Comments on `The Dalgarno - Lewis method as a perturbation theory' by Nandi *et al* (1996 ***J. Phys. A: Math. Gen.*** **29** 1101) and on `Alternate approach to non-relativistic perturbation theory' by Kim and Sukhatme (1992 ***J. Phys. A: Math. Gen.*** **25** L647)

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COMMENT

Comments on 'The Dalgarno–Lewis method as a perturbation theory' by Nandi *et al* (1996 *J. Phys. A: Math. Gen.* 29 1101) and on 'Alternate approach to non-relativistic perturbation theory' by Kim and Sukhatme (1992 *J. Phys. A: Math. Gen.* 25 L647)

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Abstract. I point out the connection between the above papers and some earlier work appearing in 1984 *Phys. Rev.* A **29** 1034 and in 1979 *Phys. Rev.* A **20** 2245.

In a recent letter in this journal, Nandi *et al* (1996) discussed the Dalgarno–Lewis method of calculating the sum rule as an independent perturbation method. The transformation they use (equation (5) of their paper) is none other than that used in the logarithmic perturbation method (Aharonov and Au 1979). The connection of the logarithmic perturbation method to the Dalgarno–Lewis (1955) method was discussed long ago by Au and Aharonov (1979) (see section 3 of their paper).

It is more convenient to view the generalized Dalgaron–Lewis method as one that involves writing the perturbed wavefunction as a scalar function f times the unperturbed wavefunction. To zeroth order, this scalar function f is of course unity. To first order, one recovers the Dalgarno–Lewis method. A perturbation method involving an expansion on f for the one-dimensional problem was given by Kim and Sukhatme (1992). In the same paper, Kim and Sukhatme also assert that since this method avoids taking the logarithm of the wavefunction, the method is applicable to excited states. This is very much an oversimplified statement. As the perturbation is introduced, the nodes of the wavefunction shift from their unperturbed position. This means that f must contain the needed singularity to cancel the zeros in the unperturbed wavefunction. This fact is indeed demonstrated in equation (29) in the example given by Kim and Sukhatme (1992). Here the singularity appears in the form of the function $\tan 3x$. In a general perturbation problem, such a singular function as a solution may not be easily identifiable. The difficulty associated with the zeros in an excited bound state wavefunction still exists in the method of Kim and Sukhatme. However, as it turns out, the straightforward logarithmic perturbation expansion method can be extended to excited bound states in one dimension. This justification was given by Au *et al* (1991).

In 1984, in an attempt to extend the logarithmic perturbation method to excited bound states in multi-dimensions, I presented a perturbation method (Au 1984) in which the

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bound state wavefunction is written as $F\exp(-G)$. For excited bound states, the nodal information on the wavefunction is all contained in F. As the perturbation is introduced, the wavefunction can respond in both F and G. If we limit the response to G, we recover the logarithmic perturbation method. If we limit the response in F and write its perturbation expansion as $F = \sum \lambda^i F_i$, we have the generalized Dalgarno–Lewis method, which was subsequently discussed by Kim and Sukhatme (1992). In Au (1984), I consider a general perturbation problem of the form

$$H\psi = \left[H_0 + \sum \lambda^i V_i\right]\psi = E\psi \tag{1}$$

with the usual expansion $E = \sum_{i=0}^{\infty} \lambda^i E_i$ and $\psi = \sum_{i=0}^{\infty} \lambda^i \psi_i$. Then in equations (1.19)–(1.25) of Au (1984) I obtain the relation

$$\boldsymbol{\nabla} \cdot [\psi_0^2 \boldsymbol{\nabla}(F_i/F_0)] = \boldsymbol{\nabla} \cdot [\psi_0^2 \boldsymbol{\nabla}(\psi_i/\psi_0)] = 2(V_i^{\text{eff}} - E_i)\psi_0^2 \tag{2}$$

where

$$V_i^{\text{eff}} = V_i + \sum_{j=1}^{i-1} F_j (V_{i-j} - E_{i-j})/F_0 \tag{3}$$

and

$$E_i = \int V_i^{\text{eff}} \psi_0^2 \, \mathrm{d}^3 r. \tag{4}$$

To first order, that is $i = 1$, we recover the Dalgarno–Lewis equation upon identifying the ratio $F_1/F_0 = \psi_1/\psi_0$ as the Dalgarno–Lewis function. It we go beyond $i = 1$, we have the generalized Dalgarno–Lewis method for multi-dimensions. For one-dimensional systems, equation (3) can be trivially integrated twice in quadrature to reproduce all the results of Kim and Sukhatme (1992). Note that in equation (2) while the ration $F_i/F_0 = \psi_1/\psi_0$ is singular at the unperturbed zeros, the solutions to F_i or ψ_i are regular, in contrast to the formulation of Kim and Sukhatme (1992) where the solutions to f_i for the excited states should be singular at the zeros of the unperturbed wavefunction.

Perturbation theory is an extremely useful tool in quantum mechanics. Many authors have contributed to the developments and refinements of this technique. The effort to obtain the perturbative corrections by direct solutions of differential equations was first attempted by Schrödinger (1926), followed by Podolsky (1928) and Sternheimer (1951), Dalgarno and Lewis (1955) and Schwartz (1959). The logarithmic perturbation method can be first attributed to Wentzel (1926) and later Price (1954), Polikanov (1967), Aharonov and Au (1979) and Turbiner (1980). I am sure that many authors have been unintentionally left out of this partial list.

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