Infinite-Order Perturbation Theory for Finite Systems

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A perturbation theory is described which leads to two alternative methods for calculating the eigenvalues and normalized eigenstates of a perturbed Hamiltonian, the results being given to all orders in the perturbation. The expansions obtained are formulated in terms of two sets of partial sums which have simple, easily characterized forms, and they combine some of the advantages of both the Rayleigh-Schrödinger and Brillouin-Wigner perturbation methods while avoiding some of the difficulties of each. In particular, one form of the perturbation expansions given here will in most cases of interest have a larger radius of convergence than the Rayleigh-Schrödinger series. As is usual for infinite-order treatments, the explicit form of the final result applies only to nondegenerate levels. However, some of the intermediate relations obtained in the derivation are of general validity. Since certain classes of unlinked diagrams appear in the expansions, the method described here is not suitable for application to systems containing a large number of particles.

I. INTRODUCTION

THE problem of time-independent perturbation theory is usually stated in approximately the following form: given a Hamiltonian

$$H=H_0+V \tag{1}$$

consisting of the sum of a part H_0 whose eigenvalue problem can be solved and a part V which may be (but is not always) assumed to be small, find an expression for the eigenvalues and eigenstates of H in terms of those of H_0 and of the matrix elements of V in the eigenstates of H_0. The solution to this problem may be obtained either by some method equivalent to use of the resolvent operator[1,2] or by means of the adiabatic hypothesis[3,4] (and possibly by some other methods[5]), and the form of the answer is highly nonunique. As a result, a sizeable number of treatments of the subject have appeared in recent years emphasizing one or another of the facets of the problem. Some of these have considered general aspects of the derivation of perturbation theories[2]; others have been interested in the formulation of a perturbation expansion which would be well adapted to treating some particular class of problems, such as studies in quantum statistical mechanics or many-particle systems[1,6,7]; and still others have done both of these.[8] The present paper must be said to belong in the second of these categories. It presents a set of perturbation expansions for a nondegenerate level which in effect steer a course midway between those of the usual Rayleigh-Schrödinger (R-S) and Brillouin-Wigner (B-W) perturbation methods, and by so doing manage to retain some of the advantages of both these techniques while avoiding some of the disadvantages of each. This form for the perturbation expansions seems to be rather advantageous in a number of problems involving systems with a finite number of particles, but is not—at least in its present form—well adapted for application to infinite systems.

The main advantages of the perturbation method considered here (aside from the simplicity of its derivation) are the following: (1) It automatically yields normalized eigenstates; (2) it gives alternative methods for calculating the state vectors and the energy; (3) it expresses all quantities of interest in terms of two sets of partial sums which have very simple, easily characterized forms; (4) when the perturbation V is a bounded operator, it yields perturbation expansions which generally have a larger radius of convergence than either the Rayleigh-Schrödinger or linked cluster series.

In its approach the development in this paper is most closely related to the work of Van Hove[1] and Hugenholtz,[7] though it may take more than a cursory glance at Refs. 1 and 7 to make this fact apparent; in particular, the procedure followed here is equivalent to use of the resolvent operator. But this fact is of no importance in the derivation, and the resolvent operator is not referred to by name again.

In the next section we shall derive the perturbation expansions proper. Section III is then devoted to a discussion of the characteristic features of these expansions and of their use in actual calculations. In order to illustrate the properties discussed, the theory is applied to a simple soluble example in Sec. IV and compared with a linked-cluster-expansion treatment of the same example.

II. DERIVATION OF THE PERTURBATION EXPANSIONS

In the following discussion we shall denote the normalized eigenstates of the Hamiltonian (1) by $|m\rangle$ and

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[1] L. Van Hove, Physica **21**, 901 (1955); **22**, 343 (1956); **23**, 441 (1957).
[2] R. Yaris, J. Chem. Phys. **40**, 1891 (1964).
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[6] K. A. Brueckner and C. A. Levinson, Phys. Rev. **97**, 1344 (1955); K. A. Brueckner, *ibid.* **100**, 36 (1955); K. A. Brueckner and J. L. Gammel, *ibid.* **109**, 1023 (1958).
[7] N. M. Hugenholtz, Physica **23**, 481 (1957).
[8] Per-Olov Löwdin, J. Math. Phys. **3**, 969 (1962); **3**, 1171 (1962); **6**, 1341 (1965); Rev. Mod. Phys. **35**, 702 (1963); J. Mol. Spectry. **13**, 326 (1964); and many others.

those of H_0 by $|m\rangle_0$. The labels of these two sets of states will be chosen so that if

$$H|m\rangle=E_m|m\rangle$$

and

$$H_0|m\rangle_0=E_m{}^0|m\rangle_0,$$

then $E_m\to E_m{}^0$ as the interaction is "turned off," in the usual sense. The basic problem is then the calculation of the energy differences

$$\delta E_m=E_m-E_m{}^0 \tag{2}$$

and transformation coefficients ${}_0\langle n|m\rangle$ for nondegenerate levels $|m\rangle_0$ in those systems for which a perturbation treatment is valid. (We shall not investigate the conditions under which the perturbation expansion is actually justified.) The approach to the problem used here depends on the fact that the quantities ${}_0\langle n|e^{-iHt}|m\rangle_0$, for all m and n, contain all the information concerning the system—and therefore, in particular, all the information needed in constructing a perturbation theory.

Consider the expression

$$-i\int_0^\infty e^{iEt}\,{}_0\langle n|e^{-iHt}|m\rangle_0 dt,\quad \mathrm{Im}E>0. \tag{3}$$

This integral defines an analytic function of the complex energy E in the upper half-plane, and this function can be analytically continued to the lower half-plane and to the points of the real axis which do not belong to the spectrum of H; this analytic continuation will actually be carried out in various expressions later without comment. By introducing the identity operator

$$I=\textstyle\sum_k|k\rangle\langle k|$$

into the matrix element in the integral one sees that, on one hand, (3) is equal to

$$\sum_k\frac{{}_0\langle n|k\rangle\langle k|m\rangle_0}{E-E_k}. \tag{4}$$

On the other hand, we can use the standard expansion

$$e^{-iHt}=e^{-iH_0t}U(0,t), \tag{5a}$$

$$U(0,t)=1+\sum_{p=1}^\infty(-i)^p\int_0^t dt_p\cdots\int_0^{t_2}dt_1V(t_p)\cdots V(t_1), \tag{5b}$$

$$V(t)=e^{iH_0t}Ve^{-iH_0t}, \tag{5c}$$

to write (3) in the form

$$\frac{{}_0\langle n|m\rangle_0}{E'}+\sum_{p=1}^\infty(-i)^{p+1}\int_0^\infty dt\int_0^t dt_p\cdots\int_0^{t_2}dt_1e^{iE't}\times{}_0\langle n|V(t_p)\cdots V(t_1)|m\rangle_0, \tag{6}$$

where $E'=E-E_n{}^0$. By introducing sums over intermediate states in the various terms and changing the variables of integration to

$$\begin{aligned}y_1&=t_1,\\ y_2&=t_2-t_1,\\ &\vdots\\ y_p&=t_p-t_{p-1},\\ y_{p+1}&=t-t_p,\end{aligned}$$

one may perform the integrations and transform (6) to the form[9]

$$\frac{{}_0\langle n|m\rangle_0}{E-E_n{}^0}+\frac{V_{nm}}{(E-E_n{}^0)(E-E_m{}^0)}+\sum_{p=2}^\infty\sum_{q_1}\cdots\sum_{q_{p-1}}\times\frac{V_{nq_{p-1}}V_{q_{p-1}q_{p-2}}\cdots V_{q_2q_1}V_{q_1m}}{(E-E_n{}^0)(E-E_{q_{p-1}}{}^0)\cdots(E-E_{q_1}{}^0)(E-E_m{}^0)}. \tag{7}$$

This result may be put in a simpler form. Suppose first that $n=m$, and define $D_m{}^p$ (D for "diagonal") as

$$D_m{}^1=V_{mm},$$

$$D_m{}^p\equiv\sum_{q_1}{}'\cdots\sum_{q_{p-1}}{}'\frac{V_{mq_{p-1}}V_{q_{p-1}q_{p-2}}\cdots V_{q_2q_1}V_{q_1m}}{(E-E_{q_{p-1}}{}^0)(E-E_{q_{p-2}}{}^0)\cdots(E-E_{q_1}{}^0)},\qquad p\geq2, \tag{8}$$

where the prime on a summation means that the term $q_i=m$ is omitted. We next define D_m in terms of the $D_m{}^p$ as

$$D_m\equiv\sum_{p=1}^\infty D_m{}^p. \tag{9}$$

Note that then $(1/E-E_m{}^0)+(D_m/(E-E_m{}^0)^2)$ contains all the terms in the sum in (7) in which $|m\rangle_0$ is not an intermediate state. Now consider the terms in (7) containing $|m\rangle_0$ as an intermediate state exactly r times, $r\geq1$; it is a straightforward matter to verify that these can be written as

$$(1/E-E_m{}^0)\left(\sum_{p=1}^\infty\frac{D_m{}^p}{E-E_m{}^0}\right)^{r+1}=(1/E-E_m{}^0)\left(\frac{D_m}{E-E_m{}^0}\right)^{r+1}.$$

From this result one concludes that (for $n=m$) (7) can be written in the form

$$[E-E_m{}^0-D_m]^{-1}\equiv\left[E-E_m{}^0-V_{mm}-\sum_{p=2}^\infty\sum_{q_1}{}'\cdots\sum_{q_{p-1}}{}'\frac{V_{mq_{p-1}}\cdots V_{q_1m}}{(E-E_{q_{p-1}}{}^0)\cdots(E-E_{q_1}{}^0)}\right]^{-1}. \tag{10}$$

Now consider the value of (7) for the case $n\neq m$, and

[9] For notational convenience we shall denote the matrix elements of V in the eigenstates of H_0 by V_{nm}: $V_{nm}\equiv{}_0\langle n|V|m\rangle_0$.

define the quantities (N for "nondiagonal")

$$N_{nm}{}^{1}=(V_{nm}/E-E_n{}^0), \tag{11}$$

$$N_{nm}{}^{p}=\sum_{q_1}{}'\cdots\sum_{q_{p-1}}{}'\frac{V_{nq_{p-1}}V_{q_{p-1}q_{p-2}}\cdots V_{q_2q_1}V_{q_1m}}{(E-E_n{}^0)(E-E_{q_{p-1}}{}^0)\cdots(E-E_{q_1}{}^0)}, \quad p\geq 2, \tag{12}$$

$$N_{nm}=\sum_{p=1}^{\infty}N_{nm}{}^{p}.$$

By the same sort of considerations as before one may show that the terms in (7) containing $|m\rangle_0$ as an intermediate state r times are $(N_{nm}/E-E_m{}^0)(D_m/E-E_m{}^0)^r$. This result and that obtained for the case $n=m$ show that (7) can be written as[10]

$$\sum_k\frac{{}_0\langle m|k\rangle\langle k|m\rangle_0}{E-E_k}=\frac{1}{E-E_m{}^0-D_m}; \tag{13}$$

$$\sum_k\frac{{}_0\langle n|k\rangle\langle k|m\rangle_0}{E-E_k}=\frac{N_{nm}}{E-E_m{}^0-D_m}, \quad n\neq m. \tag{14}$$

Note that thus far the discussion has been valid for completely general indices m and n, including those corresponding to degenerate levels, with the sole restrictions being those generated by the nature of perturbation theory itself—i.e., the requirement that the various series considered actually converge. Therefore Eqs. (13) and (14) hold with only this restriction. Now let us assume in addition that the particular index m being considered corresponds to a nondegenerate eigenvalue E_m; and let C_m be a positively directed circle in the complex energy plane which encloses E_m, but no other eigenvalues of H. Then Eqs. (13) and (14) show that

$${}_0\langle m|m\rangle\langle m|m\rangle_0=\frac{1}{2\pi i}\int_{Cm}\frac{dE}{E-E_m{}^0-D_m}, \tag{15}$$

$${}_0\langle m|m\rangle\langle m|m\rangle_0\delta E_m=\frac{1}{2\pi i}\int_{Cm}\frac{(E-E_m{}^0)dE}{E-E_m{}^0-D_m}, \tag{16}$$

$${}_0\langle n|m\rangle\langle m|m\rangle_0=\frac{1}{2\pi i}\int_{Cm}\frac{N_{nm}dE}{E-E_m{}^0-D_m}. \tag{17}$$

If in addition we assume (as is very frequently done) that $E_m{}^0$ is also a nondegenerate eigenvalue of H_0, and that C_m may be chosen so as to enclose both $E_m{}^0$ and E_m but no other eigenvalues of H_0 or H, then the integrations on the right in Eqs. (15)–(17) can be explicitly carried out. In terms of the operation

$$\partial^n\cdots\equiv\left[\frac{1}{n!}\frac{d^n}{dE^n}\cdots\right]_{E=E_m{}^0}$$

the result can be written in the form[11]

$${}_0\langle m|m\rangle\langle m|m\rangle_0=1+\partial^1D_m+\partial^2(D_m)^2+\cdots, \tag{18}$$

$${}_0\langle m|m\rangle\langle m|m\rangle_0\delta E_m=\partial^0D_m+\partial^1(D_m)^2+\partial^2(D_m)^3+\cdots, \tag{19}$$

$${}_0\langle n|m\rangle\langle m|m\rangle_0=\partial^0N_{nm}+\partial^1[N_{nm}D_m]+\partial^2[N_{nm}(D_m)^2]+\cdots. \tag{20}$$

The ratio of Eqs. (16) and (15) [or (19) and (18)] yields the energy correction δE_m immediately. In order to determine the transformation coefficients from the unperturbed to the perturbed eigenstates it is necessary to specify the phase of ${}_0\langle m|m\rangle$, which up to this point has been arbitrary. It is convenient and customary to take this phase to be zero, and once that choice has been made one obtains ${}_0\langle m|m\rangle$ as the square root of (15) [or (18)]. ${}_0\langle n|m\rangle$ is then found by dividing (17) [or (20)] by ${}_0\langle m|m\rangle$. It is perhaps worthwhile to note again that the state $|m\rangle$, now given explicitly as $|m\rangle=\sum_n|n\rangle_0\,{}_0\langle n|m\rangle$, is normalized.[12]

III. DISCUSSION OF THE PERTURBATION EXPANSIONS

Equations (15)–(20) are the relations on which perturbation calculations may be based. Since these expressions are all formulated in terms of the functions D_m and N_{nm}, it is advantageous to examine the nature of these latter quantities before considering the perturbation expansions proper. One sees from the definition in Eqs. (8) and (9) that D_m can be written as

$$D_m=\sum_{p=0}^{\infty}\sum_{S_p}\left\langle V\left(\frac{1}{E-H_0}V\right)^p\right\rangle_{S_p}, \tag{21}$$

where S_p is the set of pth-order diagrams beginning and ending at $|m\rangle_0$ in which all intermediate states are physical and different from $|m\rangle_0$. Note that the right-hand side of (21) is somewhat analogous to the linked-cluster expression for δE_m. The differences are that D_m is obtained by summing over diagrams which may be unlinked [e.g., for two-body interactions in a fermion system diagrams like those shown in Fig. 1(a), but not those in Fig. 1(b), can occur] but which are states of

[10] The expressions for (3) given by the right-hand sides of (13) and (14) seem to have been given first by L. Van Hove, Refs. 1. However, he does not appear to have written down the *left*-hand sides of these equations. Some discussion of the derivation of the expressions on the right in (13) and (14), together with an application, is given by S. Teitler, J. Math. Phys. 4, 1119 (1963).

[11] This result is obtained at once by expanding the denominators in each of the integrals and noting that, under the stated hypotheses, D_m and N_{nm} are regular inside C_m.

[12] Van Hove has obtained by a lengthier method an expression for the exact eigenstates which is closely related to that obtained from Eqs. (18) and (20); see Refs. 1 and also L. Van Hove, Lecture Notes, University of Washington, 1958 (unpublished). However, the remaining equations—and particularly the expression for the energy correction obtained from Eqs. (15) and (16) or (18) and (19)—have apparently not been stated before.

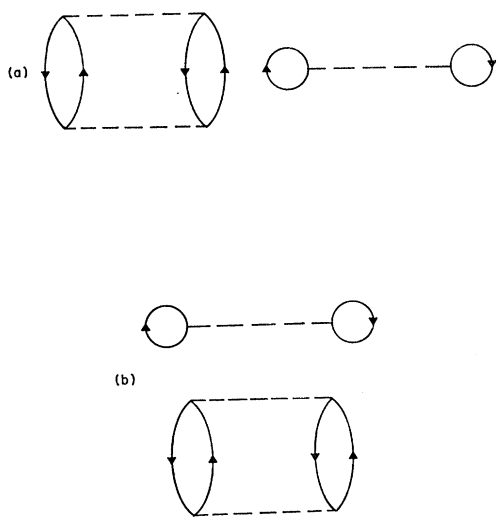

FIG. 1. (a) An unlinked diagram of the type which can occur in the summation (21). (b) An unlinked diagram which is excluded from the sum (21) by the requirement that all intermediate states differ from the initial state.

the physical system, while δE_m is obtained by summing over all linked diagrams regardless of whether or not these are exclusion principle violating or contain more internal particle lines than the number of particles in the system. In addition, D_m contains the complex variable E, instead of the $E_m{}^0$ appearing in δE_m. In the same way one can see that

$$N_{nm}=\sum_{p=1}^{\infty}\sum_{T_p}\left\langle\left(\frac{1}{E-H_0}V\right)^p\right\rangle_{T_p}, \tag{22}$$

where T_p is the set of pth order diagrams beginning at $|m\rangle_0$ and ending at $|n\rangle_0$ in which all intermediate states are physical and different from $|m\rangle_0$. This expression differs from the corresponding linked cluster expansion for the nonnormalized transformation coefficient $({}_0\langle n|m\rangle)_{NN}$ in that, once again, some unlinked diagrams but no nonphysical diagrams are contained in the sets T_p, and E appears in place of $E_m{}^0$. The appearance of the contributions of unlinked diagrams makes the perturbation theory in the form given by Eqs. (15)–(20) inappropriate for application to infinite systems.

However, in the case of finite systems the inconvenience occasioned by the appearance of unlinked diagrams can be more than offset by the fact that contributions due to nonphysical intermediate states need not be considered. In the first place, it can be the case that the number of exclusion-principle-violating diagrams one would have to sum in the linked cluster expansion is as great as or greater than the number of unlinked diagrams appearing in the series derived here.[13]

[13] It must be emphasized that there is nothing incorrect or questionable about the nonphysical diagrams which appear in the linked-cluster expansions. The point is simply that if these diagrams can be ignored then there are fewer terms to sum.

A rather extreme example of a situation of this sort will be provided by the simple problem considered in Sec. IV. A much more important consideration, however, is the fact that in the case where V is a bounded operator,[14] it is *precisely the exclusion-principle-violating diagrams* which limit the radius of convergence of the linked-cluster expansion.[15] In such a case the radius of convergence of the series (21) and (22) is generally greater than that of the linked-cluster series, a feature which might be of importance in some applications. In fact, for E in the vicinity of $E_m{}^0$ one sees immediately that the radius of convergence of (21) and (22) is $\|V\|=d$, where $\|V\|$ is the operator norm of V and d is the distance from $E_m{}^0$ to the nearest point in the remainder of the spectrum of H_0. From the manner in which D_m and N_{nm} appear in Eqs. (15)–(17) it is then clear that in most cases the radius of convergence of these expansions will be considerably larger than the best value,[16] $\|V\|=(d/2)$, which can be proved for the Rayleigh-Schrödinger expansion.[17] Finally, it might be worth pointing out that the D_m and N_{nm} are probably the simplest quantities expressed in terms of the V_{pq} from which a perturbation expansion can conveniently be constructed.

Now that the functions D_m and N_{nm} have been characterized more fully, let us consider their roles in the perturbation formulas obtained in Sec. II. The seemingly most explicit of the relations given there are Eqs. (18)–(20); these provide well-defined expressions for all the transformation coefficients and energy shifts in terms of certain series and ratios of series, and probably constitute the most convenient starting points in practical calculations where the series converge and one is interested in an accuracy corresponding to the retention of terms of only the first few orders in the perturbation expansion. Suppose, for instance, that one wishes to calculate the energy correction through fifth-order terms. It is only necessary to make V_{mm} vanish (by replacing $E_m{}^0$ by $E_m{}^0+V_{mm}$ everywhere) in order to be able to write, from Eqs. (18) and (19),

$$\delta E_m{}^{(5)}=\partial^0 D_m{}^{(5)}[1+\partial^1 D_m{}^{(3)}], \tag{23}$$

[14] It is impossible to make statements about the convergence of the perturbation series for an unbounded V without considering the nature of V in detail. One might find it reasonable to suppose that a perturbation series which had superior convergence properties for bounded V would in most cases have superior convergence properties for unbounded V as well; but this assumption would be pure conjecture.

[15] A. Katz, Nucl. Phys. **20**, 663 (1960).

[16] T. Kato has proved [Progr. Theoret. Phys. (Kyoto) **4**, 514 (1949)] that the Rayleigh-Schrödinger expansion converges for $\|V\|<d/2$; and this is the strongest possible result in terms of the norm of V, since the problem considered in Sec. IV is an example of a situation where the Rayleigh-Schrödinger expansion diverges for $\|V\|>d/2$. For finite systems the convergence properties of the Rayleigh-Schrödinger and linked-cluster expansions are the same.

[17] Note that one must use the integral relations (15)–(17) in order to take advantage of the superior convergence properties of the series for D_m and N_{nm}. The convergence properties of Eqs. (18)–(20) are similar to those of the Rayleigh-Schrödinger expansion.

where the superscripts in parentheses indicate the maximum order in the perturbation through which the superscripted quantity is correct. (This expression agrees with the Rayleigh-Schrödinger expansion through fifth-order terms, but in addition contains some higher-order contributions.) $\partial^1 D_m^{(3)}$ may be evaluated either by differentiating the defining equation for D_m and substituting values directly into the resulting expression, or—in appropriate situations—by calculating $D_m^{(3)}$ not only at E_m^0 but also at $E_m^0 \pm \delta$ and numerically differentiating. Similarly one sees that (still with $V_{mm}=0$)

$$ {}_0\langle n \,|\, m\rangle^{(3)} = \partial^0 N_{nm}^{(3)} + \tfrac{1}{2}\partial^0 N_{nm}^{(1)} \partial^1 D_m^{(2)} + \partial^0 D_m^{(2)} \partial^1 N_{nm}^{(1)} . \quad (24) $$

Calculation to higher orders than those just considered by utilization of Eqs. (18)–(20) is entirely feasible in principle. However, in practice it would quickly become an unpleasant task because of the necessity for evaluating higher-order derivatives of the D_m and N_{nm}. In situations where a greater accuracy or larger radius of convergence is desired (and perhaps even in some other cases) it is therefore convenient to use a different approach which eliminates the necessity for knowing the derivatives of D_m and N_{nm} and substitutes for it the requirement of knowing these functions for several values of E. After a preliminary calculation by means of Eq. (23) (or perhaps a lower-order expression) to determine an approximate value for E_m, one can select an appropriate curve C_m in the complex energy plane and numerically perform the integrations in Eqs. (15)–(17). For many problems this procedure can be carried out accurately and rapidly on a high-speed computer, so the technique suggested is of more than academic interest.

All of the calculational methods described here make use of the fact that Eqs. (15)–(20) express the perturbation expansions entirely in terms of the partial sums D_m and N_{nm} for which the explicit general form is easily given. The price one must pay for using only D_m and N_{nm} has been seen to be the necessity for knowing these functions for a finite set of values of the energy E, and not just for one. This is not in general a disadvantage, for it essentially amounts to a matter of transferring part of the calculational process from physicist to computer.

It is worth noting that the perturbation expansions given here share some features of both the Rayleigh-Schrödinger and Brillouin-Wigner expansions but avoid some of the difficulties of each. In particular, the series D_m and N_{nm} have the same simple structure as certain quantities appearing in the B-W method, which is a simpler structure than that encountered in the R-S method; but it is not necessary here, as it is in the ordinary B-W procedure, to be able to evaluate these series at E_m (the exact energy eigenvalue of the total Hamiltonian). Instead one may use the series (18)–(20), where everything is evaluated at E_m^0, or the integrals (15)–(17), where the only requirement is that C_m contain the one eigenvalue E_m of H in its interior. This last requirement is considerably less demanding than that of knowing E_m itself. Finally, it should be observed that the fact that the energy shifts and transformation coefficients must be calculated as ratios of the series (18)–(20) allows one to understand somewhat better the relatively complex structure of the Rayleigh-Schrödinger expansions.

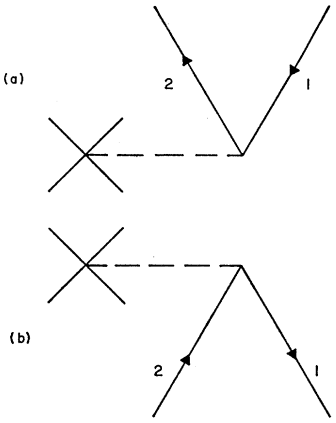

FIG. 2. The two types of vertices which can occur in the one-particle, two-level system.

IV. APPLICATION TO A SIMPLE EXAMPLE

To illustrate the matters which have been discussed, let us consider the (exactly soluble) problem of finding the ground eigenstate and eigenvalue for a simple two-level system described by the Hamiltonian matrix[18]

$$ H = \begin{pmatrix} E_1^0 & \epsilon \\ \epsilon & E_2^0 \end{pmatrix} = \begin{pmatrix} E_1^0 & 0 \\ 0 & E_2^0 \end{pmatrix} + \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix} = H_0 + V . \quad (25) $$

In order to facilitate a subsequent comparison with the linked-cluster expansion[4] it is convenient to take the eigenstate to be nonnormalized, as in that theory; the ground eigenvalue and "correctly nonnormalized" eigenstate of (27) may be seen to be

$$ E_1 = E_1^0 - (\omega/2)\{[1+(2\epsilon/\omega)^2]^{1/2} - 1\} = E_1^0 - \frac{\epsilon^2}{\omega} \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{n!(n+1)!} \left(\frac{\epsilon}{\omega}\right)^{2n} , \quad (26) $$

$$ |1\rangle_{NN} = \begin{pmatrix} 1 \\ -(\omega/2\epsilon)\{[1+(2\epsilon/\omega)^2]^{1/2} - 1)\} \end{pmatrix} , \quad (27) $$

where $\omega \equiv E_2^0 - E_1^0 > 0$.

Now let us obtain these results from the perturbation theory which has been developed in the preceding sections. Since in this case

$$ V_{12} = V_{21} = \epsilon , \quad V_{11} = V_{22} = 0 , $$

[18] An equivalent problem is treated in detail by Katz (Ref. 15).

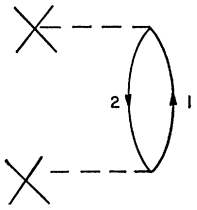

FIG. 3. The second-order contribution to δE_m in the linked-cluster expansion.

one sees that

$$D_1=(\epsilon^2/(E-E_2^0)), \tag{28}$$

$$N_{21}=(\epsilon/(E-E_2^0)); \tag{29}$$

no contributions to either quantity appear above second order. It is then a trivial matter to verify that the integrals (15)–(17) yield the correct values. A somewhat less trivial fact is that the series (18)–(20) can be written out explicitly, and after a negligible amount of computation are found to be

$${}_0\langle 1|1\rangle\langle 1|1\rangle_0=1+\sum_{n=1}^{\infty}\frac{(-1)^n(2n-1)!}{n!(n-1)!}\left(\frac{\epsilon}{\omega}\right)^{2n}, \tag{30}$$

$$\delta E_1\,{}_0\langle 1|1\rangle\langle 1|1\rangle_0=\omega\sum_{n=1}^{\infty}\frac{(-1)^n(2n-2)!}{[(n-1)!]^2}\left(\frac{\epsilon}{\omega}\right)^{2n}, \tag{31}$$

$${}_0\langle 2|1\rangle\langle 1|1\rangle_0=-\frac{\epsilon}{\omega}\sum_{n=0}^{\infty}\frac{(-1)^n(2n)!}{(n!)^2}\left(\frac{\epsilon}{\omega}\right)^{2n}. \tag{32}$$

One may easily check that the ratio of (31) to (30) agrees with (26), and the ratio of (32) to (30) (this yields the nontrivial transformation coefficient for the nonnormalized state vector) agrees with the lower component of (27).

It should be observed that though this is a trivial problem neither the Rayleigh-Schrödinger nor the linked-cluster expansions yield solutions with only a trivial amount of effort. Let us consider briefly the application of the linked-cluster expansion techniques to this system, which we shall think of as being a one-fermion system. Because of the form of the potential only the two types of vertices shown in Fig. 2 can occur. The first-order contribution to $|1\rangle_{NN}$ is given by the

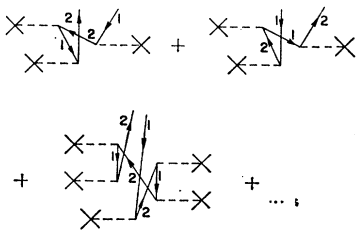

FIG. 4. Higher-order contributions to the state vector in the linked-cluster expansion.

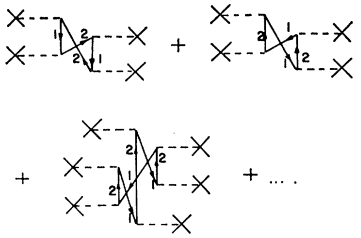

FIG. 5. Higher-order contributions to the energy in the linked-cluster expansion.

diagram of Fig. 2(a); it was noted earlier that this is the *total* contribution to N_{21}. The second-order contribution to δE_1 is shown in Fig. 3, and this in turn is the total contribution to D_1. The higher-order contributions to $|1\rangle_{NN}$ are given in Fig. 4, and the higher-order contributions to δE_1 correspond to the diagrams of Fig. 5. Note that all the diagrams in these two last series are exclusion-principle violating, and that in each case there are an infinite number of them. A comparison of the one-term expressions for D_1 and N_{21} with the infinite series above gives one some appreciation (though this is an extreme example) for the amount of simplification which can sometimes occur when nonphysical intermediate states can be ignored. The example also shows (again, in an extreme case) the difference in the radius of convergence of the series D_m, N_{nm} and the linked-cluster expansions for the energy and state vector; D_m and N_{nm} have infinite "radii of convergence" (being one-term series), while it is obvious from Eqs. (26) and (27) that, precisely because of the exclusion-principle-violating terms, the linked-cluster expansions can only converge for $\epsilon<\omega/2$.

It should be remarked that by dint of ingenuity and considerable effort the form of the general term in the linked-cluster expansions for this problem can be obtained[15]; five pages of concentrated calculation are required, as compared to the three or four lines needed to obtain Eqs. (30)–(32) by means of the methods developed here. This degree of disparity between the two methods in the amount of computational labor required is certainly not general. However, the example indicates that there are certain classes of physical problems (not all as simple as this one) which might be more advantageously treated by the method developed here than by the standard techniques.

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