A Note on Perturbation Theory*

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The perturbation theory for a stationary state is developed in the form of an implicit equation for the eigenvalue and an explicit equation (involving the eigenvalue) for the amplitudes. With the aid of a formal algebraic identity the equation for the eigenvalue is transformed into a semi-explicit form by a procedure having a wider range of validity than the more obvious iteration or power series processes.

THE physical system under discussion possesses quantum states in the space defined by the complete orthonormal set of functions $\psi_1, \psi_2, \cdots\psi_n\cdots$. These functions need not be eigenfunctions of any set of commuting operators; in particular, it is possible to dispense with the conventional separation of the Hamiltonian operator into an unperturbed part H_0, of which the ψ's are eigenfunctions, and a perturbation operator H_1 which couples the unperturbed states.

The eigenfunction of H

$$\psi=\sum a_n\psi_n \tag{1}$$

with the eigenvalue E, is determined by the system of linear homogeneous equations:

$$(E-H_{mm})a_m=\sum_{m\neq n} H_{mn}a_n. \tag{2}$$

An essential preliminary step in the solution of Eq. (2) is the reduction to diagonal form of one or more subspaces in which the diagonal matrix elements of H all have the same value. After the reduction the condition $H_{nm}=0$ for $n\neq m$ holds within each reduced subspace. Following this step Eq. (2) can be solved (at least formally) by a process of successive approximation.

If ψ_k is a good approximation to an eigenfunction of H a suitable starting point is $a_m=\delta_{km}$, $E=H_{kk}$. Successive orders of approximation are derived by inserting the values of a_m from the preceding order into the right-hand member of Eq. (2). The formal solution has the form[1]

$$\begin{aligned}
a_k&=1,\\
a_m&=[H_{mk}/(m)]+\sum_{n\neq k}[(H_{mn}H_{nk})/(m)(n)]+\cdots,\\
E&=H_{kk}+\sum_{m\neq k}[H_{km}H_{mk}/(m)]\\
&\quad+\sum_{mn\neq k}[(H_{km}H_{mn}H_{nk})/(m)(n)]+\cdots,
\end{aligned} \tag{3}$$

in which $(m)=E-H_{mm}$ and only non-diagonal matrix elements occur in the numerators of the sums. Wigner[2] has shown that the energy formula in an odd order $2\nu+1$ is precisely the expectation value of H with respect to the normalized wave function of the ν'th order.

An obvious iteration process starting from $E^{(1)}=H_{kk}$ and employing the expansion

$$[1/(E^{(\mu)}-H_{mm})]=[1/(H_{kk}-H_{mm})]\times\sum_{\nu=0}^{\infty}[(H_{kk}-E^{(\mu)})/(H_{kk}-H_{mm})]^{\nu} \tag{4}$$

transforms Eq. (3) into an explicit formula for E in which all energy denominators have been reduced to differences of diagonal matrix elements. This last form is equivalent to the Schroedinger perturbation formula[3] derived as a rule by assuming that all eigenfunctions and eigenvalues can be expressed as power series in an expansion parameter (i.e., the fine structure constant in the electromagnetic self-energy problem). In many applications the convergence condition for the infinite series of Eq. (4) fails and the explicit formula for E then embodies an

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[1] L. Brillouin, J. de phys. et rad., III, 373 (1932).

[2] E. P. Wigner, Math. u. Naturwiss. Anzeig. d. Ungar. Akad. Wiss. L III, 475 (1935).

[3] E. C. Kemble, *The Fundamental Principles of Quantum Theory* (McGraw-Hill Book Company, Inc., New York, 1937).

infinitely reiterated series of logical contradictions. One important characteristic of the iteration process is that it removes an infinite series of higher order terms (generated by the expansion of the denominators) from each summation in Eq. (3).

The present note is concerned with the transformation of Eq. (3) into a semi-explicit form by a procedure having a wider range of validity than the iteration process.

The discussion of Eq. (3) is facilitated by the introduction of the set of auxiliary functions.

$$\mathcal{E}_{km\cdots pq}\equiv H_{qq}+\sum_{r\neq km\cdots pq}\frac{H_{qr}H_{rq}}{(r)}+\sum_{rs\neq km\cdots pq}\frac{H_{qr}H_{rs}H_{sq}}{(r)(s)}+\cdots. \quad (5)$$

It is clear that $\mathcal{E}_{km\cdots q}$ can be identified with an eigenvalue only when $k=m=\cdots=q$; then $E=\mathcal{E}_{kk\cdots k}(E)\equiv\mathcal{E}_k(E)$.

The formal algebraic identity

$$\sum_{\nu=0}^{\infty}[(\mathcal{E}_{km\cdots pq}-H_{qq})/(E-H_{qq})]^{\nu}=1+\sum_{r\neq km\cdots p}[(H_{qr}H_{rq}/((q)(r))]+\sum_{rs\neq km\cdots p}[(H_{qr}H_{rs}H_{sq})/((q)(r)(s))]+\cdots. \quad (6)$$

$(q\neq km\cdots p)$ can be verified by expanding the right-hand sums as products of sums like those which appear in Eq. (5). Identical products of sums then occur on both sides of Eq. (6) multiplied by identical binomial coefficients. An essential factor in the identity is the absence of terms in Eq. (5) for which the variable indices take on the value q. If

$$|\mathcal{E}_{km\cdots pq}-H_{qq}|<|E-H_{qq}|, \quad (7)$$

Eq. (6) reduces to

$$1/(E-\mathcal{E}_{km\cdots pq})=[1/(q)][1+\sum_{r\neq km\cdots p}[(H_{qr}H_{rq})/((q)(r))]+\sum_{rs\neq km\cdots p}[(H_{qr}H_{rs}H_{sq})/((q)(r)(s))]+\cdots],\quad (q\neq km\cdots p). \quad (8)$$

If the convergence condition (7) fails, then it is suggested that the left-hand member of Eq. (8) is equivalent to the series on the right in the sense of an analytical continuation. In the application of Eq. (8) the left-hand member replaces the infinite (and possibly divergent) series on the right whereas the reverse procedure is followed in the application of Eq. (4).

The general term in the formal series for a_m is expanded in the algebraic identity

$$\sum_{np\cdots rs\neq k}\frac{H_{mn}\cdots H_{sk}}{(m)\cdots(s)}\equiv\sum_{np\cdots rs\neq km}\frac{H_{mn}\cdots H_{sk}}{(m)\cdots(s)}+\sum_{np\cdots rs\neq k}\frac{H_{mn}\cdots H_{rm}}{(m)\cdots(r)}\frac{H_{mk}}{(m)}+\cdots+\sum_{n\neq k}\frac{H_{mn}H_{nm}}{(m)(n)}\sum_{p\cdots rs\neq km}\frac{H_{mp}\cdots H_{sk}}{(m)\cdots(s)}. \quad (9)$$

With the aid of Eqs. (8) and (9) the formal series for a_m is transformed into

$$a_m=\frac{H_{mk}}{E-\mathcal{E}_{km}}+\sum_{n\neq km}\frac{H_{mn}}{E-\mathcal{E}_{km}}\left[\frac{H_{nk}}{(n)}+\sum_{p\neq km}\frac{H_{np}H_{pk}}{(n)(p)}+\sum_{pq\neq km}\frac{H_{np}H_{pq}H_{qk}}{(n)(p)(q)}+\cdots\right]. \quad (10)$$

Again employing Eq. (8) and an obvious generalization of Eq. (9), the factor in square brackets in Eq. (10) can also be transformed and the process continued indefinitely to yield the result

$$a_m=\frac{H_{mk}}{E-\mathcal{E}_{km}}+\sum_{n\neq km}\frac{H_{mn}H_{nk}}{(E-\mathcal{E}_{km})(E-\mathcal{E}_{kmn})}+\sum_{\substack{n\neq km\\ p\neq kmn}}\frac{H_{mn}H_{np}H_{pk}}{(E-\mathcal{E}_{km})(E-\mathcal{E}_{kmn})(E-\mathcal{E}_{kmnp})}+\cdots \quad (11)$$

Equation (2) now yields

$$E=H_{kk}+\sum_{m\neq k}H_{km}a_m=H_{kk}+\sum_m{}^*\frac{H_{km}H_{mk}}{E-\mathcal{E}_{km}}+\sum_{mn}{}^*\frac{H_{km}H_{mn}H_{nk}}{(E-\mathcal{E}_{km})(E-\mathcal{E}_{kmn})}+\cdots. \quad (12)$$

The star on the summation symbol signifies that there are no duplications among the variable indices $mnpq\cdots$ and furthermore that $mnpq\cdots\neq k$:

$$\sum_{mnp\cdots}{}^{*}\equiv\sum_{mnp\cdots}(m\neq k,\ n\neq km,\ p\neq kmn,\ \cdots).\tag{13}$$

Since $E=\mathcal{E}_{k\cdots k}(E)\equiv\mathcal{E}_k(E)$ the energy denominators in Eqs. (11) and (12) can be replaced by

$$\mathcal{E}_k(E)-\mathcal{E}_{km\cdots pq}(E)=H_{kk}-H_{qq}+\left[\sum_{r\neq k}\frac{H_{kr}H_{rk}}{(r)}-\sum_{r\neq km\cdots pq}\frac{H_{qr}H_{rq}}{(r)}\right]+\cdots,\tag{14}$$

which may be convergent even when $\mathcal{E}_k$ and $\mathcal{E}_{km\cdots pq}$ are separately divergent. There is also the possibility that the usual substitution of $H_{kk}-H_{qq}$ for $E-H_{qq}$ in the second- and third-order terms of Eq. (3) may be justified in particular cases even when $|E-H_{qq}|\gg|H_{kk}-H_{qq}|$.

A straightforward generalization of the procedure yielding Eqs. (11) and (12) transforms $\mathcal{E}_{km\cdots pq}$ into a form similar to Eq. (12). The result is

$$\mathcal{E}_{km\cdots pq}=H_{qq}+\sum_{r\neq km\cdots pq}\frac{H_{qr}H_{rq}}{E-\mathcal{E}_{km\cdots pqr}}+\sum_{\substack{r\neq km\cdots pq\\ s\neq km\cdots pqr}}\frac{H_{qr}H_{rs}H_{sq}}{(E-\mathcal{E}_{km\cdots pqr})(E-\mathcal{E}_{km\cdots pqrs})}+\cdots.\tag{15}$$

For computing the required energy denominators Eq. (15) may be replaced, with advantage, by

$$\mathcal{E}^{*}_{km\cdots pq}=H_{qq}+\sum_{r\neq km\cdots pq}\frac{H_{qr}H_{rq}}{\mathcal{E}_k-\mathcal{E}^{*}_{km\cdots pqr}}+\sum_{\substack{r\neq km\cdots pq\\ s\neq km\cdots pqr}}\frac{H_{qr}H_{rs}H_{sq}}{(\mathcal{E}_k-\mathcal{E}^{*}_{km\cdots pqr})(\mathcal{E}_k-\mathcal{E}^{*}_{km\cdots pqrs})}+\cdots.\tag{16}$$

Now $\mathcal{E}^{*}_{km\cdots pq}=\mathcal{E}_{km\cdots pq}$ when $E=\mathcal{E}_k(E)$ so that the physical solution of Eq. (12) is also a solution of the modified equation obtained by substituting $\mathcal{E}_k-\mathcal{E}^{*}_{km\cdots pq}$ for $E-\mathcal{E}_{km\cdots pq}$ in Eq. (12).

For the special case of a finite matrix (of order N) the right-hand members of Eqs. (11), (12), and (15) are finite rational functions of the energy and the matrix elements. In this case the analytical continuation mentioned in the sentence following Eq. (8) has a precise meaning. First suppose that all non-diagonal matrix elements are multiplied by a convergence factor λ. For a sufficiently small upper bound on the absolute value of λ, Eq. (3) is unobjectionable and can be solved rigorously by the iteration process; furthermore, all the infinite sums involved in Eqs. (6) and (8) are convergent. Adding the fact that Eq. (12) is an algebraic equation of degree N in E, the conclusion follows that it is simply a convenient way of writing the characteristic equation

$$||E\delta_{mn}-H_{mn}||=0.\tag{17}$$

Since Eqs. (12) and (17) are both algebraic equations of degree N in E, the irrelevant restriction on λ may be dropped. The special cases $N=2$ and 3 provide instructive, though trivial, illustrations of the above remarks.