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The Dalgarno–Lewis method as a perturbation theory

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Abstract. The Dalgarno–Lewis summation technique as used in the Rayleigh–Schrödinger perturbation theory is examined. It is shown that this technique forms an independent perturbation theory and can be used to deal with both bound- and continuum-state problems with some added advantage over other such approaches.

Many quantum mechanical problems are characterized by Hamiltonians (H) for which it is difficult to solve the corresponding eigenvalue problem exactly. Fortunately, there exist physical situations where the unsolvable Hamiltonian differs only slightly from the Hamiltonian (H_0) for a problem that can be solved rigorously. The small difference λH_1 between H and H_0 is referred to as a perturbation and the so-called perturbation theory provides useful techniques for constructing the eigenspectrum and/or the eigenfunction of the full Hamiltonian H by using the knowledge of corresponding quantities for H_0 and exploiting the smallness of λH_1.

The Rayleigh–Schrödinger (RS) expansion in the coupling constant λ represents the standard approach to dealing with bound-state problems of non-relativistic quantum mechanics. One typical difficulty associated with this method lies in the infinite sums that arise in all but first order, there being one in second order, two in third order and so on. In particular, higher order corrections to the energy eigenvalues involve summation over all possible eigenfunctions, which often cannot be performed explicitly even for simple situations. As opposed to this, there exists another form of the perturbation theory in which the energy corrections (ΔE) to any order are recast in an alternative simpler form such that only knowledge of the unperturbed initial state is sufficient to compute values for ΔE. This is the so-called logarithmic perturbation theory (LPT) [1] constructed for the Riccati form of the radial Schrödinger equation. Being free from summation over all unperturbed states, the LPT appears to be considerably easier to use. However, Dalgarno and Lewis [2] introduced a technique (DLT) to get around the summation problem of Rayleigh–Schrödinger perturbation theory (RSPT) raising the latter to the status of the LPT.

Traditionally, perturbation theory is developed with special reference to discrete eigenvalues. The assumption of a discrete spectrum is, in fact, unnecessary. The energy-level shift in the continuum part of the spectrun is not an observable. Thus perturbation theory for the continuous eigenvalue problem is developed for the eigenfunctions only and the well known Lippmann–Schwinger equation [3] represents the continuum version of the RS problem. Recently Au *et al* [4] have sought an analytic continuation of the bound-state LPT to calculate scattering phase shifts. This is a hierarchical approach in which the

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phase shift is expressed, order by order, as a quadrature involving known solutions of the unperturbed problem. A novel feature of the scheme is that at every stage of iteration, the phase shift is forced to be real such that the formalism is manifestly unitary.

From the above, one finds that the summation technique of DL is a mere supplement to the RS perturbation theory. One of our objectives in this work is to demonstrate that the physical implication of the DLT is more deep rooted than this. In fact, we find that the DLT forms an independent perturbation scheme by itself, with certain distinct advantages over RSPT and LPT. We also derive the corresponding continuum-state perturbation theory and examine its usefulness, particularly considering the background of the work by Au *et al* [4].

Consider the Schrödinger equation

$$H\psi(x) = E\psi(x) \tag{1}$$

with

$$H = H_0 + \lambda H_1. \tag{2}$$

As already noted, H_0 forms a simpler Hamiltonian, of which we know the spectrum, and λH_1 is a small perturbation to H_0. We are interested in generating the eigenvalues and eigenstates of H by using time-independent perturbation theory. In traditional RSPT the wavefunction and the energy eigenvalue of (1) are expanded as

$$\psi(x) = \psi^{(0)}(x) + \lambda\psi^{(1)}(x) + \lambda^2\psi^{(2)}(x) + \cdots \tag{3}$$

and

$$E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots \tag{4}$$

where $\psi^{(0)}(x)$ and $E^{(0)}$ stand for the eigenstates and eigenvalues of H_0 while $\psi^{(i)}(x)$ and $E^{(i)}$ are the ith-order corrections over $\psi^{(0)}(x)$ and $E^{(0)}$, respectively. Equations (1)–(4) provide a basis to compute the corrections, $\psi^{(i)}(x)$ and $E^{(i)}$.

In the LPT, the expansion of the energy eigenvalue remains the same as in (4). However, the wavefunction is chosen as

$$\psi(x) = \mathrm{e}^{S(x)} \tag{5}$$

with the perturbation expansion

$$S'(x) = W^{(0)}(x) + \lambda W^{(1)}(x) + \lambda^2 W^{(2)}(x) + \cdots. \tag{6}$$

The transformation (5) converts (1) to a Riccati equation for $S'(x)$ and it is clear from (6) that the perturbation expansion is sought for the logarithmic derivative of the wavefunction. In this approach the Riccati equation in conjunction with (6) yields the results for corrections to $\psi(x)$ and E.

In equation (6) the quantity $S'(x)$ represents the logarithmic derivative of the wavefunction $\psi(x)$. Interestingly, the vocabulary of supersymmetric quantum mechanics [5] can be used to give a simple physical interpretation for each term in the expansion of $S'(x)$. For example, if we restrict ourselves to the perturbation correction for the ground state of H_0, the first term of the expansion in (6), namely $W^{(0)}(x)$, will refer to the so-called 'superpotential' that plays a role in the supersymmetric realization of the Schrödinger factorization method [6]. Admittedly, the quantities $W^{(i)}(x)$ stand for the correction to $W^{(0)}(x)$ due to the perturbing potential. On a very general ground one knows that the wavefunction $\psi(x)$ is a complex quantity. Thus $S(x)$ in (5) will be complex. It is tempting to associate $\mathrm{Im}\, S(x)$ with the classical action often used to speculate on the form of the wavefunction for which the Hamilton–Jaccobi equation represents a short wavelength limit [7]. With this physical realization for $S(x)$ and the expansion of $S'(x)$, we look for a

perturbation method based on the expansion of $S(x)$ in a series of λ with coefficients in the sequence of the function $\{S^{(n)}(x)\}$. Thus we write

$$S(x) = S^{(0)}(x) + \lambda S^{(1)}(x) + \lambda^2 S^{(2)}(x) + \cdots. \tag{7}$$

Understandably, the coefficient $S^{(0)}(x)$ in (7) determines the dominant behaviour of $\psi(x)$. As with RSPT and LPT, the expansion of energy E is given in (4). The derivation of a mathematical procedure to obtain $S^{(i)}(x)$ can be facilitated by writing the Schrödinger equation (1) in the form

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + [V_0(x) + \lambda V_1(x)]\psi(x) = E\psi(x) \tag{8}$$

where we have used

$$H_0(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_0(x)$$

and $H_1(x) = V_1(x)$. Obviously, the potential $V_0(x)$ is soluble and $V_1(x)$ is the perturbing potential.

Considering the nth bound state of (8), we write (5) in the form

$$\psi_n(x) = \mathrm{e}^{S_n(x)}. \tag{9}$$

From (8) and (9) we have

$$S_n''(x) + S_n'^2(x) = \frac{2m}{\hbar^2}[V_0(x) + \lambda V_1(x) - E_n]. \tag{10}$$

Using (4) and (7) in (10) and equating the coefficients of equal power of λ on both sides, we obtain the series of equations

$$S_n^{(0)\prime\prime}(x) + S_n^{(0)\prime 2}(x) = \frac{2m}{\hbar^2}[V_0(x) - E_n^{(0}] \tag{11}$$

$$S_n^{(1)\prime\prime}(x) + 2S_n^{(0)\prime}(x)S_n^{(1)\prime}(x) = \frac{2m}{\hbar^2}[V_1(x) - E_n^{(1)}] \tag{12}$$

$$S_n^{(2)\prime\prime}(x) + 2S_n^{(0)\prime}(x)S_n^{(2)\prime}(x) = -\frac{2m}{\hbar^2}E_n^{(2)} - S_n^{(1)\prime 2}(x) \qquad \text{etc.} \tag{13}$$

Equation (11) for the unperturbed system is a nonlinear differential equation while the others, namely (12) and so on, form a set of linear inhomogeneous differential equations. Fortunately, the solution of (11) is known. For example,

$$S_n^{(0)}(x) = \ln \psi_n^{(0)}(x). \tag{14}$$

Given (14), the linear equations can be solved easily.

In order to make contact between (11)–(13) etc and the work of DL, we express $\psi_n(x)$ as

$$\psi_n(x) = \mathrm{e}^{S_n^{(0)}(x)}[1 + \lambda S_n^{(1)}(x) + \lambda^2\{S_n^{(2)}(x) + \tfrac{1}{2}S_n^{(1)^2}\} + \cdots]. \tag{15}$$

Clearly, the first-order correction to the wavefunction in (3) is given by

$$\psi_n^{(1)}(x) = \psi_n^{(0)}(x)S_n^{(1)}(x) \tag{16}$$

which, in the usual RSPT, involves a summation over the discrete set together with an integration over the continuous set of eigenfunctions. In the technique of DL, $\psi_n^{(1)}(x)$ is obtained as the solution of an inhomogeneous differential equation. It is of interest to note that (12) and (16) can be combined to get this equation and we have

$$(H_0 - E_n^{(0)})\psi_n^{(1)}(x) = (E_n^{(1)} - V_1(x))\psi_n^{(0)}(x). \tag{17}$$

Equation (17) has been written for the first-order correction to the wavefunction. The higher order correction terms can also be identified from (15) so as to write equations such as (16) and combine them with the appropriate equations for $S_n^{(i)}(x)$. This will lead to DL-type equations for $\psi_n^{(i)}(x)$. Thus we see that the ingredients of the DL summation technique are embedded in our perturbation theoretic equations. In other words, one would like to assert that the DLT constitutes an independent perturbation scheme.

As with RSPT and LPT, we now proceed to derive a continuum version of the perturbation theory described above. To that end, we introduce the continuum analogue of (11)–(13) etc as

$$S^{(0)\prime\prime}(k,x) + S^{(0)\prime 2}(k,x) = \frac{2m}{\hbar^2}V_0(x) - k^2 \tag{18}$$

$$S^{(1)\prime\prime}(k,x) + 2S^{(0)\prime}(k,x)S^{(1)\prime}(k,x) = \frac{2m}{\hbar^2}V_1(x) \tag{19}$$

$$S^{(2)\prime\prime}(k,x) + 2S^{(0)\prime}(k,x)S^{(2)\prime}(k,x) = -S^{(1)\prime 2}(k,x) \qquad \text{etc} \tag{20}$$

where $k^2 = 2mE/\hbar^2$. As in the bound case we have

$$S^{(0)}(k,x) = \ln \psi^{(0)}(k,x). \tag{21}$$

In the following we propose to work with the Jost boundary condition such that [9]

$$\psi(k,x) = h(k,x)\mathrm{e}^{-\mathrm{i}k\delta(k,x)} \tag{22}$$

with $\delta \sim -x$ and $h \sim 1$ as $x \to \infty$. For the wavefunction in (21) the quantity $k\delta(k,0)$ stands for the scattering phase shift.

Equation (19) can be solved to get

$$S^{(1)}(k) = -\frac{2m}{\hbar^2}\int_0^\infty \frac{\mathrm{d}x}{\psi^{(0)^2}(k,x)}\int_x^\infty V_1(x')\psi^{(0)^2}(k,x')\,\mathrm{d}x'. \tag{23}$$

In writing (21) we have used $S^{(1)\prime}(k,\infty) = S^{(1)}(k,\infty) = 0$ and $S^{(1)}(k,0) = S^{(1)}(k)$ by assuming that the perturbing potential is of finite range. The results in (22) and (23) can now be combined to write the first-order correction to the scattering phase shift $\eta^{(1)}(k)$ $(= k\delta^{(1)}(k,0))$ as

$$\eta^{(1)}(k) \equiv \mathrm{Im}\, S^{(1)}(k) = -\frac{2m}{\hbar^2}\,\mathrm{Im}\left[\int_0^\infty \frac{\mathrm{d}x}{\psi^{(0)^2}(k,x)}\int_x^\infty V_1(x')\psi^{(0)^2}(k,x')\,\mathrm{d}x'\right]. \tag{24}$$

Similarly, beginning from the differential equation (20) one can get the second-order correction to the phase shift in the form

$$\eta^{(2)}(k) \equiv \mathrm{Im}\, S^{(2)}(k) = -\,\mathrm{Im}\left[\int_0^\infty \frac{\mathrm{d}x}{\psi^{(0)^2}(k,x)}\int_x^\infty S^{(1)\prime 2}(k,x')\psi^{(0)^2}(k,x')\,\mathrm{d}x'\right]. \tag{25}$$

The general result for $\eta^{(i)}(k)$ can also be obtained in a similar manner. The results we have presented for the scattering phase shifts are in agreement with those quoted by Au *et al* [4]. For the bound-state case, DLT and LPT have been shown to be equivalent [10] and we have found a similar expected result for the scattering phase shift. As an added advantage over the continuum version of LPT, we demonstrate that our basic equations in (18), (19) etc provide a natural basis to calculate scattering phase shifts without performing the multiple integrals involved in the expressions for $\eta^{(i)}$s. We take $V_0(x) = 0$ and $V_1(x) = -V_0\mathrm{e}^{-x}$. For this case (18) gives

$$S^{(0)}(k,x) = \mathrm{i}kx \tag{26}$$

which, when substituted in (19), leads to the first-order correction to the scattering phase shift as

$$\eta^{(1)}(k) = \frac{2mV_0}{\hbar^2}\frac{2k}{1+4k^2}. \tag{27}$$

Similarly, one can get

$$\eta^{(2)}(k) = -\left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{k(5-4k^2)}{4(1+4k^2)^2(1+k^2)}. \tag{28}$$

Flügge [11] has quoted the results in (27) and (28) calculated by the use of the Born approximation.

We conclude by noting that the technique of Dalgarno and Lewis has always been regarded as a supplement to the RSPT. This is perhaps the reason why the DLT has been less widely used in the past than it has deserved to be. However, with our demonstration that the Dalgarno–Lewis method is an independent perturbation technique to be treated on an equal footing with RSPT and LPT, one would like to emphasize further physical applications of the method developed in this work.

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References

[1] Zel'dovich Ia B 1957 *Sov. Phys.–JETP* **4** 942
Polikanov V S 1967 *Sov. Phys.–JETP* **25** 882
Imbo T and Sukhatme U 1984 *Am. J. Phys.* **52** 140
[2] Dalgarno A and Lewis J T 1955 *Proc. R. Soc.* A **233** 70
[3] Lippmann B A and Schwinger J 1950 *Phys. Rev.* **79** 469
Bohm A 1993 *Quantum Mechanics Foundations and Applications* (New York: Springer)
[4] Au C K, Chow C K, Chu C S, Leung P T and Young K 1992 *Phys. Lett.* **164A** 23
[5] Witten E 1981 *Nucl. Phys.* B **185** 513
[6] Infled L and Hull T E 1951 *Rev. Mod. Phys.* **23** 21
Sukumar C V 1988 *J. Phys. A: Math. Gen.* **21** L455
[7] Goldstein H 1985 *Classical Mechanics* (New Delhi: Addison-Wesley/Norasa)
[8] Schiff L I 1968 *Quantum Mechanics* (New York: McGraw-Hill)
[9] Newton R G 1982 *Scattering Theory of Waves and Particles* (New York: Springer) p 349
[10] Mavromatis H A 1991 *Am. J. Phys.* **59** 738
[11] Flügge S 1974 *Practical Quantum Mechanics* (New York: Springer)