chem Phys 64:4541; Weiner B, Goscinski O (1977) Int J Quantum Chem 12 (Suppl 1):299; Calles A, Goscinski O (1979) Rev Mxicana de Física 26:23; Weiner B, Goscinski O (1980) Phys Rev A22:2374; Goscinski O, Weiner B (1980) Phys Scripta 21:385; Goscinski O (1980) in: Fukui K, Pullman B (eds) Horizons in quantum chemistry. Reidel, Dordrecht, p 17; (1982) Int J Quantum Chem 16:591; Weiner B, Goscinski O (1980) Int J Quantum Chem 18:1109; ibid (1982) 21:369; (1983) Phys Rev A27:57
5. Löwdin P-O (1985) Adv quantum chem 17:285; Löwdin PO (1986) Proc 5th ICQC in Montreal, Int J Quantum Chem 29:1651
6. Löwdin PO (1962) J Math Phys 3:969; ibid (1962) 1171
7. Löwdin PO (1983) J Math Phys 24:70
8. See e.g. Löwdin PO (1971) Int J Quantum Chem 4S:231 and references in this paper
9. Löwdin PO (1965) J Math Phys 6:1341; (1968) Phys Rev A357:139; (1969) J Chem Phys 34:S175.
10. Löwdin PO (1989) in: Carbo R (ed.) Quantum chemistry, basic aspects, actual trends, 1. Elsevier, Amsterdam; See also Cizek J, Vrscay ER (1985) Int J Quantum Chem 28:665; ibid (1986) S20:65; Vinette F, Cizek J, Vrscay ER (1987) Int J Quantum Chem 32:663; (1988) Comp Rend 306:21; Cizek J, Vinette F, Vrscay ER (1987) Int J Quantum Chem S21:757; Cizek J, Vinette F (1988) Int J Quantum Chem S22:537; (1988) Chem Phys Letters 149:516; Vinette F, Cizek J (1988) Lecture notes in computer science, Vol 385. Springer, Berlin; Cizek J, Vinette F, Paldus J (1988) in: Kaldor U (ed) Proc Symp Many-Body Methods in Quantum Chemistry, Tel-Aviv 1988, 23 Springer, Berlin; Pieruchi P, Zarrabian S, Paldus J, Cizek J (1990) Phys Rev A42:3351; Vinette F, Cizek J (1991) J Math Phys 32:3392; Cizek J, Vinette F, Weniger EJ (1991) Int J Quantum Chem S25:209; (1993) J Mod Phys C4:257
11. von Neumann J (1932) Mathematische Grundlagen der Quantenmechanik Springer, Berlin