regions.

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[1]A. M. Friedman, H. J. Fortune, G. C. Morrison, and R. H. Siemssen, in *Proceedings of the International Conference on Nuclear Reactions Induced by Heavy Ions, Heidelberg, July 1969,* edited by R. Bock and W. R. Hering (North-Holland, Amsterdam, 1970), p. 171.

[2]H. Faraggi, A. Jaffrin, M. C. Mermaz, J. C. Faivre, J. Gastebois, B. G. Harvey, J. M. Loiseaux, and A. Papineau, Ann. Phys. (New York) 66, 905 (1971).

[3]H. Faraggi, M. C. Lemaire, J. M. Loiseaux, M. C. Mermaz, and A. Papineau, Phys. Rev. C 4, 1375 (1971).

[4]A. Cunsolo *et al.*, J. Phys. (Paris), Colloq. 6, 171 (1971).

[5]I. Rotter, Nucl. Phys. A122, 567 (1968), and A135, 378 (1969), and Fortschr. Phys. 16, 195 (1968); D. Robson, Comments Nucl. Particle Phys. 5, 16 (1972).

[6]K. Bethge, Annu. Rev. Nucl. Sci. 20, 255 (1970), and references therein.

[7]L. J. Denes, W. W. Daehnick, and R. M. Drisko, Phys. Rev. 148, 1097 (1966).

[8]H. W. Fulbright and J. A. Robbin, University of Rochester Report No. UR-NSRL-9, 1969 (unpublished), and Nucl. Instrum. Methods 71, 237 (1969).

[9]L. C. Farwell, J. J. Kraushaar, and W. W. Baer, Nucl. Phys. A186, 545 (1972).

[10]P. D. Kunz, Code DWUCK, Boulder, Colo.

[11]C. Mairle *et al.*, Nucl. Phys. A134, 180 (1969).

[12]U. C. Voos, W. von Oertzern, and R. Bock, Nucl. Phys. A135, 207 (1969).

[13]H. H. Gutbrod, H. Yoshida, and R. Bock, Nucl. Phys. A165, 240 (1971).

[14]G. Bassani, N. M. Hintz, and C. P. Kavaloski, Phys. Rev. 136, B1006 (1969).

[15]W. P. Alford, R. Lindgren, and D. Elmore, private communication.

Continued-Fraction Method for Perturbation Theory

D. F. Scofield*

Aerospace Research Laboratories, Wright-Patterson Air Force Base, Ohio 45433

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A direct operational approach to the solution of the Schrödinger equation has led to an iterative nonperturbative method for its solution. The method, when applied to the Mathieu equation and the anharmonic-oscillator equation, is superior to the perturbation-iteration method and to Rayleigh-Schrödinger perturbation theory both in terms of rate of convergence and range of coupling constant allowed.

In the application of the linked-cluster many-body perturbation theory (LCMBPT) to atoms[1] one must evaluate ever more topologically complicated diagrams. Moreover, the theory is not especially rapidly convergent if precise results are desired. In addition, special techniques must be employed to sum to infinite order certain classes of diagrams. Thus, it would be of advantage for practical calculations to develop a formalism which eliminates many of the difficulties with LCMBPT, but which retains as many of the virtues of LCMBPT as possible. This Letter presents a summary of a contribution to this endeavor. The method reported has as its asymptotic expansion the Rayleigh-Schrödinger perturbation theory (RSPT), but converges for the case of the anharmonic oscillator in three iterations where RSPT diverges. The method provides more rapidly convergent results for the Mathieu equation than perturbative approaches.

We begin by considering the motivation which led to the continued-fraction method (CFM) which has provided these results. Consider the time-independent Schrödinger equation $H|\alpha\rangle = E_\alpha|\alpha\rangle$ for any state $|\alpha\rangle$, assumed for simplicity to be nondegenerate and not necessarily the ground state. A splitting of the Hamiltonian is assumed of the form $H = H_0 + \lambda V$ with $H_0|\alpha\rangle_0 = E_\alpha{}^0|\alpha\rangle_0$. From here on we will suppress the α subscripts and the explicit indication of the dependence of the perturbation (λV) on the coupling constant λ. Let $P_0 = |\alpha\rangle_{00}\langle\alpha|$ and $Q_0 = 1 - P_0$ with $P_0{}^2 = P_0$ and $P_0{}^\dagger = P_0$ be projection operators onto and out of the space spanned by $|\alpha\rangle_0$. Then with the introduction of the reduced resolvent $T_0(E) = Q_0/(E - H_0)$, we can obtain the reaction operator (or transition operator) $t(E)$ for the state $|\alpha\rangle$, whose matrix elements give the level shifts

$$E - E^0 = {}_0\langle\alpha|t(E)|\alpha\rangle_0, \tag{1}$$

where

$$t(E) = V + VT_0(E)t(E). \tag{2}$$

The Lippman-Schwinger equation (2)[2] may be

solved for $t(E)$, yielding

$$t(E) = (1 - VT_0)^{-1}V = V(1 - T_0V)^{-1}$$
$$= V^{1/2}(1 - V^{1/2}T_0V^{1/2})^{-1}V^{1/2}. \quad (3)$$

Then, using the Cauchy formula, Eq. (1) may be transformed to

$$_0\langle\alpha|\, E - E^0 - \frac{1}{2\pi i}\oint \frac{t(\epsilon)P_0 d\epsilon}{\epsilon - E}\,|\alpha\rangle_0 = 0. \quad (4)$$

The contour includes the eigenvalue E. If we then introduce an equivalent operator h such that $E|\alpha\rangle_0 = (E^0+h)|\alpha\rangle_0$, then Eq. (4) may be written as

$$_0\langle\alpha|\, E - E^0 - \frac{1}{2\pi i}\oint \frac{t(\epsilon)P_0 d\epsilon}{\epsilon - E^0 - h}\,|\alpha\rangle_0 = 0.$$

This equation will be satisfied if h satisfies

$$h = \frac{1}{2\pi i}\oint \frac{t(\epsilon)P_0 d\epsilon}{\epsilon - E^0 - h}. \quad (5)$$

Since $\epsilon = E^0 + h$ merely shifts the denominator of $T_0(\epsilon_0)$ from ϵ_0, h will exist anywhere in virtue of Eq. (5) except at those points where λ is an eigenvalue λ_k of the operator $1 - \lambda T_0(E^0+h)V$. Thus, it is seen that h will exist whenever $t(E^0+h_k)$ exists, where h_k is an eigenvalue of h.

Now if in Eq. (5) we were dealing only with scalar functions instead of noncommuting operators, $t(\epsilon)$ would have the form of a linear fractional transformation. This would lead to a continued-fraction expansion for h. In our case, even though it can be shown that $t(\epsilon)$ may be expressed as a composition of two successive operator-valued linear fractional transformations, thus leading to a continued fraction for operators, a simpler method may be employed. We merely note that a continued-fraction expansion can also be obtained from developing the continued-fraction solution to the quadratic equation

$$Bh^2 + h = A. \quad (6)$$

Our task is then to obtain the operators B and A from which we can find the $n+1$st approximant from the nth via the recursion relation

$$h_{n+1} = (1 + Bh_n)^{-1}A, \quad h_0 = y, \quad (7)$$

which has the continued-fraction form

$$h = [1 + B(1 + B\cdots)^{-1}A]^{-1}A, \quad h_0 = A.$$

An equation of the required form of Eq. (6) leading to the determination of the operators B and A may be obtained using the methods developed by Löwdin,[3] Block and Des Cloizeaux,[4] and others.[5] The equation is obtained as follows: Consider

$$(H - E^\alpha - e)|\alpha\rangle = 0, \quad (8)$$

where $E^\alpha + e = E$ and $e = E^0$ is the eigenvalue associated with the unperturbed eigenfunction $|\alpha\rangle_0$ whose adiabatic transform is $|\alpha\rangle$. In Eq. (8) if we multiply on the left-hand side by P_0, we obtain

$$P_0V|\alpha\rangle = E^\alpha|\alpha\rangle_0, \quad (9)$$

since $P_0(H - e) = P_0(H_0 - e + V) = P_0V$. The normalization of $|\alpha\rangle$ is chosen so that $P_0|\alpha\rangle = |\alpha\rangle_0$. By multiplying Eq. (9) by the operator U (assumed existent), which is defined to satisfy

$$U|\alpha\rangle_0 = |\alpha\rangle, \quad UP_0 = U, \quad (10)$$

we then obtain $UV|\alpha\rangle = E^\alpha|\alpha\rangle$. When this relation is substituted into Eq. (8), we obtain

$$(H - e - UV)|\alpha\rangle = 0. \quad (11)$$

Because of the first relation of Eq. (10), we have for the representation of U

$$U = |\alpha\rangle\, {}_0\langle\alpha|. \quad (12)$$

Therefore, multiplying on the right-hand side of Eq. (11) by $_0\langle\alpha|$, we obtain

$$(H - e - UV)U = 0$$

or (13)

$$(e - H_0)U = VU - UVU.$$

Since $U = (P_0 + Q_0)U$ and $P_0U = P_0$, we obtain

$$(e - H_0)Q_0U = VU - UVU.$$

Hence

$$Q_0U = T_0(e)(VU - UVU). \quad (14)$$

Equation (14) may be rewritten with the help of the definition $h \equiv VU$ as

$$t(e)T_0(e)V^{-1}h^2 + h = t(e)P_0. \quad (15)$$

It can be shown that the operator h appearing in Eq. (15) is the same one as in Eq. (5).[6] Clearly Eq. (15) is of the desired form. A proof of convergence of the recursive process in Eq. (4) for Eq. (15) can be obtained by a modification of a proof of McFarland.[7] The following criteria is obtained as a by-product of the proof when the initial approximation is $h_0 = t(e)P_0$:

$$\|[1 - VT_0(e)]^{-1}\|^2\|VT_0(e)\| < y_A. \quad (16)$$

In relation (16) $\|\cdots\|$ denotes the norm of the linear operator appearing between the pair of vertical double bars. The norm of the operator is defined relative to the norm of a vector in the Hilbert space by using the inner product defined on the space in the following manner: Let $|u\rangle$ and $|v\rangle$ be the vectors in the space, then the norm of

TABLE I. Mathieu-equation comparison of RSPT, PI, and CFM level-shift results for $\lambda = 2.0$ ($\|\lambda V\|/d = \frac{1}{2}$) for the ground state. The exact result by eighth-order CFM is 0.878 234.

CFM	PI	RSPT	Order
0.8788	0.8333	0.8750	2
0.8783	0.8920	0.8750	3
0.8782	0.8737	0.8784	4

TABLE II. Mathieu-equation comparison of RSPT, PI, and CFM level-shift results for $\lambda = 4.0$ ($\|\lambda V\|/d = 1$) for the ground state. The exact result by eighth-order CFM is 1.544 86.

CFM	PI	RSPT	Order
1.5552	1.0000	1.5000	2
1.5466	1.7778	1.5000	3
1.5452	1.1541	1.5547	4

a vector $u = \|u\| \equiv \langle u|u\rangle^{1/2}$. Let L be a linear operator defined on some subspace of the Hilbert space, then the norm of the operator $L = \|L\|$, defined as the greatest lower bound of the non-negative numbers C in the set S, where the set $S = \{C: \|Lu\| = \|v\| \leq C\|u\|$, for any vector $|u\rangle$ in the domain of the operator $L\}$. Relation (16) then yields the following two minimal regions of convergence:

$$0 < \|V\|/d < 3 - 2\sqrt{2}$$

and

$$\|V\|/d > 3 + 2\sqrt{2}.$$

In the above V is the perturbation and d is the distance of isolation of the eigenvalue e from the nearest different eigenvalue e' in the spectrum of H_0. That is, $d = |e - e'|$.

It can be shown[6] that in the solution of Eq. (15) via the recurrence given by Eq. (7), all disconnected diagrams cancel, leaving a result that depends linearly upon the number of particles N of the system. A time-dependent version of the theory has been constructed and the application of the method to potential scattering has been considered. The application of CFM to the calculation of the nonrelativistic bound-state spectrum of fluorine has begun. The extension of the method to the degenerate case has been completed, as has been the considerations necessary to calculate the expectation values of other operators than the level-shift operator h.[6]

In order to indicate the possible usefulness of the method we present a comparison of CFM, RSPT, and perturbation-iteration (PI) results for various coupling constants for the Mathieu equation ($H_0 = -d^2/d\theta^2$, $\lambda V = \lambda \cos^2\theta$). Formulas for the RSPT and PI results can be found in Morse and Feshbach.[8] We also present some results on the anharmonic-oscillator problem ($H_0 = -d^2/dx^2 + x^2$, $\lambda V = \lambda x^4$). All calculations were done in sigle precision using 20×20 matrices to represent the operators involved except for the anharmonic-oscillator results where 10×10 matrices were used. No attempt has been made to be especially numerically accurate. The aim has been merely to show that the method works. In passing, it is interesting to note that the Feenberg perturbation theory[9] in the case of the Mathieu equation yields a continued fraction which can also be obtained from the PI method using Padé approximants to the PI series. The continued fraction, however, is different from the one used in the CFM.

In the case of the Mathieu equation, from Tables I and II for the ground state, and III and IV for the sixth excited state, we see that RSPT is better than the PI method for the cases shown, and that CFM gives better results than either RSPT or the PI method. For the anharmonic oscillator, CFM gives rapid convergence to correct eigenvalues (see Table V). In the case of the anharmonic oscillator the proof of the convergence for CFM, together with the proof of the asymptotic equivalence of the RSPT to CFM, gives an alternate proof for the asymptotic convergence of RSPT for the anharmonic oscillator.[6] This does not prove that RSPT converges though. A general point may be made in closing, that is, the level-shift operator h satisfies a quadratic equation; hence, a perturbation theory or a data-fitting method, such as the usual Padé method for this problem,[10] may lead to excess computation if this is not taken into account.[6]

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TABLE III. Mathieu-equation comparison of RSPT, PI, and CFM level-shift results for $\lambda = 2.0$ ($\|\lambda V\|/d = \frac{1}{10}$) for the sixth excited state ($E_0^6 = 36.0$). All methods are rapidly convergent.

CFM	PI	RSPT	Order
1.003 55	1.000 00	1.000 00	1
1.003 57	1.003 56	1.003 57	2

TABLE IV. Mathieu-equation comparison of RSPT, PI, and CFM level-shift results for $\lambda = 30.0$ ($\|\lambda V\|/d = \frac{3}{2}$) for sixth excited state ($E_0^6 = 36.0$).

Order	RSPT	PI	CFM
n	Diverges	Questionable convergence	Converges to a solution in the second Riemann sheet which when transformed to the first sheet gives 15.8290

TABLE V. Anharmonic-oscillator comparison of CFM level-shift results for the ground state with rigorous upper and lower bounds given by Bazley and Fox and by Reid. The first 41 terms of RSPT give a level shift of approximately 10^{26} (Ref. 10).

λ	Upper bound[a]	CFM	Lower bound[b]
0.1	0.065 286	0.065 285 5	0.065 285
0.2	0.118 293	0.118 292 6	0.118 292
0.5	0.241 957	0.241 854 0	0.241 811
0.8	0.338 096	0.337 545 5	0.337 397
1.0	0.393 371	0.392 353 1	0.392 131

[a]Ref. 11. [b]Ref. 12.

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*National Academy of Sciences–National Research Council postdoctoral associate.

[1]K. A. Brueckner, Phys. Rev. 97, 1353 (1955); K. Goldstone, Proc. Roy. Soc., Ser. A 239, 267 (1957); H. P. Kelly, Advan. Chem. Phys. 14, 129 (1969).

[2]B. A. Lippman and J. Schwinger, Phys. Rev. 79, 469 (1950).

[3]For example, P.-O. Löwdin, in *Perturbation Theory and its Applications in Quantum Mechanics*, edited by C. H. Wilcox (Wiley, New York, 1966).

[4]C. Bloch, Nucl. Phys. 6, 329 (1958); J. Des Cloizeaux, Nucl. Phys. 20, 321 (1960).

[5]O. Goscinski and E. Brandas, Int. J. Quantum Chem. 5, 131 (1971); E. Brandas and O. Goscinski, Phys. Rev. A 1, 552 (1970); J. O. Hirshfelder, Int. J. Quantum Chem. 3, 731 (1969); H. Silverstone and T. T. Holloway, Phys. Rev. A 4, 2191 (1971).

[6]D. F. Scofield, to be published.

[7]J. E. McFarland, Proc. Amer. Math. Soc. 9, 824 (1958).

[8]P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. II, Chap. 9.

[9]E. Feenberg, Phys. Rev. 74, 206 (1948).

[10]J. J. Loeffel, A. Martin, B. Simon, and A. S. Wightman, Phys. Lett. 30B, 656 (1969).

[11]N. Bazley and D. Fox, Phys. Rev. 124, 483 (1961).

[12]C. Reid, J. Chem. Phys. 43, S186 (1965).

Transition Counter*

C. L. Wang, G. F. Dell, Jr., H. Uto, and Luke C. L. Yuan
Brookhaven National Laboratory, Upton, New York 11973
(Received 30 June 1972)

We report a new type of counter based on the transition radiation from ultrarelativistic charged particles. The efficiency of the "transition counter" depends almost linearly on the Lorentz factor of the particle in the energy region covered and is over 80% for 2-GeV electrons. Particles heavier than electrons in a 2-GeV unseparated beam are effectively rejected. A possible application of the counter at multihundred-GeV accelerators is discussed.

In the ultrarelativistic region, where the particle velocities approach the velocity of light, conventional Cherenkov and time-of-flight detectors lose their effectiveness in particle identification. It is important therefore to develop new methods of particle identification based on effects which do not approach a limit or "saturate" at very high energies. The transition radiation, which is emitted by a moving charge crossing the interface of different media,[1] and the intensity of which in the