The Göteborg atomic-theory group

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1 Introduction

In this report we wish to describe the background and development of the atomic-theory group in Göteborg and to put its achievements in an international perspective. Of particular interest to us, living in a small country, remote from the main research centers, is how our works are being received and commented upon in the scientific literature. One source of information is the citation index on the *Web of Science*, a system that evidently has been considerably improved during the last few years. The system has its advantages and disadvantages, though, as the following memo will demonstrate.

2 Early work

2.1 Uppsala period

The leader of the group, Ingvar Lindgren, started his scientific career in 1955 as a graduate student in Uppsala under the auspices of the Nobel laureate to be Kai Siegbahn, working with atomic-beam determinations of nuclear spin and moments via the atomic hyperfine structure. His theoretical work started at the beginning of the 1960's, when the IBM 1620 computer was installed at the Physics Department. One of his early works was to develop a self-consistent-field (SCF) program, using the Slater exchange approximation [1, 2, 3]

$$V_{\rm ex}^{\rm S} \propto \rho^{1/3} \tag{1}$$

where ρ is the total electron density (of a certain spin direction). This exchange potential is combined with the direct (Coulomb) part of the Hartree-Fock (HF) potential and termed *Hartree-Fock-Slater* potential. Ingvar modified this potential by means of two parameters to minimize the total energy. This *Optimized Hartree-Fock-Slater* improved the agreement with HF considerably, and it was found that the same set of parameters could be used with negligible loss of accuracy over half the periodic table (22, 39)[1] (74 and 56 citations). Arne Rosén, one of Ingvar's first students, developed a relativistic version of the SCF program, which they together applied to many atomic systems. Later Slater introduced a similarly modified exchange potential with a single parameter, which is the famous and widely used *X-α method* [4]. The disadvantage with this is that the optimum value of α strongly varies with the nuclear charge (see further below).

In the late 1950's and early 1960's the method for *Electron Spectroscopy for Chemical Analysis* (ESCA) was developed in Uppsala by Kai Siegbahn and his team. In the first ESCA book [5] we contributed with an extensive comparison of the experimental electron binding energies for atoms with our theoretical results. Early calculations were also performed of

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[1] The numbers refer to the list below of our most cited works.

Figure 1: Ingvar teaching some graduate students in the early 1960's. (Foto taken by one of the students.)

the chemical shifts observed in the spectra, using a simple atomic model. Some of these results were reported at the 40:th anniversary of the ESCA method in 2003 [6].

(In the early days there was in certain important circles quite a negative attitude towards local potentials, particularly if these were parameterized. The Slater-type of exchange was frequently used for some time, mainly for band-structure calculations, where the non-local and long-ranged HF exchange was known to work very badly. However, the X-α method later came into bad reputation, largely because it was oversold together with the muffin-tin potential. Later, the situation changed drastically by the advent of the Density-Functional Theory (DFT) in the mid 1960's [7, 8] and its increased popularity in the 1970's. It then became fashionable to use local potentials again, even parameterized ones. Nowadays, however, no-one talks any longer about the Slater exchange or X-α. Instead, when this kind of approximation is used, it is fashionable to refer to it as *"DFT in the local-density-approximation"*, which, of course, is essentially the same thing. It should be remembered that the Slater local exchange—together with the Thomas-Fermi atomic model—were the first density-functional models, predating the theories of Hohenberg-Kohn-Sham by several decades.)

In 1959-60 Ingvar spent a post.-doc. year with Bill Nierenberg, Dick Marrus, Amado Cabezas and coworkers at Berkeley, working with atomic-beam experiments on rare-earth elements (24) (72 cit.). Together with Brian Judd he performed the corresponding theoretical analysis, which is one of our most cited paper (164 cit.). The experiments together with the theoretical analysis led in several cases to new determination or confirmation of the electronic ground-state configuration of these elements. This was difficult to determine by optical spectroscopy due to the fact that several of the atoms have very low lying states with different parity.

Of great importance for the early development of our group were the *Brookhaven Conferences on Atomic Beams* that were arranged essentially yearly from 1955 and a number of years forward with Bill Cohen from Brookhaven Nat. Lab. as the driving force. Most leading atomic physicists in experiments as well as in theory attended these conferences. Ingvar attended several of them, starting from the second conference in 1956, and he presented the first experimental results in 1957. One conference in the series was arranged in Uppsala in 1964 by Ingvar together with Bill Cohen (Fig.2). This was the first in the series with an extended scope, including also optical resonance spectroscopy (optical pumping, optical double resonance etc—laser spectroscopy was not yet invented) as well as corresponding theory. The conference was preceded by one week of introductory lectures, particularly aimed for graduate students, given by Brian Judd, Johns Hopkins Univ., (atomic physics) and Gunnar Sørensen, Aarhus university (nuclear physics). This conference series was in

Figure 2: "Brookhaven conference" in Uppsala 1964 (from left: Bill Cohen, I.I.Rabi, D.A.Jackson, Paris, S.Penselin, Bonn, and I.L.). (Foto: Upplandsmuséet)

1968 transformed into the *International Conference on Atomic Physics* (ICAP) with the first conference in New York. This is nowadays the main international conference in atomic physics and has been held every second year since the start.

Atomic-beam spectroscopy was in the middle of the century the modern form of experimental atomic physics, particularly due to the discovery of the microwave-resonance phenomenon by Rabi in the late 1930's. In the 1950's it was practitioned by several leading scientists, like Norman Ramsey, Wolfgang Paul, Willis Lamb, Polykarp Kusch, Vernon Hughes, Julian Zacharias, Dan Kleppner and Pat Sandars.

2.2 Move to Göteborg

In 1966 Ingvar was appointed professor at Chalmers University of Technology (CTH), and moved with Arne Rosén and one more graduate student to Göteborg to set up an atomic-physics group at the joint physics department of CTH and University of Gothenburg. There they continued the experimental atomic-beam work and Ingvar and Arne the atomic calculations. A report on the relativistic OHFS calculations was given at the first ICAP conference in 1968, and a Phys. Rev. paper on the subject the same year (7) has been frequently cited (154 cit.) They also developed HF versions of both the non-relativistic and the relativistic programs. A comprehensive report on relativistic SCF calculations and the analysis of the hyperfine structure in particular was published in *Case Studies in Atomic Physics* in 1974. This our most cited article (452 citations). Later, Arne has performed extensive SCF calculations on molecular systems.

In 1970-71 Ingvar spent a sabbatical year at Yale university with Vernon Hughes and at Gainesville in Florida with Per-Olof Löwdin and John Slater. Together with Karl-Heinz Schwarz in Florida—following a suggestion from Slater— he analysed the X-α method in order to explain the variation of the parameter α (19) (83 cit.). They found that the variation was primarily due to the self interaction, which has higher relative weight for light elements.

At the Sanibel symposium in 1971 Ingvar presented a new local potential (9) (120 cit.) This work was partly done together with Arne. Here, the electronic self interaction is removed from the Slater exchange

$$V_{\text{ex}}^{\text{HS}} \propto \rho^{1/3} - \rho_i^{1/3} \tag{2}$$

where ρ_i is the electron density due to the electron considered. This modified exchange potential was combined with the Hartree potential without self interaction (rather than the Coulomb part of the HF potential) and termed *Hartree-Slater* (HS) potential. This gave very good agreement with HF without any adjustable parameter. The disadvantage is that the potential is orbital dependent and therefore leads to non-orthogonal orbitals. The potential has been used in solid-state and surface physics [9]. In 1981 Perdew and Zunger [10] introduced this idea into DFT under the name *"SIC—self-interaction correction"*.

When the approximation Eq. (2) appeared, solid-state physicists showed very little interest in it. It took some ten years before it was realized by Perdew and Zunger that the potential could be useful in DFT. Their paper has to date received 6585 citations!

The group in Göteborg has been a combined experimental and theoretical group. In addition to the atomic-beam work that Ingvar and Arne continued, an optical-spectroscopy group was set up with Sune Svanberg—at that time a graduate student—as group leader. In the 1970's the work of that subgroup was more and more directed towards laser spectroscopy. In that decade Svanberg built up an impressive research group in this field. Around 1980 he became professor in Lund and has there set up one of the world-leading laser centra. At about the same time Arne started to set up a large separate experimental group on molecular spectroscopy in Göteborg.

In the 1970's Ingvar started to concentrate more and more on theoretical work. Some atomic-beam work was still performed by Ingvar and Arne together with graduate students. Extensive atomic-beam work was also performed at CERN under the leadership of Curt Ektröm, who started as a graduate student in the group. Later he moved to Uppsala and became the head to the The Svedberg laboratory.

3 Many-body theory

3.1 Early many-body-perturbation calculations

In 1972 John Morrison from USA joined our group in Göteborg—and stayed for nearly 10 years—and we started atomic many-body calculations, primarily by means of single-particle and pair programs John had brought with him [11, 12]. We modified the programs to make them more efficient and more adopted to the problems we had in mind. The first graduate students in the theory group were Johannes Lindgren, Sten Garpman, and Lennart Holmgren and a few years later Ann-Marie Mårtensson(-Pendrill) and Sten Salomonson joined the group, followed by Jean-Louis Heully, Eva Lindroth, Per Öster, and Anders Ynnerman. John and Ingvar gave several courses on Atomic Many-Body Theory, and at the end of John's stay in Göteborg their book appeared (see below).

In the mid 1970's we applied the many-body programs particularly to the atomic hyperfine structure (15) (91 cit.), and we developed all-order single-particle programs, which gave the core polarization to all orders (14, 20) (96 and 82 cit.). Of particular interest is that we noticed early the importance of Brueckner orbitals on the hyperfine structure of alkali atoms (14). Lennart Holmgren developed a program for evaluating the fine structure, treated by means of a full two-body operator and applied this to the alkali atoms (42) (53 cit.). Subsequently, Ann-Marie developed an iterative, all-order pair program (29) (64 cit.)—a procedure nowadays sometimes inadequately termed *"linear coupled-cluster"*—and tested it on the He atom, treated as an open-shell system. This program formed the basis for our work for a long time.

3.2 Coupled-cluster approach

Nowadays, the most effective method for many-body calculations in atomic physics and quantum chemistry is assumed to be the coupled-cluster method, which is based upon the exponential Ansatz with the wave operator of the form

$$\Omega = \mathrm{e}^{S} \tag{3}$$

S (by chemists often denoted by T) is the *cluster operator*, which was shown to be *connected* for closed-shell systems (single reference function). The idea of the exponential Ansatz was probably first communicated by Hubbard in the late 1950's [13]. It was introduced into nuclear physics by Kümmel and Coester around 1960 [14] and into quantum chemistry by Čižek in 1966 [15] (1297 cit.).

The pair program developed by Ann-Marie was modified by Sten Salomonson into a full coupled-cluster program with double excitations (CCD), and our first results were reported in 1979 at the Nobel symposium at Lerum outside Göteborg, organized by us together with Stig Lundquist [16]. Our almost 30 years old calculations with numerical basis on the Be and Ne atoms (16) (88 cit.) are still being used as benchmark for accurate finite-basis-set calculations [17]. We also reported at the symposium one of the very first multi-reference coupled-cluster calculation (on Be-like ions) (13) (99 cit.). There we experienced the famous intruder-state problem (see below) for the neutral atom but we could find a solution for the B^+ ion. Such problems had been observed earlier in nuclear physics [18], but our observation was probably the first in an atomic/molecular system. We have, as well as several other groups, later approached the Be problem, as will be discussed later.

Our coupled-cluster calculations appeared shortly after the first results of similar (closed-shell) programs, appearing in 1978, by Bartlett et al. [19] (730 cit.) and by Pople et al. [20] (674 cit.), but our procedure was applicable and also applied to open-shell (quasi-degenerate) problems. From our observation of the importance of Brueckner orbitals, we included early single excitations into the CC equations (CCSD). Our first application of the (open-shell) CCSD procedure was the calculation of the ionization energy and hyperfine structure of the Li atom, published in 1985 (18) (84 cit.). Internationally, the first CCSD calculation was reported by Purvis and Bartlett in 1982 [21], which with 2237 citations is the most cited of all papers on coupled clusters! They used a single-reference approach, which was claimed to work well also for quasi-degenerate cases like the Be atom.

3.3 Relativistic MBPT. Improved numerical procedure

In the mid 1980's we started looking at the relativistic many-body problem. An analysis of the Dirac equation, based on the Foldy-Wouthuysen transformation, was performed, and pair equations were derived also with electron-positron-pair creation (142 cit.). We did not pursue this line of work, instead Eva Lindroth developed a first version of a pair program based on full four-component Dirac functions (40) (55 cit.). The problem with virtual-pair creation has very recently been taken up in our group (see below). It is interesting to note that our original approach to the relativistic problem by means of the Foldy-Wouthuysen transformation has been frequently used by other groups, mainly chemists, and the paper is one of our most cited ones.

In the late 1980's Sten and Per Öster introduced a new procedure for generating the numerical basis functions, based upon *space discretization*, and new non-relativistic and relativistic (10, 11) (106 cit.) pair programs were constructed. Here, the single-electron Schrödinger and Dirac equations are solved essentially exactly in this space, and the completeness relation is satisfied with extreme precision. This new procedure improved our numerical accuracy considerably. Both programs were tested on the helium atom, treated as closed- as well as open-shell system, and the correlation energies obtained agreed with very accurate calculations of Drake within 1 part in 10^7 [22]. In the closed-shell case it was important to include single excitations (CCSD). The results agreed well with the somewhat less accurate results of Johnson et al. [23].

Sten and Per also performed very accurate (non-relativistic) CCSD calculations of the ionization energies of the Be atom and the affinity of the Li atom (26) (68 cit.). Li^- is a delicate system due to the weak binding of the last electron. The calculation of Sten and Per yielded the correlation energy of the system to more than 99%. These calculation are supposed to be among the most accurate ones available in the literature even today, and they have been used as benchmarks for accurate finite-basis-set calculations [24, 25, 17]. Jankowski and Malinowski state: *...we took advantage of the possibility of comparing our results ... with their extremely accurate counterparts recently calculated by Salomonson and Öster ....*

Sten and Anders Ynnerman performed similar calculations of the ionization energy of the sodium atom, a problem more complicated than it first might seem [26] (41 cit.), and here it turned out necessary to include certain triple excitations to reach reasonable agreement with experiment (CCSD(T)). This work represents the most accurate calculation of this quantity performed. Another delicate problem is the electron affinity of elements of the second group of the periodic table (Ca, Sr), where several conflicting experimental and theoretical results have appeared. Together with Håkan Warston, Sten performed the most accurate calculation at the time [27] (24 cit.).

3.4 Complex rotation

In the early 1990's, shortly before leaving the group for a permanent position in Stockholm, Eva Lindroth made important improvements of the computer programs of Salomonson and Öster by including the method of *complex rotation.* This method was first applied to double excited states of the helium atom [28], and a little later to solving the above-mentioned intruder problem in the excited state of the beryllium atom [29] $\mathrm{e}^{-\mathrm{i}t(\varepsilon_a-\varepsilon_r+\mathrm{i}\gamma)}$. In contrast to other approaches to this problem [30, 31], the method of complex scaling also give the life-time of the auto-ionizing states.

3.5 Other applications

(Incomplete)

In his post-doc. years at Charlottesville 1984-85 Sten applied the numerical technique he and his coworkers had developed in Göteborg to the photoionization process together with Hugh Kelly [32] (49 cit.).

Ann-Marie started during her post.-doc. time in Seattle 1980-81 to work on the parity and time-reversal violation in atomic systems [33, 34] (24 and 32 cit.). Together with Sten she also used the technique to evaluate specific mass shifts (36) (60 cit.).

3.6 The Bloch equation

In 1974 Ingvar modified the original *Bloch equation*, valid for a degenerate model space,

$$[E_0 - H_0]\Omega P = V\Omega P - \Omega V_{\mathrm{eff}} \tag{4}$$

into the commutator form (”*generalized Bloch equation*”)

$$[\Omega, H_0]P = V\Omega P - \Omega V_{\mathrm{eff}} \tag{5}$$

valid also for a *quasi-degenerate* model space (302 cit.). Here, $H = H_0 + V$ and the effective Hamiltonian $H_{\mathrm{eff}} = H_0P + V_{\mathrm{eff}}$. Per-Olov Löwdin sometimes referred to this equation as the *”Bloch-Lindgren equation”* [35]. This form of the Bloch equation yields directly the Rayleigh-Schrödinger perturbation expansion for an arbitrary model space and it leads to the *linked diagram* or *linked-cluster theorem* (LDE), when the model space is complete,

$$[\Omega, H_0]P = \Big(V\Omega P - \Omega V_{\text{eff}}\Big)_{\text{linked}} \tag{6}$$

The LDE theorem, first shown in the 1950's by Brueckner and Goldstone for a single-reference model space, was extended by Brandow to the multi-reference (quasi-degenerate) case in 1967 [36] (978 cit.). Brandow introduced a second perturbation to generate the separation of the model space, leading to a complicated double expansion, and his proof of the LDE is very complex. With the commutator form Eq. (5) the treatment is more transparent. A relation equivalent to the generalized Bloch equation was derived at about the same time by Kvasnička [37]. Although he used diagrammatic representation, the elimination of unlinked diagrams was never demonstrated.

The equation (5) is nowadays often expressed in one of the equivalent compact forms

$$H\Omega P = \Omega H_{\text{eff}} \qquad \text{or} \qquad H_{\text{eff}} = \Omega^{-1} H\Omega P \tag{7}$$

and all forms are normally referred to as the *"generalized Bloch equation"*. It is now the starting point for most open-shell MBPT and coupled-cluster calculations, and it is often used without reference to the original work.

(In spite of the fact that the Bloch equation (5,7) is often used without reference, the 1974 paper is our third most cited paper (302 cit.). Most citations are from Mukherjee et al., Kolkata (33), Göteborg (25), Torun (Meissner, Jankowski) (17), Bratislava (Kvasnička, Hubač) (17), Toulouse (Malrieu et al.) (12), Chicago (Freed, Chauhuri) (12), Finley (New Mexico, Tokyo, Lund etc) (12). The technique with extended model space has not been generally recognized, however. As late as 1994—20 years after the appearance of the Bloch equation (5)—in their relativistic calculation on the $1s2p$ state of He-like ions, the Notre-Dame group (Walter Johnson, Sapirstein) used a single reference with the consequence that they had great convergence problems for low Z, due to the close degeneracy [38]. In a comment to their paper we showed that the convergence problem was easily remedied by using the extended model space and the generalized Bloch equation [39].)

3.7 Open-shell coupled-cluster models

Several attempts have been made to solve the open-shell coupled-cluster problem, and the first results appeared in the late 1970's.

There are essentially two approaches to the general, quasi-degenerate multi-reference open-shell CC, the *valence-universal (VU) or Fock-space approach*, and the *state-universal (SU) or Hilbert-space approach.* In VU the same wave or cluster operator is used for all valence sectors (all stages of valence ionization), while in SU only a single valence sector with a fixed number of valence electrons is considered. Both approaches normally employ a *multi-reference* (MR) model space.

In 1976-78 Offermann et al. [40, 41] presented a coupled-cluster formalism for a single open shell (degenerate model space), while the first proposal to handle the full MR CC was made by in 1977 Mukherjee et al. [42, 43]. (An earlier version turned out not to be entirely correct.) They introduced a double cluster expansion

$$\Psi_k = \exp(T_c)\exp(T_v)\Psi_k^0 \tag{8}$$

where T_c is the cluster operator for the core and T_v for the valence.

In 1978 Ingvar proposed at the Sanibel meeting the *normal-ordered form* of the exponential Ansatz

$$\Omega = \{\mathrm{e}^S\} \tag{9}$$

The normal ordering avoids the unwanted contractions between cluster operators, which appear in other open-shell approaches. (Related ideas were presented at about the same time by Ey [41].) This form of the wave operator leads to a Bloch-type of equation for the cluster operator, and it can be shown that all diagrams are *connected* for a complete model space

$$[S,H_0]P=\Big(V\Omega P-\Omega V_{\rm eff}\Big)_{\rm conn} \tag{10}$$

in close analogy with the wave-operator equation for standard MBPT Eq. (5). For us with our background in many-body theory, working entirely with normal-ordered operators, the normal-ordered exponential Ansatz was quite natural. Nevertheless, it took quite some time before the approach was generally accepted, and initially it was even heavily criticized (see below). (The 1978 paper is our second most cited paper with 437 citations.)

In 1980 Kvasnička extended the normal-ordered approach, Eq. (9), to a hermitian formulation [44]. In 1984 Mukherjee et al. [45] analysed the size-consistency of an open-shell energy functional, based upon the normal-ordered approach. In 1985 Haque and Kaldor [46] reported on open-shell CCD calculations also using normal-ordering. In the same year they also reported on open-shell calculations with first-order singles and some triple excitations [47].

Our work as well as most of Mukherjee et al. are of VU type. Also the works of Stolarczyk and Monkhorst [48] in the second half of the 1980's are of VU type, although without normal ordering.

The work of Jeziorski and Monkhorst in 1981 [49] (390 cit.) and of Jeziorski and Paldus in 1989 [50] are of SU type, and here a specific cluster operator is used for each reference state, leading to a large number of cluster parameters.

There is also a third approach to the open-shell CC, advocated particularly by Li and Paldus and first introduced in 1978 [51, 52]. This is known as the *state-selective or state-specific approach* (SS). Here, a relation of the type

$$\Psi_k=S_k\exp(T_c)\Psi_k^0 \tag{11}$$

is used, where the cluster component for the core (T_c) is kept frozen and the valence part is given by the non-cluster operator S_k. One reference state at a time is considered. This approach does not work well, if there is a strong interaction between the reference states.

Bartlett et al. have in a series of papers developed a procedure for open-shell systems, using a single reference function of restricted or unrestricted open-shell HF basis functions [53].

Very recently, Mukherjee has shown that certain valence-shell contractions are actually desired, particularly when valence holes are involved [54]. He then introduced a modified normal ordering

$$\Omega=\{\{\exp(S)\}\} \tag{12}$$

where contractions involving passive (spectator) valence lines are reintroduced compared to the original normal ordering Eq. (9).

A major problem with the multi-reference open-shell coupled cluster approach for a complete model space is that the above-mentioned "*intruder states*" often destroy the convergence. This problem is particularly severe when the approach is treated perturbatively. In a non-perturbative approach it can be avoided [30, 55]. Several specific methods have also been developed to avoid or reduce this problem. The *intermediate-effective-Hamiltonian approach* was developed by the Toulouse group (Malrieu, Durand et al.) in the mid 1980's [56]. Here only a limited number of roots of the secular equation are being looked for. Another approach, developed at about the same time by Mukherjee [57] is to work with an *incomplete model space*. In a comprehensive Physics Report Ingvar and Mukherjee analyzed in 1987 the connectivity criteria for the normal-ordered coupled-cluster expansion for arbitrary incomplete model spaces. (This paper is our fourth most cited work with 244 citations.) The intruder problem is avoided in the state-specific (SS) approach, but here other problems appear instead. As mentioned previously, Eva Lindtoth and Ann-Marie were able to solve the problem by means of complex rotation [29].

(The 1978 paper on the normal-ordered Ansatz is our second most cited article (437 cit.)—a few years ago this paper had only one single citation registered on the Web of Science, the reason being that the journal where it was published, International Journal of Quantum Chemistry, was only sporadically included in the search. This has evidently recently been changed. Now, out of about 475 papers found on the Web of Science on the subjects ”*open-shell coupled cluster*” or ”*multi-reference coupled cluster*” our paper is the third most cited. Most citations are from Torun (53), Mukherjee et al. (43), Bartlett et al. (40), Paldus et al. (37), Tel Aviv (Kaldor et al.) (33), Göteborg (26), other Indian groups (21), Bratislava (Kvasnička, Hubač) (17), Nooijen (Florida, Princeton, Waterloo) (14).)

3.8 Comments on open-shell coupled-cluster approaches

There are strongly different opinions expressed in the literature about the best way to proceed with open-shell CC, and we shall comment on a few of them.

Our normal-ordered coupled-cluster approach, Eq. (9), was at first strongly criticized by Jeziorski and Monkhorst in 1981 [49]. They claimed that our cluster amplitudes are not uniquely defined and that the *”development of the theory relies heavily on somewhat vague, graphical arguments”*. Later, in a paper from 1989 Jeziorski and Paldus [50] express quite a different opinion (to say the least!). There it is stated that the *”introduction of the normal ordered exponential ansatz represented an important advantage in existing CC formalism to open shells”* and *”using purely diagrammatic arguments, Lindgren obtained correct working equations for the valence-universal amplitudes* $S^{\alpha\beta\cdot\cdot}_{\rho\sigma\cdot\cdot}$. *His 1978 paper may be viewed as a good illustration to the t'Hooft and Veltman 'principle' that 'the diagrams contain more information than the underlying formalism'”*.

In another paper from 1992 Jankowski, Paldus et al. [58] devote an entire section to comparing their algebraic equations with our diagrammatic procedure. Actually, we do not understand why people felt that they had to do this kind of analysis. If you are acquainted with the diagrammatic representation, it is trivial to transform the diagrams to algebraic form, and furthermore, complete algebraic equations are found in the Lindgren-Morrison book as well as in most of our CC papers.

In a paper from 1984 Haque and Mukherjee [59] conclude that *”One attractive feature of the [normal-ordered] development is its direct correspondence with the open-shell perturbation theory of Brandow and Lindgren, a feature not shared by Refs [42, 43] and [51].”* Concerning the SS approach, Eq. (11), it is stated that *”the non-cluster nature of* S_k *(which is not an exponential type of operator) will tend to make theory progressively unsuitable for states with very many valence occupancies”*.

Li and Paldus express in later papers [52] criticism about both the valence-universal (VU) and the state-universal (SU) approaches. They emphasize that for methods based on the effective Hamiltonian formalism and generalized Bloch equation and *”relying on the valence universal or state universal cluster Ansatz”*, the implementation is very demanding and *”often plagued with intruder state and multiple solution problems”*. Instead they claim that the SS approach is free from intruder problems and simpler to employ.

Quite a different opinion was expressed by Nooijen and Bartlett in two papers from 1996 [60, 61]. They are critical to the approach of Li and Paldus, who start from a non-normal-ordered similarity transformation. Due to the fact that the open-shell cluster operators do not generally commute, they find that *”the apparent simplicity of their approach is misleading”*, and they *”doubt that this scheme will lead to a widely applicable computational scheme”*. They are also critical to the approach of Stolarczyk and Monkhorst [48], who use the same transformation, and claim that the use of non-commuting operators *”would render the formalism very cumbersome in practical application. The logical step is to replace the exponential form of the similarity transform by the normal ordered exponential* $\{\mathrm{e}^T\}$*, as introduced by Lindgren”*.

Figure 3: Five Nobel laureates at ICAP 8 in Göteborg 1982. From left: Art Schawlow (1981), Kai Siegbahn (1981), Alexandr Prokhorov (1964), Isaak Rabi (1944), and Nicolas Bloembergen (1981) (GP Foto).

4 Later work

4.1 QED calculations

In the 1990's we started quantum-electrodynamical (QED) calculations on atomic systems together with the graduate students Hans Persson and Per Sunnergren. These calculations were performed by means of the S-matrix technique [62] and applied to highly charged ions. At that time accurate experimental results were appearing from various accelerator laboratories, at Berkeley, Livermore and GSI in Darmstadt. The first calculation we performed was of the Lamb shift of Li-like uranium (34) (61 cit.), where accurate result had been obtained from Berkeley [63]. We found good agreement with the experimental result, which was one of the first confirmations of the validity of QED at very strong field. Similar, but less complete results were at the same time obtained by the Notre-Dame group [64]. We also performed accurate calculations of the g-factor of hydrogenic ions, results that later were experimentally confirmed to 9 digits— of which 3 do represent QED effect (36, 27) (61 and 66 cit.). These calculations have later been further refined by the Russian group (Shabaev, Yerokhin) together with Thomas Beier (who was post.doc. in our group for two years), and this has led to an improved value of the electron mass [65]. We also performed a complete two-photon analysis of He-like ions, using Feynman as well as Coulomb gauges (11) (106 cit.), calculated the two-electron Lamb shift of highly charged He-like ions (28) (66 cit.) and QED effects of the hyperfine structure of hydrogen-like ions (33) (62 cit.).

For the renomalization procedure we developed the simple *partial-wave normalization procedure* (25) (68 cit.). In this procedure the normalization was performed separately for each partial wave, which had the advantage that no singularities appear. This works well in low order, but we have shown that the procedure is not completely exact in higher orders [66]. In later works we applied the more correct *dimensional regularization.*

A problem with the S-matrix formulation is that it is not applicable to the quasi-degenerate situation with closely spaced unperturbed states, such as the fine-structure separations. For standard many-body calculations we had for a long tome been able to handle this situation by means to the generalized Bloch equation Eq. (5). At the turn of the century we were able to develop a new procedure, which had this property also for QED calculations. This is referred to as the *"covariant-evolution-operator method"*. Our graduate student, Björn

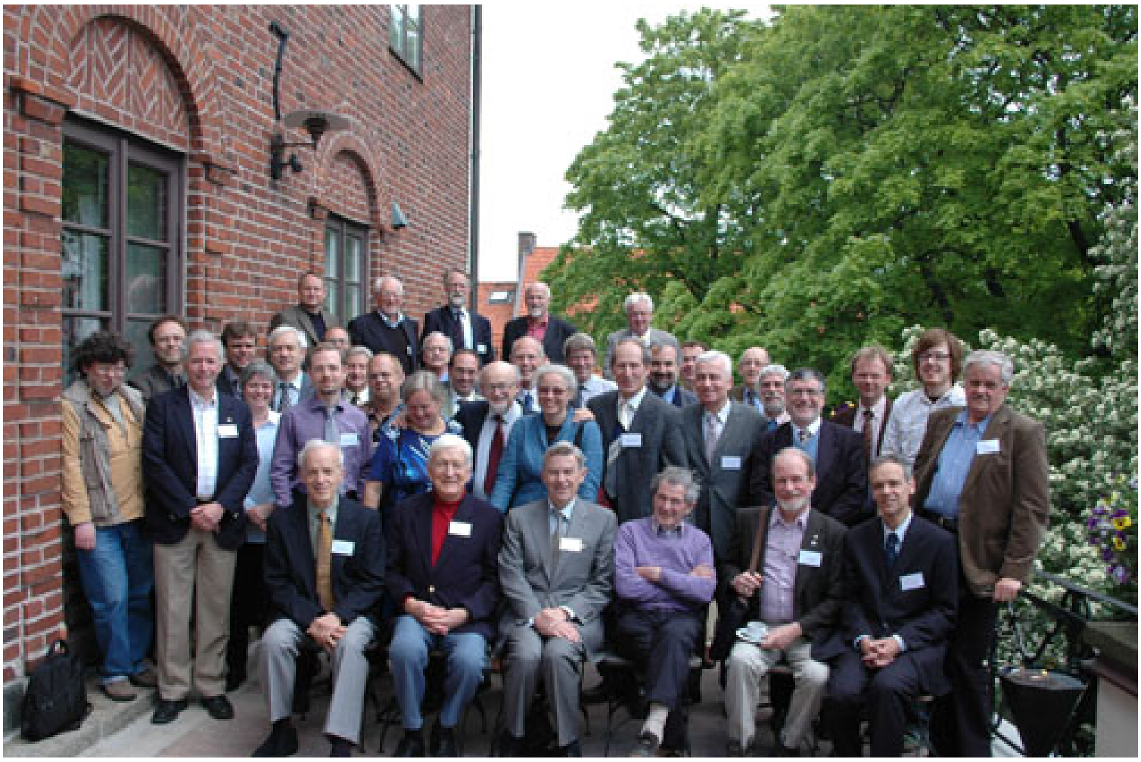

Figure 4: Conference arranged in Göteborg in connection with Ingvar's 75:th birthday in 2006.

Åsén, applied this new technique to the fine structure of some light He-like ions [67]. A comprehensive report on the method has appeared in Physics Reports [68]. Our calculations represented the first QED calculation of the fine-structure. These calculations have later been extended by Shabaev et al., using their two-times Green's-function technique, which is the only other technique available for this kind of work [69].

Our QED calculations have been reported at numerous conferences on highly charged ions, starting with the Nobel Symposium in Sweden 1992 (see below).

For a number of years we participated in an European project *Eurotrap* together with groups in Germany and France, which gave us good possibility to the exchange of ideas with these groups as well as the exchange of graduate students and post.docs. Presently, we have joined the SPARC collaboration, which coordinates the heavy-ion research in Europe.

4.2 Combining MBPT and QED

The covariant-evolution-operator technique has—in contrast to other available techniques for QED calculations—a structure that is quite similar to that of standard many-body perturbation theory (MBPT). Therefore, this technique has the potential for combining QED with MBPT, a combination that for a long time has been looked for. Together with our graduate student Daniel Hedendahl, we are presently constructing and testing such an approach. The work performed so far is described in two recent publications [70, 71] and reported at several conferences.

The standard techniques for QED calculations can presently handle the exchange of maximum two photons. For highly charged ions this is normally quite sufficient, but in many other cases the electron correlation plays a more important role so that two photons are not sufficient. With our new technique it is possible to combine QED effects with an arbitrary number of instantaneous Coulomb interactions.

Principally, the procedure leads to a strictly covariant form of relativistic MBPT and CCA, and is has been demonstrated that it ultimately leads for two-particle systems to the Bethe-Salpeter equation [72, 73], thereby verifying the relativistic covariance of the procedure. The numerical evaluation follows closely the technique used in our previous works, the main difference being that the retarded, time-dependent interactions are handled by separating them into two single-particle interactions, following an idea of Sten. Treating each of them as a separate perturbation, the standard many-body rules can be used.

The calculations are very time consuming and so far only limited numerical results have appeared. The results obtained do show, though, that the combination of low-order QED and electron correlation is quite significant for a system like He-like neon. This kind of result has never appeared before. Presently, we are working with the inclusion of the effects of virtual pairs (positron creation) as well as of radiative effects (self energy, vacuum polarization etc.) This kind of effects will probably not for a long time be of interest to quantum chemists. On the other hand, these works will probably be of more interest to the physics community (highly-charged-ion research). Fritzsche, Indelicato and Stöhlker have in a recent review [74] stated that *"At present, interplay between QED and the many-body effects constitutes the greatest challenge posed to the accurate theoretical evaluation of transition energies in the field of highly charged ions"*.

4.3 Density-Functional Theory

In recent years we (Sten and Ingvar) have also done some work on *density-functional theory* (DFT). We have mainly been interested in fundamental problems (differentiability etc.) and have not performed any real calculations. DFT is now frequently used by (quantum) chemists, and the theory rests on a firm ground, particularly after the works of Levy [75] and Lieb [76] and of English and English [77, 78]. According to these works the Kohn-Sham (KS) potential is a *local* potential, known as the *locality theorem*. This theorem has recently been questioned, particularly by Nesbet. In a paper from 1998 [79] he claims that the KS potential is generally *orbital dependent* and hence cannot be a strictly local potential that depends only on the space coordinates. Nesbet's ideas have been challenged by several authors, Holas and March [80] and Gál [81]. We have also commented upon this and shown that Nesbet's conclusion is incorrect [82]. In his argument he uses expressions for the kinetic energy and the density that are not correct outside the normalized regime where he works. With correct expressions in the entire region we showed that the potential is in fact *orbital independent* and therefore strictly local. Nesbet has in a series of papers persistently argued that our results are incorrect, since they disagree with his—in our opinion incorrect—result from 1998. No counterarguments are given. We have in two more papers [83, 84] analysed this matter in greater detail. In the DFT community it is now generally agreed that that the locality theorem is rigorous.

With the help of an undergraduate student, Fredrik Möller, we have also shown that the theorem, saying that the Kohn-Sham orbital eigenvalue of the highest occupied orbital (HOMO) equals the ionization energy, is valid to at least some 8-9 digits [85, 86]. Some leading scientists in the field claim that this theorem is not very accurate, but the point is that one needs a very good potential to reach high accuracy—standard approximations are not sufficient. We constructed an accurate KS potential for the ground and first excited states of the helium atom from the electron density obtained with our coupled-cluster program and compared the resulting KS eigenvalue with our many-body ionization energy. The results agreed within the numerical accuracy. As far as we know, our result is several orders of magnitude more accurate than any earlier or later demonstration of this theorem for any system, but our publications have so far remained essentially unnoticed by the DFT community. This numerical calculation also verifies the above-mentioned locality theorem to very high degree.

In 1993 Ingvar received a research award from the Alexander-von-Humboldt Stiftung in Germany with the possibility of spending a full year at German universities. Ingvar utilized this award during the years 1999-2002 with stays primarily at the universities of Frankfurt and Erlangen, particularly learning about DFT.

5 Other activities

5.1 Books

5.1.1 Atomfysik

In the 1960's Ingvar wrote an intermediate-level book in Swedish on Atomic Physics, *Atomfysik*, which could be regarded as a modernized version of the classical book by Condon and Shortley [87]. Later the book was augmented with an experimental part by Sune Svanberg [88]. This was used for many years as textbook for senior undergraduate and junior graduate students. This then formed the basis for a more extensive monograph by Svanberg on *Atomic and Molecular Spectroscopy* [89].

5.1.2 Atomic Many-Body theory

In 1982 the first edition of the book by Ingvar and John Morrison on *"Atomic Many-Body Perturbation Theory"* appeared. This represents a comprehensive account of perturbation theory, with particularly atomic systems in mind. This gives a fairly extensive background to the field and summarizes the developments made in our group during the 1970's. The presentation is heavily based upon graphical technique, angular-momentum graphs and Goldstone-Brandow perturbation diagrams. When it appeared, the book was quite up-to-date with linked-diagram representation of quasi-degenerate perturbation theory, based on the generalized Bloch equation (Eq.5), and the open-shell coupled-cluster theory, based upon the normal-ordered approach (Eq.9). Complete algebraic equations for CCSD are given for a multi-reference model space. The second edition in 1986 got a wider distribution, and the book is still to a large extent considered as the standard work in the field. The two editions have received 750 citations and represent our most cited work. Unfortunately, Springer Verlag stopped keeping the book in stock some years back, but the book will soon be available on the internet.

5.2 Conferences

In 1979 we arranged together with Stig Lundquist in Göteborg a Nobel Symposium at Lerum outside Göteborg on *Many-Body Effects in Atoms and Solids*, where many of the first coupled-cluster calculations from various groups were reported [16].

In 1992 we arranged together with experimental groups in Stockholm and Lund a Nobel Symposium on *Heavy ions spectroscopy and QED effects in atomic systems* at Saltsjöbaden, outside Stockholm, where many early experimental and theoretical results on highly-charged ions were reported [90].

In 1982 we arranged in Göteborg the general atomic-physics conference ICAP 8—*Eights International Conference on Atomic Physics*—with some 400 participants, among them five Nobel laureates [91] (Fig.3).

In connection with Ingvar's retirement in 1996 an international conference *Modern Trends in Atomic Physics* was arranged by the Göteborg group at Hindås outside Göteborg [92], and in connection with his 75:th birthday in 2006 a second conference *Current Trends in Atomic Physics* was arranged in Göteborg [93] (See Figs 4 and 5).

6 Concluding remarks

In this account we have described the development and some achievements of our atomic-theory group in Göteborg and how our works have been received by the scientific community. One measure of the latter is the number of citations as registered on the *Web of Science*. Generally, we find that our works are well received, and that many old papers, even those published in European journals, are quite frequently cited. Even if papers in journals publish by AIP (Phys. Rev., Phys. Rev Lett., J. Chem. Phys. etc.) are still favoured, due to the dominating role these journals have, we find that the situation is not as unbalanced as it was some time ago. Presently, essentially all scientific journals—with some important exceptions[2]—are available electronically and most of them seem to be scanned for citations. Nevertheless, the citation index should still be handle with great care.

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Figure 5: Norman Ramsey, Dan Kleppner and Eleanor Campbell (top left), Ann-Marie and Joe Sucher (top right), Sten and Norman Ramsey (bottom left), and Ingvar talking to some participants, in the front Peter Mohr and Dan Kleppner (bottom right) at the Göteborg symposium 2006. (Foto:IL and AP)