THE TRANSITION FROM MATHEMATICIAN TO ASTROPHYSICIST

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Various landmarks in the evolution of Alexander Dalgarno from a gifted mathematician to becoming the acknowledged Father of Molecular Astrophysics are noted. His researches in basic atomic and molecular physics, aeronomy (the study of the upper atmosphere) and astrophysics are highlighted.

Keywords: atomic and molecular physics, aeronomy, astrophysics, Dalgarno-Lewis method, associative detachment, rotational excitation.

1. Some Distinct Landmarks

As this "Dalgarno Celebratory Symposium" in honor of Alex Dalgarno's 80^{th} birthday continues, I would like to welcome you all to this morning's session "*Calculation of Atomic and Molecular Properties*". This title is particularly well suited to Alex's philosophy because, in a recent reminiscence[1] of his career, he mentions that, " ... It is often said, by theorists, that physics is embodied in its equations, but I think it is to be found in the solutions to the equations". And so, emboldened/accelerated by this realization, Alex embarked on making landmark advances in all of the following subjects:

(1) Atomic and Molecular Structure (perturbation variational and expansion methods)
(2) Interactions (polarization, dispersion, model, pseudo and long-range potentials) and
(3) Collisions (near-resonant electronic transfer, excitation and charge transfer radiative transitions, rotational and vibrational excitation in molecules, spin-exchange).

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to be covered today by this title. Those advances began with hard work in the 1950's and still continue today,[2] particularly in relation to ultracold gases.[3]

1.1. *The Dalgarno-Lewis Method*

I first met Alex when I entered Queen's University, Belfast as an undergraduate in 1958. In my second year, Alex taught me Classical Mechanics out of Goldstein's book[4] and, in my third (honours) year, David Bates taught me Quantum Mechanics and Scattering Theory, using his notes later published.[5] Even by that time–from when he accepted Bates's invitation to become a faculty member at Queen's in 1951– Alex had already made many valuable contributions to the subjects I have enumerated above in Sect. 1. One that I particularly liked was the Dalgarno-Lewis method[6] developed for "The exact calculation of long-range forces between atoms by perturbation theory". It provides an elegant method which enabled exact results to be obtained for various orders in perturbation theory, and which replaced the infinite sums that arise in each order by the solution of differential equations. Its popularity became further enhanced by its detailed inclusion in the book "*Quantum Mechanics*" by Leonard Schiff[7] and it is still being used today.

1.2. *Associative Detachment*

Also during that year (1958), Alex pointed out that it was the process of associative detachment

$$H^- + H \rightarrow H_2 + e^- \qquad (1)$$

that controlled the ionization balance in the solar atmosphere and he gave a verbal estimate of its relatively rapid rate ($3 \times 10^{-10} cm^3 s^{-1}$), later quoted by Pagel.[8] His suggestion led to a new picture of the solar atmosphere. Alex commented that associative detachment (1) is a source of H_2. Others later recognized that (1) is the major source of H_2 in the early universe. Alex's recognition that associative detachment would ordinarily be a fast reaction[9] also led to a new picture of the D-region of the terrestrial ionosphere. After Alex's suggestion, the associative detachment reaction has been included in all discussions of weakly ionized plasmas, laboratory as well as astrophysical.

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1.3. *The Arthurs-Dalgarno Method*

Molecular hydrogen, H_2, is the most abundant molecule in the Universe and, because of Alex's studies of its properties, H_2 has become a potent diagnostic probe. Recognizing the need from his work on diffuse interstellar clouds, Alex then embarked on extensive investigations of the radiative and collisional properties of H_2. They involved the formulation of quantum-mechanical scattering theory for rotational excitation by Arthurs and Dalgarno[10] and the development of numerical procedures to solve the resulting close- coupling equations. Allison and Dalgarno[11] reported the first solutions of close-coupled equations for rotational excitation and gave results for rotational excitation of H_2 in collision with H, He and H_2. It initiated an industry of such calculations by chemical physicists which continues today. Indeed, Alex is still involved, with calculations of rotational-vibrational molecular collisional transitions at ultralow temperatures,[12] exploring the Wigner regime.

1.4. *The Founding of Molecular Astrophysics*

Key to the founding of Molecular Astrophysics were Alex's studies of the radiative properties of molecular hydrogen beginning with the determination of the oscillator strengths and transition probabilities of the Lyman and Werner systems[13] which were essential elements in the interpretation of the observational data expected from the ultraviolet spectrometer on the Copernicus satellite.

2. The Modus Operandi

The four examples above perhaps serve to illustrate some of the hallmarks of Alex's successful *modus operandi*, which, if possible, may be summarized as follows:

(a) Identify the great variety of atomic and molecular quantum processes of significance to the physics and chemistry of the environment under consideration.
(b) Perform calculations to understand the reaction mechanisms and determine the rate coefficients either from existing theory or from theoretical methods he would invent for their study. Often this involved extending quantum mechanical theory for application to a diverse range of processes that operate in astrophysical environments where conditions are extreme.

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(c) Construct models of the particular environment, and then,
(d) Conduct rigorous investigations.

The wide array of applications has included:

(1) Early Universe
(2) Planetary and Stellar Atmospheres
(3) Interstellar Clouds
(4) Shocked Gases
(5) Photon-dominated regions (PDR's), or photo-dissociation regions, and X-ray dominated regions (XDR's). Responses of molecular material to UV and X-rays and to magneto-hydrodynamic (MHD) shocks
(6) Planetary Nebulae, Planetary Atmospheres and Comets, Supernova ejecta (SN1987A).

3. The Result of the Transition

Alex has made landmark advances and provided major contributions not only to the development and application of Atomic, Molecular and Optical Physics but also to the interpretation of astrophysical phenomena from the early Universe to planetary atmospheres, covered within the array of applications above. His method of construction of models of interstellar clouds, for example, with the close interplay of molecular physics and astrophysics has become part of the fabric of molecular astrophysics. His combination of quantum-mechanical theory and analyses of astrophysical data with the identification of the relevant molecular processes and recognition of their consequences is molecular astrophysics at work. And so the evolution of *Molecular Astrophysics* into a unified discipline of inquiry continues to be dominated by Alex and his students. Sir David Bates (my mentor at Queen's and afterward) and George Victor summed it up quite nicely when they wrote[14] 20 years ago that "There is no greater figure than Alex in the history of Atomic Physics and its applications" Also, 10 years ago, Alex's pioneering contributions to Molecular Astrophysics were acknowledged[15] by describing him as "*The Father of Molecular Astrophysics*".

Alex, now more than ever, has earned these accolades. This three-day Symposium is indeed testament to the fact that Alex's career has essentially embodied three spectacular careers, each in (a) Theoretical Atomic and Molecular Physics, (b) Aeronomy (the study of the upper atmosphere), Planetary Atmospheres and Comets and (c) Astrophysics. Any one of us would consider ourselves most fortunate to be successful in any one of these endeavors and to have, at most, a one-day celebration, as acknowledgment.

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4. The Beginning and End of the Transition

And Alex did all of this without the benefit of any formal undergraduate courses/training in Physics, Chemistry or Astronomy. Alex graduated in 1947 with a degree in Mathematics at University College, London (UCL) and had a fellowship to do whatever he pleased for the year afterward. According to Alex's recent account[1,16] of this time at UCL, he considered further work in geometry, a subject he thoroughly enjoyed, almost, as entertainment. But he thought of geometry more as an intellectual exercise, as he readily solved hypothetical problems and puzzles. Because he wanted to solve real physical problems, he identified Physics as a possible area for him to apply his considerable mathematical skills. He choose an appropriate graduate Physics course for study at UCL. One day, the Department head, then Sir Harrie Massey, happened to meet Alex by chance in the corridor and asked him what he wanted to do after finishing his Physics course. Alex had no idea, until Massey suggested Atomic Physics, a subject Alex, at that time, knew little about. But to Alex, Atomic Physics "sounded different" and "it might be interesting".[16] Massey offered Alex a Fellowship to pursue his Ph.D (with advisor R. A. Buckingham, an expert in interatomic forces). And so, it was this serendipitous encounter with Massey in the corridor of UCL that turned out to be the key event that led Alex from the study of Mathematics to Physics and subsequently, in later years, to Aeronomy, Chemistry, Astronomy and Astrophysics. And David Bates, who was about to leave UCL in 1951 to reinstate the Dept. of Applied Mathematics at Queen's, offered Alex, on completion of his Ph.D, a faculty position at Queen's.

Bates later introduced him to Aeronomy and Planetary Atmospheres. Then, as they say, the rest is history. He occupied his chair at Queen's until 1967 when he accepted the invitation of Leo Goldberg and Fred Whipple to a chaired position at, what is now, the Harvard-Smithsonian Center for Astrophysics. I linked up again with Alex in 1968 at Harvard, ten years after we first met in Belfast and I spent three very productive years there under his wise counsel and tutorship. And so, we are now back to the beginning of my talk. The circle is completed. On reviewing all his monumental advances and contributions to these vast fields, researchers in each of these areas must now be all extremely grateful that Alex easily and successfully made the transition from gifted mathematician to astrophysicist with such astonishing rapidity and spectacular success. I consider Alex's role in molecular astrophysics to be analogous to the roles played by Bethe, Chandrasekhar and Fowler in stellar and nuclear astrophysics. Alex has

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established Molecular Astrophysics as a unified intellectual field of great scientific endeavor, impact and achievement.

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16. Listen to and view Harry Kreisler's Conversation with Alexander Dalgarno at: `http://globetrotter.berkeley.edu/people3/Dalgarno/dalgarno-con0.html`.

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First row, kneeling: Graeme Lister, David Schultz, Vasili Kharchenko, Hossein Sadeghpour. **First row, standing:** John Black, Ionel Simbotin, Evelyne Roueff, Kate Kirby, James Babb, Lisa Bastille, Michael Jamieson, Thomas Rescigno, Bernard Zygelman, Françoise Masnou-Seeuws. **Second row:** Tom Cravens, William Stwalley, Stephen Lepp, Paul Rimmer, Alfred Msezane, Donghui Quan, Amiel Sternberg, Neal Lane, Franco Gianturco, Alex Dalgarno, Deborah Watson, Ray Flannery, Jane Fox, Bidhan Saha, Peter Beiersdorfer, Richard Pratt, Barry Schneider, Ewine van Dishoeck, Bill McCurdy, Verne Jacobs, Stefano Bovino. **Third row:** Ronald Pepino, John Raymond, Derrick Crothers, Jacob Taylor, William McConkey, Jean Turner, Phillip Stancil, Jaan Lepson, Tom Hartquist, Steven Manson, Cecil Laughlin, Shih-I Chu, Guo-Xin Chen, Turgay Uzer, Robert Kurucz, Kelly Chance, Eric Heller, Walter Johnson, Daniel Vrinceanu, Roman Krems. **Fourth row:** Enrico Bodo, unknown, Charles Weatherford, Balakrishnan Naduvalath, Timur Tscherbul, Philippe Pellegrini, Robert Forrey, Gordon Drake, Brian Burrows, Maurice Cohen, Brendan McLaughlin, Tom Gorczyca, Marko Gacesa, Hyun-Kyung Chung, Xi Chu, Peng Zhang.

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