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[9]For some interesting ways to visualize (photographically) the instantaneous center in the motion of a wheel that rolls without slipping, see P. L. Tea, Jr., "On seeing instantaneous centers of velocity," Am. J. Phys. **58**, 495–497 (1990).

[10]See, for example, A. S. Ramsey, *Dynamics, Part I* (Cambridge U.P., Cambridge, England, 1959), 2nd ed., p. 240; Brian H. Chirgwin and Charles Plumpton, *A Course of Mathematics for Engineers and Scientists, Volume 3, Theoretical Mechanics* (Pergamon, New York, 1963), pp. 278–280

[11]Since the body is at any instant undergoing pure rotation around the instantaneous center, the velocity of any point of the body must clearly be perpendicular to the line joining the point to the instantaneous center. If the directions of the (nonparallel) velocities of any two points are known at some instant, the instantaneous center at that instant can be obtained as the intersection of the lines through these points, perpendicular to the velocities.

[12]I am indebted to Prof. Harry Soodak for suggesting this simple proof.

The Dalgarno–Lewis summation technique: Some comments and examples

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The Dalgarno–Lewis technique [A. Dalgarno and J. T. Lewis, "The exact calculation of long-range forces between atoms by perturbation theory," Proc. R. Soc. London Ser. A **233**, 70–74 (1955)] provides an elegant method to obtain exact results for various orders in perturbation theory, while avoiding the infinite sums which arise in each order. In the present paper this technique, which perhaps has not been exploited as much as it could be, is first reviewed with attention to some of its not-so-straightforward details, and then six examples of the method are given using three different one-dimensional bases.

I. INTRODUCTION

For most problems in quantum mechanics, with notable exceptions being the particle in a box, the hydrogen atom, and the harmonic oscillator, one must eventually have recourse to some approximation scheme. One systematic approximation approach involves using standard perturbation theory.[1] The difficulty with this approach, however, lies in the infinite sums that arise in all but first order, there being one in second order, two in third order, etc. If, on the other hand, one takes only a few terms in a particular order, one does not usually feel very comfortable with this truncation since one is then uncertain whether or not one has obtained a good enough approximation to the correct energy, or wave function, to that order. In some cases, one can get around this summation problem by using the Dalgarno–Lewis (DL) approach[2,3] or by the equivalent logarithmic perturbation theory approach (LPT).[4] The present paper concentrates on the Dalgarno–Lewis formalism but the interested reader may also consult Ref. 4, which gives a derivation of the LPT method, applies it to seven examples, and lists previous papers on this method. In the Appendix, it is further shown that the (one-dimensional) second-order LPT ground-state energy expression and the corresponding Dalgarno–Lewis expression are in fact identical. The Dalgarno–Lewis method and the LPT method involve formalisms of roughly equivalent complexity. Thus, though the LPT method does not require obtaining the "Dalgarno–Lewis function" F_n it instead involves solving a nonlinear Ricatti differential equation.

The ingenious and convenient Dalgarno–Lewis technique, which includes all terms in a given order, has been applied to some interesting problems, notably the Stark effect,[5] and in the evaluation of the rotational contribution to the energy of N noninteracting, spinless particles moving in a common deformed, harmonic oscillator potential,[6] and has made its way into some quantum mechanics textbooks.[5,7] It is not, however, an approach most students of quantum mechanics are as comfortable with as they could be. Section II reviews and comments on this technique and on some of its not-so-straightforward details. In Sec. III the formalism is then illustrated in three different one-dimensional bases, namely, those of the infinite square well, the one-dimensional Coulomb potential, and the one-dimensional harmonic oscillator.

II. THE DALGARNO–LEWIS FORMALISM

Given a Hamiltonian that may be decomposed into an "unperturbed" part H_0 and a "perturbation" h, i.e.,

$$H = H_0 + h, \tag{1}$$

the Schrödinger equation one wishes to solve is

$$H\Psi_n = E_n\Psi_n, \tag{2}$$

where it is assumed one knows the solutions of the unperturbed Schrödinger equation,

$$H_0\Phi_n^{(0)} = E_n^{(0)}\Phi_n^{(0)}, \tag{3}$$

and the solution Ψ_n reduces to $\Phi_n^{(0)}$ as the perturbation becomes vanishingly small. In Eq. (3) the solutions $\Phi_n^{(0)}$ are all assumed to be nondegenerate. If this is not the case, the subsequent discussion is restricted to those levels that are nondegenerate and, if it happens that all the excited states are degenerate, the discussion must be restricted to the ground state which is always nondegenerate.[7] Then

$$E_n^{(1)} = \langle n|h|n\rangle, \tag{4}$$

where for any state r, $|r\rangle \equiv \Phi_r^{(0)}$, and $E_n^{(0)}$, $E_n^{(1)}$ are the zeroth- and first-order terms in an expansion

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + E_n^{(3)} + \cdots, \quad (5)$$

where

$$E_n^{(2)} = \sum_{m\neq n} \frac{\langle n|h|m\rangle\langle m|h|n\rangle}{E_n^{(0)} - E_m^{(0)}}, \quad (6)$$

$$E_n^{(3)} = \sum_{m,p\neq n} \frac{\langle n|h|m\rangle\langle m|h|p\rangle\langle p|h|n\rangle}{(E_n^{(0)} - E_m^{(0)})(E_n^{(0)} - E_p^{(0)})} - E_n^{(1)} \sum_{q\neq n} \frac{\langle n|h|q\rangle\langle q|h|n\rangle}{(E_n^{(0)} - E_q^{(0)})^2}. \quad (7)$$

Similarly,

$$\Psi_n = N(\Phi_n^{(0)} + \Phi_n^{(1)} + \cdots), \quad (8)$$

where

$$\Phi_n^{(1)} = \sum_{p\neq n} \frac{|p\rangle\langle p|h|n\rangle}{E_n^{(0)} - E_p^{(0)}}, \quad (9)$$

while for any Hermitian operator O,

$$\langle \Psi_n|O|\Psi_n\rangle = N^2\biggl(\langle n|O|n\rangle + 2\sum_{p\neq n} \frac{\langle n|O|p\rangle\langle p|h|n\rangle}{E_n^{(0)} - E_p^{(0)}} + \sum_{p,p'\neq n} \frac{\langle n|h|p\rangle\langle p|O|p'\rangle\langle p'|h|n\rangle}{(E_n^{(0)} - E_p^{(0)})(E_n^{(0)} - E_{p'}^{(0)})} + \cdots\biggr), \quad (10)$$

where the matrix elements $\langle p'|O|p\rangle$, $\langle p'|h|p\rangle$ have been assumed real and

$$N^2 = \left\{1 + \sum_{p\neq n} \frac{\langle n|h|p\rangle\langle p|h|n\rangle}{(E_n^{(0)} - E_p^{(0)})^2} + \cdots\right\}^{-1}.$$

In the above perturbation theory framework, the basic equation that defines the state-dependent Dalgarno–Lewis operator F_n is a commutator relationship, namely,

$$(F_nH_0 - H_0F_n)\Phi_n^{(0)} = [F_n,H_0]\Phi_n^{(0)} = (h - E_n^{(1)})\Phi_n^{(0)}. \quad (11)$$

From this equation one sees that F_n is uncertain to within a constant C since $[C,H_0] = 0$. Additionally, from Eq. (11), F_n is seen to be dimensionless. Moreover, if H_0 commutes with the parity operator, and h has definite parity, F_n has the same parity as h. The definition of F_n is consistent since, using Eq. (3) and the Hermitivity of H_0, Eq. (11) gives correct results for diagonal matrix elements:

$$\langle n|[F_n,H_0]|n\rangle = \langle n|F_nE_n^{(0)} - E_n^{(0)}F_n|n\rangle = \langle n|h - E_n^{(1)}|n\rangle = 0, \quad (12)$$

while for nondiagonal matrix elements, again using Eq. (3):

$$\langle m|F_n|n\rangle = \langle m|h|n\rangle/(E_n^{(0)} - E_m^{(0)}) \quad (m\neq n). \quad (13)$$

Equation (13) shows why F_n is a useful quantity since, for instance, in terms of F_n one can write

$$E_n^{(2)} = \sum_{m\neq n} \langle n|h|m\rangle\langle m|F_n|n\rangle, \quad (14)$$

i.e., the energy denominator has disappeared enabling one to use closure in Eq. (14), i.e.,

$$\sum_m |m\rangle\langle m| = 1$$

or

$$\sum_m |m\rangle\langle m| + \int dk\,|k\rangle\langle k| = 1, \quad (15)$$

if there are also continuum states in the basis. Hence

$$E_n^{(2)} = \langle n|hF_n|n\rangle - E_n^{(1)}\langle n|F_n|n\rangle, \quad (16)$$

i.e., instead of the, in principle, infinite number of summations in Eq. (6) one need only evaluate at most two integrals $\langle n|hF_n|n\rangle$, $\langle n|F_n|n\rangle$ or only one if $E_n^{(1)}$ is zero for some reason, e.g., parity considerations, as is the case in Examples 1 and 4 of Sec. III.

By similar manipulations one obtains

$$E_n^{(3)} = \langle n|F_nhF_n|n\rangle - 2E_n^{(2)}\langle n|F_n|n\rangle - E_n^{(1)}\langle n|F_n^2|n\rangle \quad (17)$$

and to first order

$$\Psi_n = N(1 + F_n - \langle n|F_n|n\rangle)\Phi_n^{(0)}, \quad (18)$$

with $N = 1$ if one requires "cross normalization," i.e., $\langle n|\Psi_n\rangle = 1$. Alternatively $N = (1 + \Delta F_n^2)^{-1/2}$, where the variance of F_n, $\Delta F_n^2 \equiv \langle n|F_n^2|n\rangle - \langle n|F_n|n\rangle^2$, if the Ψ's are normalized, i.e., if $\langle\Psi_n|\Psi_n\rangle = 1$. Also, assuming O and F commute

$$\langle\Psi_n|O|\Psi_n\rangle = N^2(\langle n|O|n\rangle + 2\langle n|OF_n|n\rangle - 2\langle n|O|n\rangle\langle n|F_n|n\rangle + \langle n|F_nOF_n|n\rangle - 2\langle n|OF_n|n\rangle\langle n|F_n|n\rangle + \langle n|F_n|n\rangle^2\langle n|O|n\rangle + \cdots), \quad (19)$$

where, in this case, since the Ψ's are normalized

$$N = (1 + \Delta F_n^2 + \cdots)^{-1/2}.$$

The central problem is thus to obtain the function F_n.

From the defining commutator relationship, Eq. (11), if h does not involve differential operators, in the one-dimensional case one obtains the differential equation:

$$\Phi_n^{(0)}\frac{d^2F_n}{dx^2} + 2\frac{dF_n}{dx}\frac{d\Phi_n^{(0)}}{dx} = \frac{2m}{\hbar^2}(h - E_n^{(1)})\Phi_n^{(0)} = \frac{1}{\Phi_n^{(0)}}\frac{d}{dx}\left(\Phi_n^{(0)^2}\frac{dF_n}{dx}\right), \quad (20)$$

and, with a little manipulation, this leads to

$$\Phi_n^{(0)}(x)^2\frac{dF_n(x)}{dx}\bigg|_a^x = \frac{2m}{\hbar^2}\int_a^x [h(x) - E_n^{(1)}]\Phi_n^{(0)}(x)^2\,dx.$$

If a is chosen such that $\Phi_n^{(0)}(a)$ is zero, after a further integration one obtains the closed-form expression

$$F_n(x) = \int^x \frac{1}{\Phi_n^{(0)}(x)^2} \times\left(\frac{2m}{\hbar^2}\int_a^x [h(\zeta) - E_n^{(1)}]\Phi_n^{(0)}(\zeta)^2\,d\zeta\right)dx + K, \quad (21)$$

where K is an arbitrary constant.

One notes that in Eq. (21) the integral over $d\zeta$ is a definite integral with ζ varying from a to x while the integral over dx is indefinite. The constant K can be chosen to be zero with no loss of generality because the commutator definition, Eq. (11), leaves F_n undetermined to within an arbitrary constant. The choice of the lower limit a in the ζ integral is, however, more problematic. This is because the choice of a determines the value of an additional variable contribution to F_n, namely,

$$D\int^x \Phi_n^{(0)}(x)^{-2}\,dx,$$

where

$$D=-\frac{2m}{\hbar^2}\int^a [h(\zeta)-E_n^{(1)})\Phi_n^{(0)}(\zeta)^2\,d\zeta.$$

The correct choice for a may, however, be determined by noting that F_n must satisfy Eq. (13) for any $m\neq n$, and that $\Phi_n^{(0)}(a)=0$.

Another way to see why there is this uncertainty is to note that from Eq. (20) dF_n/dx is undetermined to within the variable $D/\Phi_n^{(0)}(x)^2$, since

$$\frac{d}{dx}\left(\Phi_n^{(0)}(x)^2\frac{D}{\Phi_n^{(0)}(x)^2}\right)=0.$$

Thus F_n is undetermined to within

$$D\int^x \Phi_n^{(0)}(x)^{-2}\,dx.$$

This matter is further illustrated in the examples of Sec. III.

An additional interesting fact about F_n is that its definition involves a linear relationship. Thus, for a given H_0 if F_{n1} is the F function for h_1, while F_{n2} is the F function for h_2, then automatically $F_{n1}+F_{n2}$ is the F function for $h=h_1+h_2$. Therefore, complicated systems may sometimes be analyzed with the help of simpler ones. This is illustrated in Example 5 of Sec. III. The reader should not, however, be left with the impression that for all one-dimensional systems Eq. (21) will result in a simple expression that will obviate the need to do sums. In fact, for some systems, the F_n which results from performing this integral is itself only expressible as an infinite sum.

With techniques similar to those illustrated above, it is also possible to get simplified higher-order expressions, e.g., for $E_n^{(4)}$, $E_n^{(5)}$, which do not explicitly involve infinite series. Unfortunately, however, only in the one-dimensional case can a simple integral expression be obtained for F_n and the additional operators that are needed for these higher-order expressions.

III. EXAMPLES

A. Infinite square-well basis

Example 1. Consider a one-dimensional system with Hamiltonian:

$$\begin{aligned}H&=p^2/2m+V(x),\\ V(x)&=\alpha(m^2c^3/\hbar)x\quad(|x|\leqslant\pi/2),\\ &=\infty\quad(|x|>\pi/2),\end{aligned}\tag{22}$$

where α is a dimensionless constant.

The obvious perturbation theory decomposition of this system (which cannot be treated exactly analytically) is

$$\begin{aligned}H&=H_0+h(x),\\ H_0&=p^2/2m+V_1(x),\\ V_1(x)&=0\quad(|x|\leqslant\pi/2),\\ &=\infty\quad(|x|>\pi/2),\\ h(x)&=\alpha(m^2c^3/\hbar)x\quad(|x|\leqslant\pi/2),\\ &=0\quad(|x|>\pi/2).\end{aligned}\tag{23}$$

Here,

$$\Phi_0^{(0)}(x)=\sqrt{2/\pi}\cos x,\quad \Phi_1^{(0)}(x)=\sqrt{2/\pi}\sin 2x,$$

$$\Phi_3^{(0)}(x)=\sqrt{2/\pi}\sin 4x,\quad E_n^{(0)}=(n+1)^2\hbar^2/2m.$$

One immediately obtains

$$E_n^{(1)}=\langle n|\alpha(m^2c^3/\hbar)x|n\rangle=0,\tag{24}$$

since $h(x)$ has odd parity. [Using Eq. (17) one also obtains $E_n^{(3)}=0$, in this case, since h and F_n have the same parity.] Substituting into Eq. (21) for $F_0(x)$,

$$\begin{aligned}F_0(x)&=\frac{2m}{\hbar^2}\frac{\alpha m^2c^3}{\hbar}\int^x\frac{1}{\cos^2 x}\int_a^x(\zeta\cos^2\zeta)d\zeta\,dx\\ &=\alpha\left(\frac{mc}{\hbar}\right)^3\int^x\sec^2 x\left(\frac{\zeta^2}{2}+\frac{1}{4}(2\zeta\sin 2\zeta+\cos 2\zeta)\right)\Big|_a^x dx\\ &=\frac{\alpha}{2}\left(\frac{mc}{\hbar}\right)^3\int^x\left[x^2\sec^2 x+2x\tan x+1-\frac{\sec^2 x}{2}-\sec^2 x\left(a^2+a\sin 2a+\frac{\cos 2a}{2}\right)\right]dx.\end{aligned}\tag{25}$$

Here, the ambiguity mentioned in Sec. II arises as to the correct choice for a. The condition $\Phi_0^{(0)}(a)=0$, however, restricts a to two possible values, namely, $a=\pi/2$ and $a=-\pi/2$. Both these choices result in

$$F_0(x)=\frac{\alpha}{2}\left(\frac{mc}{\hbar}\right)^3\left[\left(x^2-\frac{\pi^2}{4}\right)\tan x+x\right].\tag{26}$$

As mentioned in Sec. II, this ambiguity arises because, for this example, $dF_0(x)/dx$ in Eq. (20) is uncertain to within $D\sec^2 x$, i.e., $F_0(x)$ is uncertain to within the variable $D\tan x$, with D an unknown constant. To verify the choice for a is correct, one notes, for instance, that a condition on F_0 is

$$\begin{aligned}\langle 0|F_0|1\rangle&=\frac{\langle 0|h|1\rangle}{E_0^{(0)}-E_1^{(0)}}=\frac{2^4\alpha m^2c^3/3^2\pi\hbar}{-3\hbar^2/2m}\\ &=(-2^5/3^3\pi)\alpha(mc/\hbar)^3.\end{aligned}\tag{27}$$

Evaluating this expression shows that the choice which yields Eq. (26), namely, $a=\pm\pi/2$, is the correct one. Once one has evaluated this expression one can also immediately display the first term contributing to the second-order energy, namely, from Eq. (6),

$$E_0^{(2)}=\frac{\langle 0|h|1\rangle\langle 1|h|0\rangle}{E_0^{(0)}-E_1^{(0)}}+\cdots$$
$$=-\frac{2^9}{3^5}\frac{\alpha^2m^5c^6}{\hbar^4\pi^2}+\cdots. \quad (28)$$

One may additionally confirm that ($\langle 0|F_0|2\rangle$ being zero from parity considerations),

$$\langle 0|F_0|3\rangle=\frac{\langle 0|h|3\rangle}{E_0^{(0)}-E_3^{(0)}}=\frac{-2^5\alpha m^2c^3/3^25^2\pi\hbar}{-15\hbar^2/2m}. \quad (29)$$

Thus

$$E_0^{(2)}=-\frac{2^9}{1^53^5}\frac{\alpha^2m^5c^6}{\hbar^4\pi^2}-\frac{2^{11}}{3^55^5}\frac{\alpha^2m^5c^6}{\hbar^4\pi^2}-\cdots$$
$$=-(2.1070+0.0027+\cdots)(m^5c^6\alpha^2/\hbar^4\pi^2)$$
$$\sim -2.1097(\alpha^2m^5c^6/\hbar^4\pi^2) \quad (30)$$

versus the exact second-order contribution from Eq. (16):

$$E_0^{(2)}=\frac{2}{\pi}\int_{-\pi/2}^{\pi/2}\frac{\alpha m^2c^3}{\hbar}x\frac{\alpha}{2}\left(\frac{mc}{\hbar}\right)^3\times\left[\left(x^2-\frac{\pi^2}{4}\right)\tan x+x\right]\cos^2 x\,dx$$
$$=-\frac{\pi^2}{24}(15-\pi^2)\frac{\alpha^2m^5c^6}{\hbar^4\pi^2}=-2.1098\frac{\alpha^2m^5c^6}{\hbar^4\pi^2}, \quad (31)$$

showing that almost all the correction in this case comes from the first excited state and incidentally that

$$\pi^2(1-\pi^2/15)=\frac{2^{12}}{5}\left(\frac{1}{(1\times 3)^5}+\frac{2^2}{(3\times 5)^5}+\frac{3^2}{(5\times 7)^5}+\frac{4^2}{(7\times 9)^5}+\cdots\right) \quad (32)$$

is a very quickly converging series relation (giving five-digit agreement after three terms) which to the knowledge of the author is not quoted in the literature.[8,9]

B. One-dimensional Coulomb basis

Example 2. Consider a one-dimensional system with Hamiltonian

$$H=p^2/2m-\alpha\hbar c/x+V(x),$$
$$V(x)=C[(2\alpha mc/\hbar)x]^n \quad (x\geqslant 0;\ n=1,2,...), \quad (33)$$
$$=\infty \quad (x<0),$$

where C is a constant that has units of energy. The obvious perturbation theory decomposition of this system, which cannot be treated exactly analytically (see, however, Example 3 where the problem can also be solved analytically if $n=-1$) is

$$H=H_0+h(x),$$
$$H_0=p^2/2m+V_1(x),$$
$$V_1(x)=-\alpha\hbar c/x \quad (x\geqslant 0),$$
$$=\infty \quad (x<0), \quad (34)$$
$$h(x)=C[(2\alpha mc/\hbar)x]^n \quad (x\geqslant 0;\ n=1,2,...),$$
$$=0 \quad (x<0).$$

Here,

$$\Phi_0^{(0)}(x)=2\sqrt{(\alpha mc/\hbar)^3}\,xe^{-\alpha mcx/\hbar},$$
$$\Phi_1^{(0)}(x)=\sqrt{\frac{1}{2}\left(\frac{\alpha mc}{\hbar}\right)^3}\,x\left(1-\frac{x}{2}\frac{\alpha mc}{\hbar}\right)e^{-\alpha mcx/2\hbar},$$
$$\Phi_2^{(0)}(x)=2\sqrt{\left(\frac{\alpha mc}{3\hbar}\right)^3}\times x\left(1-2x\frac{\alpha mc}{3\hbar}+2x^2\frac{\alpha^2m^2c^2}{27\hbar^2}\right)e^{-\alpha mcx/3\hbar},$$
$$E_q^{(0)}=-\tfrac{1}{2}\alpha^2mc^2[1/(q+1)^2].$$

One immediately obtains:

$$E_0^{(1)}=4\left(\frac{\alpha mc}{\hbar}\right)^3C\int_0^\infty\left(\frac{2\alpha mcx}{\hbar}\right)^n e^{-2\alpha mcx/\hbar}x^2\,dx$$
$$=\frac{C}{2}\int_0^\infty u^{n+2}e^{-u}\,du=\frac{C}{2}(n+2)! \quad (35)$$

Substituting into Eq. (21) for $F_0(x)$ with the choice $a=\infty$ [the only other choice for which $\Phi_0^{(0)}(a)=0$ being $a=0$, which yields the same result for $F_0(x)$],

$$F_0(x)=\frac{2m}{\hbar^2}\frac{\hbar^2C}{4\alpha^2m^2c^2}\int^{2\alpha mcx/\hbar}\frac{1}{y'^2e^{-y'}}\int_\infty^{y'}\left((\zeta')^n-\frac{(n+2)!}{2}\right)\zeta'^2e^{-\zeta'}\,d\zeta'\,dy'$$
$$=-\frac{C}{2\alpha^2mc^2}\int^{2\alpha mcx/\hbar}\frac{1}{y'^2}\left\{\sum_{k=0}^{n+2}\frac{(n+2)!}{(n+2-k)!}y'^{n+2-k}-\frac{(n+2)!}{2}\sum_{k=0}^{2}\frac{2!}{(2-k)!}y'^{2-k}\right\}dy'$$
$$=-\frac{C}{2\alpha^2mc^2}\int^{2\alpha mcx/\hbar}y'^{-2}\sum_{k=0}^{n-1}\frac{(n+2)!}{(n+2-k)!}y'^{n+2-k}\,dy'$$
$$=-\frac{C(n+2)!}{2\alpha^2mc^2}\sum_{k=0}^{n-1}\frac{1}{(n+2-k)!(n+1-k)}\left(\frac{2\alpha mcx}{\hbar}\right)^{n+1-k}, \quad (36)$$

where use was made of the expression[10]

$$\int x^ne^{-x}\,dx=-e^{-x}\sum_{k=0}^{n}\frac{n!}{(n-k)!}x^{n-k}.$$

One can confirm that the choice $a=\infty$ in Eq. (36) is the correct one by verifying that for this value of a

$$\langle 0|F_0|1\rangle=\frac{\langle 0|h|1\rangle}{E_0^{(0)}-E_1^{(0)}}=\frac{\sqrt{2}2^{2n+6}(n+2)!nC}{3^{n+5}\alpha^2mc^2}. \quad (37)$$

Hence, using $E_0^{(0)}-E_1^{(0)}=-\tfrac{3}{8}\alpha^2mc^2$,

$$E_0^{(2)} = \frac{\langle 0|h|1\rangle\langle 1|h|0\rangle}{E_0^{(0)} - E_1^{(0)}} + \cdots$$
$$= -\frac{2^{4n+10}(n+2)!^2 n^2 C^2}{3^{2n+9}\alpha^2 mc^2} + \cdots, \quad (38)$$

whereas the exact second-order result from Eq. (16) is

$$E_0^{(2)} = -C^2(n+2)!/2^3\alpha^2 mc^2 \times \sum_{k=0}^{n-1} \frac{2(2n+3-k)! - (n+2)!(n+3-k)!}{(n+2-k)!(n+1-k)}. \quad (39)$$

A feeling for the rate of convergence may be obtained by comparing the exact second-order result for the case $n = 1$, where $F_0(x) = -Cx^2m/\hbar^2$,

$$E_0^{(2)} = \langle 0|hF_0|0\rangle - E_0^{(1)}\langle 0|F_0|0\rangle$$
$$= -\frac{15C^2}{\alpha^2 mc^2} + \frac{9C^2}{\alpha^2 mc^2} = -\frac{6C^2}{\alpha^2 mc^2} \quad (40)$$

versus the first term in the second-order expansion in this case, namely, $-2^{16}C^2/3^9\alpha^2mc^2 \sim -3.3296(C^2/\alpha^2mc^2)$. Thus, for $n = 1$, the first term is little over half the total second-order value which also includes a contribution from the term

$$\int dk \frac{\langle 0|h|k\rangle\langle k|h|0\rangle}{E_0^{(0)} - E_k^{(0)}},$$

since there are also continuum states in this basis. As noted in Sec. II, Eqs. (39) and (40) also automatically include this contribution. For $n = 3$, however, one obtains $E_0^{(2)} = -42\,780C^2/\alpha^2mc^2$ from Eq. (39), versus the first second-order term, Eq. (38) $\sim -37\,883.15C^2/\alpha^2mc^2$, indicating that the convergence improves with increasing n.

Example 3. Consider the Hamiltonian in Example 2,

$$H = p^2/2m - \alpha\hbar c/x + V(x), \quad (41)$$

but with

$$V(x) = C(2\alpha mcx/\hbar)^{-1} \quad (x \geqslant 0),$$
$$= \infty \quad (x < 0). \quad (42)$$

Rewriting this Hamiltonian as

$$H = H_0 + h(x),$$
$$H_0 = p^2/2m + V_1(x),$$
$$V_1(x) = -\alpha\hbar c/x \quad (x \geqslant 0),$$
$$= \infty \quad (x < 0),$$
$$h(x) = C(2\alpha mcx/\hbar)^{-1} \quad (x \geqslant 0),$$
$$= 0 \quad (x < 0),$$

the same unperturbed energies and eigenstates arise as in Example 2 and

$$E_0^{(1)} = C/2. \quad (43)$$

Additionally, with $a = \infty$ (the same choice as in Example 2),

$$F_0(x) = \frac{C}{2\alpha^2 mc^2}\int^{2\alpha mcx/\hbar} \frac{1}{y'^2 e^{-y'}} \times \int_\infty^{y'} \left(\zeta' - \frac{\zeta'^2}{2}\right) e^{-\zeta'} d\zeta'\, dy'$$
$$= \frac{C}{2\alpha^2 mc^2}\int^{2\alpha mcx/\hbar} \frac{1}{2} dy'$$
$$= Cx/2\alpha\hbar c, \quad (44)$$

where $hF_0 = C^2/4\alpha^2mc^2$ is a constant in this case. This yields

$$E_0^{(2)} = \langle 0|hF_0|0\rangle - E_0^{(1)}\langle 0|F_0|0\rangle$$
$$= C^2/4\alpha^2mc^2 - 3C^2/8\alpha^2mc^2$$
$$= -C^2/8\alpha^2mc^2. \quad (45)$$

Using Eq. (17) one can also obtain the third-order contribution to the ground-state energy,

$$E_0^{(3)} = \langle 0|F_0hF_0|0\rangle - 2E_0^{(2)}\langle 0|F_0|0\rangle - E_0^{(1)}\langle 0|F_0^2|0\rangle$$
$$= \frac{C^3}{\alpha^4 m^2 c^4}\left(\frac{3}{16} + \frac{3}{16} - \frac{3}{8}\right)$$
$$= 0.$$

In this case one can also trivially solve this problem exactly by writing the Hamiltonian as

$$H = \frac{p^2}{2m} - \frac{\alpha\hbar c}{x}\left(1 - \frac{C}{2\alpha^2 mc^2}\right) = \frac{p^2}{2m} - \frac{\alpha'\hbar c}{x},$$

where $\alpha' = \alpha(1 - C/2\alpha^2mc^2)$ which has exact ground-state energy:

$$E_0 = -\frac{1}{2}mc^2\alpha'^2 = -\frac{1}{2}mc^2\alpha^2 + \frac{C}{2} - \frac{C^2}{8\alpha^2 mc^2},$$

in agreement with the result obtained by the Dalgarno–Lewis approach above, verifying also that the choice $a = \infty$ was the correct one. One may also write

$$-\frac{C^2}{8\alpha^2 mc^2} = \frac{\langle 0|h|1\rangle\langle 1|h|0\rangle}{E_0^{(0)} - E_1^{(0)}} + \frac{\langle 0|h|2\rangle\langle 2|h|0\rangle}{E_0^{(0)} - E_2^{(0)}} + \cdots + \int \frac{dk\,\langle 0|h|k\rangle\langle k|h|0\rangle}{E_0^{(0)} - E_k^{(0)}}$$
$$= -\frac{2^6}{3^7}\frac{C^2}{\alpha^2 mc^2} - \frac{3^3}{2^{12}}\frac{C^2}{\alpha^2 mc^2} + \cdots,$$
$$-0.125\frac{C^2}{\alpha^2 mc^2} \sim -0.029\frac{C^2}{\alpha^2 mc^2} - 0.007\frac{C^2}{\alpha^2 mc^2} + \cdots, \quad (46)$$

indicating the series is slowly convergent in this case.

C. One-dimensional harmonic oscillator

Example 4. Consider the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 + \lambda\hbar\omega\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)^3 \quad (-\infty \leqslant x \leqslant \infty), \quad (47)$$

where λ is a dimensionless constant. The obvious perturbation theory decomposition of this system, which cannot be treated exactly analytically, is

$$H_0 = p^2/2m + \tfrac{1}{2}m\omega^2x^2,$$
$$h(x) = \lambda\hbar\omega(\sqrt{m\omega/\hbar}\,x)^3 \quad (-\infty \leqslant x \leqslant \infty). \quad (48)$$

For this H_0,

$$\Phi_0^{(0)}(x) = (m\omega/\pi\hbar)^{1/4} e^{-m\omega x^2/2\hbar},$$

$$\Phi_1^{(0)}(x) = (\sqrt{2}/\pi^{1/4})(m\omega/\hbar)^{3/4} x e^{-m\omega x^2/2\hbar},$$

$$\Phi_3^{(0)}(x) = \frac{1}{2\sqrt{12}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \times\left[8\left(\sqrt{\frac{m\omega}{\hbar}}x\right)^3 - 12\sqrt{\frac{m\omega}{\hbar}}x\right]e^{-m\omega x^2/2\hbar},$$

$$E_n^{(0)} = (n+\tfrac{1}{2})\hbar\omega.$$

Both $E_n^{(1)}$ and $E_n^{(3)}$ are again zero (as in Example 1) from parity considerations. With the choice $a=\infty$ [the only other choice for which $\Phi_0^{(0)}(x)=0$ being $a=-\infty$ which yields the same result for $F_0(x)$]:

$$F_0(x) = \lambda\hbar\omega\frac{2m}{\hbar^2}\frac{\hbar}{m\omega}\int^{\sqrt{m\omega/\hbar}x}\frac{1}{e^{-y'^2}}\int_\infty^{y'}\zeta'^3 e^{-\zeta'^2}d\zeta'\,dy'$$

$$= \lambda\int^{\sqrt{m\omega/\hbar}x}\frac{1}{e^{-y'^2}}\int_\infty^{y'}\zeta'^2 e^{-\zeta'^2}d\zeta'^2\,dy'$$

$$= -\lambda\int^{\sqrt{m\omega/\hbar}x}(y'^2+1)dy'$$

$$= -\lambda\left[\frac{1}{3}\left(\sqrt{\frac{m\omega}{\hbar}}x\right)^3 + \sqrt{\frac{m\omega}{\hbar}}x\right]. \quad (49)$$

By evaluating

$$\frac{\langle 0|h|1\rangle}{E_0^{(0)}-E_1^{(0)}} = \frac{(3\sqrt{2}/4)\lambda\hbar\omega}{-\hbar\omega} = -\frac{3\sqrt{2}\lambda}{4} = \langle 0|F_0|1\rangle$$

one finds that the choice $a=\infty$ is okay. Evaluating Eq. (16) yields $E_0^{(2)} = -(11\hbar\omega/8)\lambda^2$. There are only two nonvanishing terms in the second-order series expansion in this case, namely,

$$E_0^{(2)} = \frac{\langle 0|h|1\rangle\langle 1|h|0\rangle}{E_0^{(0)}-E_1^{(0)}} + \frac{\langle 0|h|3\rangle\langle 3|h|0\rangle}{E_0^{(0)}-E_3^{(0)}}$$

$$= -\tfrac{9}{8}\lambda^2\hbar\omega - \tfrac{1}{4}\lambda^2\hbar\omega = -\tfrac{11}{8}\lambda^2\hbar\omega,$$

in agreement with the above result.

Example 5. Consider the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 + \lambda\hbar\omega\left(\sqrt{\frac{m\omega}{\hbar}}x\right)^3 + \delta\hbar\omega\sqrt{\frac{m\omega}{\hbar}}x \quad (-\infty\leqslant x\leqslant\infty), \quad (50)$$

where λ and δ are dimensionless constants. With the perturbation theory decomposition

$$H_0 = p^2/2m + \tfrac{1}{2}m\omega^2x^2,$$

$$h(x) = \lambda\hbar\omega\left(\sqrt{\frac{m\omega}{\hbar}}x\right)^3 + \delta\hbar\omega\sqrt{\frac{m\omega}{\hbar}}x \quad (-\infty\leqslant x\leqslant\infty), \quad (51)$$

this problem may be simplified by writing $h = h_1 + h_2$ where $h_1 = \lambda\hbar\omega(\sqrt{m\omega/\hbar}x)^3$, for which $F_{01}(x)$ was obtained in Example 4, and $h_2 = \delta\hbar\omega\sqrt{m\omega/\hbar}x$, for which it is easy to show $F_{02}(x) = -\delta\sqrt{m\omega/\hbar}x$. Thus, in this case,

$$F_0(x) = -\lambda\left[\frac{1}{3}\left(\sqrt{\frac{m\omega}{\hbar}}x\right)^3 + \sqrt{\frac{m\omega}{\hbar}}x\right] - \delta\sqrt{\frac{m\omega}{\hbar}}x \quad (52)$$

and $E_0^{(2)} = -\hbar\omega(\tfrac{11}{8}\lambda^2 + \tfrac{3}{2}\lambda\delta + \tfrac{1}{2}\delta^2)$.

Example 6. Consider the Hamiltonian in Example 4,

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 + \lambda\hbar\omega\left(\sqrt{\frac{m\omega}{\hbar}}x\right)^3 \quad (-\infty\leqslant x\leqslant\infty),$$

where λ is a dimensionless constant.

With the same decomposition as in Example 4 one may evaluate $F_1(x)$ and hence obtain $E_1^{(2)}$.

From Example 4, $E_1^{(1)} = 0$, while

$$\Phi_1^{(0)}(x) = \frac{\sqrt{2}}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{3/4} x e^{-m\omega x^2/2\hbar}.$$

Substituting into Eq. (21) with $a=\infty$ (as in Example 4) one obtains

$$F_1(x) = -\lambda\left[\frac{1}{3}\left(\sqrt{\frac{m\omega}{\hbar}}x\right)^3 + 2\left(\sqrt{\frac{m\omega}{\hbar}}x\right) - 2\left(\frac{1}{\sqrt{m\omega/\hbar}x}\right)\right]. \quad (53)$$

One can verify that Eq. (53) is correct by calculating

$$\frac{\langle 1|h|0\rangle}{E_1^{(0)}-E_0^{(0)}} = \frac{3\sqrt{2}\lambda}{4} = \langle 1|F_1|0\rangle.$$

Using F_1 one can obtain $E_1^{(2)}$ by evaluating Eq. (16), with the result

$$E_1^{(2)} = -\tfrac{71}{8}\lambda^2\hbar\omega. \quad (54)$$

IV. CONCLUSIONS

In this paper the Dalgarno–Lewis summation technique was reviewed. It was shown how to eliminate the ambiguities that arise in the definition of the relevant function F_n, and additionally a useful consequence of the linear relationship by which it is defined was pointed out. Finally, six examples of the technique in three bases, those of a particle in a box, the one-dimensional Coulomb potential, and a one-dimensional harmonic oscillator, were given. These are only a few of the many interesting problems the reader can investigate with this technique.

APPENDIX

The second-order ground-state energy expression according to the Dalgarno–Lewis approach is given by Eq. (16) of the text:

$$E_{0(\mathrm{DL})}^{(2)} = \langle 0|hF_0|0\rangle - E_0^{(1)}\langle 0|F_0|0\rangle. \quad (\mathrm{A1})$$

Assuming h and F_0 do not involve differential operators, for a one-dimensional system this may be written

$$E_{0(\mathrm{DL})}^{(2)} = \int_{-\infty}^{\infty} F_0(x)|\Phi_0^{(0)}(x)|^2[h(x) - E_0^{(1)}]dx. \quad (\mathrm{A2})$$

For the case $\Phi_0^{(0)}(x)\to 0$, as $x\to-\infty$, (i.e., "a" $= -\infty$), the corresponding LPT expression is given in Eq. (20) of Ref. 4, namely (using the same notation),

$$E_{0(\mathrm{LPT})}^{(2)} = -\frac{2m}{\hbar^2}\int_{-\infty}^{\infty} |\Phi_0^{(0)}(x)|^{-2} \times \left| \int_{-\infty}^{x} |\Phi_0^{(0)}(\zeta)|^2 [h(\zeta) - E_0^{(1)}] d\zeta \right|^2 dx. \quad \text{(A3)}$$

Assuming $\Phi_0^{(0)}$ is real and integrating (A2) by parts, one obtains

$$E_{0(\mathrm{DL})}^{(2)} = F_0(x) \int_{-\infty}^{x} \Phi_0^{(0)}(x)^2 [h(x) - E_0^{(1)}] dx \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{dF_0(x)}{dx} \int_{-\infty}^{x} \Phi_0^{(0)}(\zeta)^2 [h(\zeta) - E_0^{(1)}] d\zeta \, dx.$$

But using Eq. (4) in the text, and the fact that $\Phi_0^{(0)}(x)$ is a normalized wave function,

$$\int_{-\infty}^{\infty} \Phi_0^{(0)}(x)^2 [h(x) - E_0^{(1)}] dx = E_0^{(1)} - E_0^{(1)} \int_{-\infty}^{\infty} \Phi_0^{(0)}(x)^2 dx = 0.$$

Thus one can also write

$$E_{0(\mathrm{DL})}^{(2)} = -\int_{-\infty}^{\infty} \frac{dF_0(x)}{dx} \times \int_{-\infty}^{x} \Phi_0^{(0)}(\zeta)^2 [h(\zeta) - E_0^{(1)}] d\zeta \, dx. \quad \text{(A4)}$$

Differentiating Eq. (21) and substituting the resulting expression for $dF_0(x)/dx$ in (A4) one obtains

$$E_{0(\mathrm{DL})}^{(2)} = -\int_{-\infty}^{\infty} \frac{1}{\Phi_0^{(0)}(x)^2} \frac{2m}{\hbar^2} \times \int_{-\infty}^{x} \Phi_0^{(0)}(\zeta)^2 [h(\zeta) - E_0^{(1)}] d\zeta \times \int_{-\infty}^{x} \Phi_0^{(0)}(\zeta)^2 [h(\zeta) - E_0^{(1)}] d\zeta \, dx, \quad \text{(A5)}$$

which is just Eq. (A3), the corresponding LPT expression.

Generalizing these results to complex Φ's presents no problem.

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The role of amplitude and phase of the Fourier transform in the digital image processing

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The analysis of the importance of the amplitude and the phase of Fourier transform has been carried out by means of combining these functions between two images and observing the reconstructed image after a second transform. This processing has been studied by taking into account several possibilities, especially for very structurally different images. It is proved that the phase carries the most relevant information, but when common images are combined with images constituted by strongly marked geometric forms it is not so evident and the amplitude could play a more important role.

I. INTRODUCTION

In digital image processing the Fourier transform provides a powerful method of analyzing and manipulating the spatial frequency plane of an image.[1]

In the Fourier representation of images, the spectral amplitude and phase tend to play different roles. Oppenheim and Lim[2] showed that in many contexts the phase contains much of the essential information in an image and that the phase is sufficient to reconstruct the image completely. This fact has been successfully applied to pattern recognition, using only the phase information of the Fourier transform of the model to be detected in order to elaborate a filter for recognition with greater efficiency than the usual matched filter.[3]

In this paper, we review and discuss the aforementioned