Arab J. Math. Sc.
Volume 1, Number 1, June 1995
pp. 95-111

GENERAL FORMULATION OF THE PADÉ APPROXIMANTS TO THE PERTURBATION SERIES IN NON-RELATIVISTIC QUANTUM MECHANICS

A.B. KHALIL

ABSTRACT. The aim of this work is two fold: First, to bring into focus a unified formulation of perturbation theory as used in nonrelativistic quantum mechanics. This enables us to obtain the different types of perturbation methods used to calculate the energy level shift, in the discrete spectrum, produced by the perturbation and, one should emphasize, the scattering phase shift in the continuous spectrum. Secondly, as an application to this unified formulation, we report some new results for a general formulation of the theory of the application of Padé approximants in nonrelativistic quantum mechanics which, in the case of a singular potential, is a preliminary working laboratory for the non-renormalizable field theories.

1. REVIEW OF STATIONARY STATE PERTURBATION THEORY

Quantum mechanical systems with a finite number of degrees of freedom are usually described by a Hamiltonian H which is self-adjoint and semi-bounded below. The spectrum of H often consists of two parts: a monotonic increasing sequence of discrete eigenvalues $E_0, E_1, \ldots, E_n, \ldots$ with only one point of accumulation, and a continuum above them. The lowest lying or minimum, eigenvalue E_0, commonly called the ground state eigenvalue, is, in most practical cases of interest, nondegenerate.

Assume that H can be decomposed into the sum of two parts each of which is self- adjoint:

(i) an unperturbed part H_0 having known discrete and nondegenerate eigenvalues E_n^0, $n = 0, 1, 2, \ldots$, below the continuous spectrum. We arrange the eigenvalues of H_0 in an ascending order

$$E_0^0 < E_1^0 < \ldots < E_n^0 < \ldots,$$

the corresponding set of eigenvectors $\{|\phi_n >, n = 0, 1, 2, \ldots\}$ of H_0 are othonormalized such that

$$H_0|\phi_n >= E_n^0|\phi_n >, \quad <\phi_m|\phi_n >= \delta_{mn} \tag{1.1}$$

We assume that the unperturbed eigenvectors of H_0, the $|\phi_n >$'s, form a complete set and that together with the eigenvalues, the E_n^0's, are known.

(ii) A perturbing part $V = H - H_0$, which in practice represents the potential, that is the interaction between the different constituents of the quantum mechanical system.

In general one introduces a perturbation parameter, g, commonly known as the coupling constant, such that

$$H(g) = H_0 + gV \tag{1.2}$$

with the corresponding discrete part of the spectrum $E_0(g) < H_1(g) < \ldots < E_n(g) < \ldots$ and corresponding eigenvectors $|\psi_0(g) >, |\psi_1(g) >, \ldots, |\psi_n(g) >, \ldots$, respectively such that

$$H(g)|\psi_n(g) >= E_n(g)|\psi_n(g) > \tag{1.3}$$

The original Hamiltonian, H, is obtained by putting $g = 1$ in $H(g)$, while the unperturbed Hamiltonian H_0 is obtained by switching off the perturbation, that is putting $g = 0$ in $H(g)$, i.e. $H_0 = H(0)$.

The several, seemingly different, devised perturbation methods, evaluate the unknown perturbed eigenvalues E_n and eigenvectors $|\psi_n>$ of the perturbed Hamiltonian H in terms of the known perturbed eigenvalues E_n^0 and eigenvectors $|\phi_n>$ of the unperturbed Hamiltonian H_0. This may be achieved either explicitly as in the Rayleigh-Schrödinger (RS) known perturbation expansion, or implicitly as in the Brillouin-Wigner (BW) ([1],[2]) scheme. There are other methods of interest like the Eden-Francis method [3] and the Tanaka-Fukuda method ([4],[5]). Each has its advantages and disadvantages and one generally selects the method which is appropriate when applied to a certain field of application. However, they all have a common origin. One obtains the different perturbation methods by making different choices for a certain arbitrary operator in a general formulation given by Watson [6] and by Watson and Riesenfeld [7]. This general formulation has the advantage of being readily suitable for the passage from the bound state perturbation theories of discrete (energy) eigenvalues to the case of the continuous scattering states of continuous eigenvalues. The details of this methods will be laid down in what follows.

Although the present formal considerations will not be so limited, it is convenient - for later discussions - to require that the quantum mechanical system under considerations be confined to a box of finite volume v. This is consistent with the assumption that the eigenfunctions $|\phi_n>$ and $|\psi_n>$ and their corresponding eigenvalues E_n^0 and E_n, $n = 0, 1, 2, \ldots,$ are discrete.

To solve equation (3) - dropping the parameter g for simplicity -

$$H|\psi_n>= E_n|\psi_n>, \tag{1.3}$$

one introduces the Green's function operator - or equivalently the resolvent of equation (3),

$$G(E) = (E - H)^{-1} \tag{3a}$$

satisfying the relation $(E-H)G = I$, I being the identity operator. Here, one looks upon E as a complex variable. The matrix elements of $G(E)$ in the $|\phi>$ representation are

(3b) $$< \phi_m|G|\phi_n >=< \phi_m|(E-H)^{-1}|\phi_n >$$

and by inserting the identity operate I and expanding it in terms of the assumed complete set of eigenfunctions $|\psi_n >$ and their corresponding eigenvalues E_n, $n = 0, 1, 2, \ldots$, of H, we may write

(3c) $$< \phi_m|G(E)|\phi_n >= \sum_s \frac{< \phi_m|\psi_s >< \psi_s|\phi_n >}{E - E_s}.$$

Clearly $G(E)$ has poles at $E = E_s$ for all values of s.

The task of finding the eigenvalues E_s of equation (3) is clearly seen to be equivalent to that of finding the poles at $E = E_s$ of the matrix elements of $G(E)$. Alternatively one may formulate this as a search for the zeros of the - reciprocal - algebraic equation.

(4a) $$[< \phi_m|G(E)|\phi_n >]^{-1} = 0$$

for the eigenvalue $E = E_n$ say. The diagonal matrix elements of G are particularly convenient for this purpose. Let us therefore define

(5) $$G_{nn}(E) \equiv < \phi_n|G(E)|\phi_n >,$$

and we have, as a special case of equation (4a),

(4b) $$[G_{nn}(E)]^{-1} = 0.$$

To evaluate $G_{nn}(E)$ ([8]), we have from equation (3)

(6) $$(E - H_0)G = I + VG.$$

Equivalently we may write

(6a) $$G = (E - H_0)^{-1} + (E - H_0)^{-1}VG$$

The preceding equation shows that to know the diagonal matrix elements of G requires the knowledge of its off-diagonal matrix elements. One then can show that equation (6a) may be put into a more convenient form by introducing a new operator F defined by the equation (cf.[9])

$$< \phi_m|G(E)|\phi_n >=< \phi_m|F|\phi_n > G_{nn} \tag{7a}$$

where G_{nn} is defined by equation (5). Equivalently one may write equation (7a) in an operator form

$$G = FY, \tag{7b}$$

where Y is the diagonal matrix,

$$< \phi_m|Y|\phi_n >= G_{nn}\delta_{mn} \tag{8}$$

From equations (7b) and (8) one sees that the diagonal matrix elements of F are unity, that is

$$< \phi_n|F|\phi_n >= 1 \tag{9}$$

Substituting from equation (7b) into equation (6) one gets

$$(E - H_0)FY = I + VFY \tag{10}$$

The diagonal matrix element of this equation would give by inserting the identity operator between F and Y and using equations (7b), (8) and (9)

$$(E - E_n^0)G_{nn} = 1 + X_{nn}G_{nn} \tag{11}$$

where

$$X_{nn} =< \phi_n|VF|\phi_n > \tag{12a}$$

is the diagonal matrix element of the operator

$$X = VF \tag{12b}$$

One can readily solve the simple algebraic equation (11) for G_{nn} and thus gets

(13) $$G_{nn} = [E - E_n^0 - X_{nn}(E)]^{-1}$$

We have previously seen that to look for the eigenvalues E_n of H, one has to look for the poles of the matrix elements of $G(E)$ which turned to be the solution of the algebraic equation $[G_{nn}(E)]^{-1} = 0$. Thus in view of equation (13), the required eigenvalues are solutions of the algebraic equation

(14a) $$E_n = E_n^0 + X_{nn}(E_n)$$

This equation may be explicitly solved for the eigenvalue E_n and thus plays a fundamental role in perturbation theory.

Equation (14a) may be alternatively written as

(14b) $$\Delta E_n \equiv E_n - E_n^0 = X_{nn}(E_n) =< \phi_n|VF|\phi_n >$$

and the left hand side of this equation is the shift in the corresponding eigenvalues due to switching on the perturbation V. That is why $X = VF$ is commonly called the "level shift" operator. That is, its diagonal matrix elements represent the shift between the "unperturbed" (energy) eigenvalue E_n^0 and corresponding the perturbed (energy) eigenvalue E_n.

We have seen that in the process of arriving at equation (14), that we have repeatedly inserted the identity operator I and expanded it in terms of the complete set of eigenfunctions $\{|\phi_n >, n = 0, 1, 2, \ldots\}$. In fact one can use any complete set of functions for this expansion. However, preference for using the unperturbed eigenfunctions stems from the fact that in practice one generally takes $|\phi_n >$ to be a reasonable approximation of $|\psi_n >$, since the latter tends to the former when the perturbation is switched off [10]. Also in the theory of Padé approximants $|\phi_n >$ plays a fundamental role of relating the approximants to the diagonal matrix elements of the resolvent of the eigenvalue equation [11].

Our task now is to solve equation (14) to obtain the level shift X_{nn}. To achieve that let us go back to equation (10).

$$(E - H_0)FY = I + VFY \tag{10}$$

For a solution one tries to invert the operator $(E - H_0)$, and since we are assuming that E - from a mathematical point of view - is a complex quantity, this operator is in general singular [12]. So to invert $(E - H_0)$, and making use the experience gained from the theory of complex contour integration, one begins first by "displacing" it in an (essentially) arbitrary manner. So introducing an arbitrary operator D, equation (10) may evidently be rewritten in the form

$$(E - H_0 - D)FY = I + (V - D)FY \tag{15}$$

For our purpose it is simple, sufficient and convenient to assume that D is diagonal with respect to $\{|\phi_n>, n = 0, 1, 2, \ldots\}$; so

$$<\phi_m|D|\phi_n> = \delta_{mn}D_{mn} \tag{16}$$

Equation (15) may then be "solved" and written in the form:

$$F = \frac{1}{(E - H_0 - D)}\frac{1}{Y} + \frac{1}{E - H_0 - D}(V - D)F \tag{17a}$$

which is an integral equation for F. For the vector $F|\phi>$, we have,

$$F|\phi> = \frac{1}{(E - H_0 - D)}Y^{-1}|\phi> + \frac{1}{E - H_0 - D}(V - D)F|\phi> \tag{17b}$$

It is convenient to get rid of the operator Y^{-1} and replace it by other known or desirable operators. To do that we make use of the fact that Y is diagonal in the $|\phi>$-representation. So, Y^{-1} is also diagonal, again in the $|\phi>$-representation, and its diagonal, matrix elements are the inverses of the corresponding diagonal matrix elements of Y. Consider now the first term of the right hand side of equation (17b). Inserting the expansion of the identity in terms of the complete set $\{|\phi>\}$ and making use of equations (8), (13) and (16) we have

$$\frac{1}{E - H_0 - D}Y^{-1}|\phi_n> \;=\; \sum_m \frac{1}{E - H_0 - D}|\phi_m><\phi_m|Y^{-1}|\phi_n>$$

$$
\begin{aligned}
&= \sum_m \frac{1}{E-H_0-D}|\phi_m> G_{nn}^{-1}(E)\delta_{mn} \\
&= \sum_m \frac{1}{E-H_0-D_{mm}}|\phi_m> G_{nn}^{-1}(E)\delta_{mn} \\
&= \frac{1}{E-H_0-D_{nn}} G_{nn}^{-1}(E)|\phi_n> \\
&= \frac{1}{E-H_0-D_{nn}}[E-E_n^0-X_{nn}(E)]|\phi_n> \\
&= \frac{1}{E-H_0-D_{nn}}[E-H_0-X_{nn}(E)]|\phi_n>
\end{aligned}
$$

So equation (17b) for the vector $F|\phi>$ now takes the form:

$$
\begin{aligned}
F|\phi_n> &= \frac{1}{E-H_0-D_{nn}}[E-H_0-X_{nn}(E)]|\phi_n> \\
&+\frac{1}{E-H_0-D}(V-D)F|\phi_n>
\end{aligned}
\tag{17c}
$$

One should bear in mind that $F|\phi_n>$ given by equation (17c) does not depend on the choice of the arbitrary operator D apart from the restrictions imposed on it e.g. the operator D being diagonal in the $|\phi>$ - representation as expressed by equation (16). An obvious simplification of equation (17c) results if one chooses

$$
D_{nn} = X_{nn}(E) \tag{18}
$$

So we get

$$
F|\phi_n> = |\phi_n> + \frac{1}{E-H_0-D}(V-D)F|\phi_n> \tag{19a}
$$

Again $F|\phi_n>$ does not depend on the choice of D apart from the restrictions imposed on its form by equations (16) and (18). Equation (19a) provides an integral equation for F which may be used in turn to find $X_{nn} =< \phi_n|VF|\phi_n>$, leading to the evaluation of the level shift operator.

Now taking the scalar product of both sides of equation (19a) with $<\phi_m|$, the matrix elements of F may be written as

$$(19b) \qquad F_{mn} = <\phi_m|F|\phi_n>= \delta_{mn} + \frac{<\phi_m|(V-D)F|\phi_n>}{E - E_m^0 - X_{mm}}$$

$$(19c) \qquad = \delta_{mn} + \sum_s \frac{1}{E - E_m^0 - X_{mm}}[V_{ms} - D_{mm}\delta_{ms}]F_{sn}$$

where $V_{ms} =<\phi_m|V|\phi_s>$,

From equation (19b) the diagonal matrix elements F_{nn} are given by

$$(19d) \qquad F_{nn} = 1 + \frac{<\phi_n|(V-D)F|\phi_n>}{E - E_n^0 - X_{nn}}$$

Owing to the fact that $<\phi_n|F|\phi_n>= 1$ - see equation (9) -one deduces that,

$$(19e) \qquad <\phi_n|(V-D)F|\phi_n>= 0$$

This equation proves to be useful in simplifying detailed calculations in certain particular methods of perturbation theory. Inserting the identity operator in the right hand side of equation (19a) and expanding it in terms of the complete set $\{|\phi_n>, n = 0, 1, 2, \ldots\}$ and making use of equation (19c), equation (19a) may be written in the form

$$(19f) \qquad F|\phi_n>= |\phi_n> + \frac{1}{E - H_0 - D}(I - \wedge_n)(V-D)F|\phi_n>$$

where

$$(20) \qquad \wedge_n = |\phi_n><|\phi_n|$$

is the projection operator onto the state $|\phi_n>$.

The perturbation scheme for evaluating the eigenvalues, the E_n's, of H may now be formulated as follows:

Suppose the eigenvalues E_n^0 and the eigenfunctions $|\phi_n>$ of the unperturbed Hamiltonian H_0 are all known. A perturbation V is then switched on Equation (17a)

$$F = (E - H_0 - D)^{-1}Y^{-1} + (E - H_0 - D)^{-1}(V - D)F, \tag{17a}$$

when acting on the eigenfunction $|\phi_n>$, can be used to evaluate equation (12a),

$$X_{nn} =< \phi_n|VF|\phi_n > \tag{12a}$$

Using this equation, equation (14a)

$$E_n = E_n^0 + X_{nn}(E_n) \tag{14a}$$

may then be solved for the E_n's which are the eigenvalues of the perturbed Hamiltonian $H = H_0 + V$.

Moreover, as was asserted, the arbitrary operator D is subjected only to the condition (16) which states that it is diagonal:

$$< \phi_m|D|\,\phi_n >= \delta_{mn}D_{nn} \tag{14a}$$

it is usually desirable to choose the operator D in such a manner that

$$< \phi_n|(E - H_0 - D)^{-1}Y^{-1}|\phi_n >= 1 \tag{18a}$$

This usually involves a limiting procedure which should be done properly. This choice is equivalent to the previous simplification expressed by the choice given by equation (18),

$$D_{nn} = X_{nn}(E) \tag{18}$$

Condition (18) or (18a) in general cannot always be satisfied. When this condition is met, equation (17a) may be replaced by the simpler equation

$$F = I + \frac{1}{E - H_0 - D}(V - D)F \tag{17d}$$

Again, when F acts on $|\phi_n >$, one gets the convenient equation (19a)

$$F|\phi_n >= |\phi_n > + \frac{1}{E - H_0 - D}(V - D)F|\phi_n > \tag{19a}$$

and the perturbation procedure goes as usual.

It is to be noticed that the structure of equation (19a) is similar to that of the outgoing and ingoing wave functions $|\psi_n^{\pm} >$. Indeed, if we let $E = E_n^0 \pm i \in$ and set $D_{mn} = 0$ for all $m \neq n$, equation (19f) for $F|\phi_n >$ is identical with that for $|\psi_n^{\pm} >$ when the volume v of the encasing box tends to infinity followed by the limit of $\in$ tending to plus zero.

2. APPLICATIONS

Different commonly used perturbation forms are obtained by making different choices of the operator D. The general rule is normally the suitability to the specific problem encountered and the simplification of the evaluation of equations (19). In what follows examples of known methods are given as special cases of the formulation outlined in part I.

1. Brillouin - Wigner Method (BW). Let

$$D = X_{nn}\Lambda_n \tag{21}$$

Then equation (19f) may be written as

$$\begin{aligned}(E - H_0 - X_{nn}\Lambda_n)F|\phi_n > &= (E - H_0 - X_{nn}\Lambda_n)|\phi_n > \\ &\quad +(1 - \Lambda_n)(V - X_{nn}\Lambda_n)F|\phi_n >\end{aligned} \tag{22}$$

Since $\Lambda_n^2 = \Lambda_n = |\phi_n >< \phi_n|$ and we have $< \phi_n|F|\phi_n = 1$, equation (22) may be simplified, as the terms containing X_{nn} cancel, and we are permitted to write

$$F|\phi_n >= |\phi_n > + \frac{1}{E - H_0}(I - \Lambda_n)VF|\phi_n > \tag{23}$$

The level shift operator X, given by equation (12b), may now be written in the form

$$X = V + V\frac{I - \Lambda_n}{E - H_0}X \tag{24}$$

By iteration one gets the useful symmetric form for the level shift operator

$$X = V + V\frac{1-\Lambda_n}{E-H_0}V + V\frac{I-\Lambda_n}{E-H_0}V\frac{I-\Lambda_n}{E-H_0}V + \dots \tag{25}$$

From equation (14b) we get for the perturbed eigenvalue E the implicit form:

$$E_n = E_n^0 + <\phi_n|V|\phi_n> + \sum_{m\neq n}\frac{|<\phi_n|V|\phi_m>|^2}{E_n - E_m^0} + \dots \tag{26}$$

which is the BW implicit form of the perturbation expansion of E_n.

2. Rayleigh - Schrödinger Method (ES). Let us put

$$D = X_{nn}(E)\,\Lambda_n + (E - E_n^0)(I - \Lambda_n) \tag{27}$$

Using the simplification procedure used in the special case of BW method equation (19f) becomes

$$F|\phi_n> = |\phi_n> + \frac{1}{E_n^0 - H_0}(I-\Lambda_n)(V-\delta E)F|\phi_n> \tag{28a}$$

where $\delta E = E - E_n^0$. Again from equation (14) we get for X_{nn} as a function of δE,

$$X_{nn}(\delta E + E_n^0) = \delta E, \tag{28b}$$

A systematic expansion of equation (28) in powers of V gives the known RS series expansion for the eigenfunctions E_n.

Other specific methods used in certain models like the Eden-Francis method, the Feenberg and the Tanaka-Fukuda method may also be deduced [13].

3. Passage from Discrete to Continuous Spectra. The preceeding discussion has dealt with the shift in the discrete eigenvalues of the Hamiltonian due to switching on a perturbation. Evaluation of this shift was accomplished through the "level shift" operator $X = VF$. The system under consideration was assumed to be enclosed in a large box of volume v.

In some quantum mechanical stationary state problems of great complexity, it is a very useful approximation to replace the part of the discrete spectrum, which becomes continuous when the boundary of the enclosure recedes to infinity, by that continuum. One needs for this purpose to understand the manner in which one formalism goes over to the other; that is, how quantities of one formalism are connected with those of the other and the nature of this connection. Two such quantities of great physical interest are the level shift in the energy eigenvalues caused by the application of a perturbation in the case of stationary bound states and the phase shifts $\delta(E)$ in the region of the continuum of the scattering states.

It has been shown that ([7],[14],[15]) when the volume v of the enclosure tends to infinity in a suitable manner the perturbation induced shift in the energy levels becomes proportional to the corresponding scattering phase shift. Moreover this result holds even when the total Hamiltonian is not separable. Stated explicitly the limit of the level shift ΔE is given by

$$\lim_{v \to \infty} \quad \Delta E(E) = X(p, \Delta E) = -\frac{2E}{p}\delta(E) \tag{30}$$

where p is the corresponding momentum of the scattering system.

We have seen that the level shift operator $X = VF$ plays an important general role in quantum theory. For suitable choice of the operator D we can deduce the various known methods of the bound state stationary perturbation theory. Moreover when going the continuous state, the level shift operator X gives rise to the important phase shift which plays a prominent role in scattering theory.

4. The General Formulation of the Padé Approximants to the Perturbation Series [16]. The importance of the application of Padé approximants (PA) in nonrelativistic quantum mechanics, specially to potential scattering lies in the fact that it offers a proving ground for the possible application of the same techniques to quantum field theory. In this content a large number of these trials have been made and many of them are reviewed by Basdevant [17].

The power of the application of Padé Approximants in non-relativistic quantum mechanics lies in a theorem [18] which states that, $[N-1/N]$ Padé Approximant to the mean value of the resolvent R of H, symmetrized in a certain way, is equal to the exact mean value of the resolvent of the finite rank symmetric operator $\wedge_N H \wedge_N$. That is, from equation (3):

$$H(g)|\psi_n(g)>= E_n(g)|\psi_n(g)>, \tag{31}$$

its resolvent is defined by

$$R(E,g) = [E - H(g)]^{-1} = [(E - H_0) - gV]^{-1}. \tag{32}$$

The above mentioned theorem for the Padé Approximant of the resolvent $[N-1/N]R_{\phi(g)}$ may be stated explicitly as

$$\begin{aligned} [N-1/N]R_{\phi(g)} &= <\phi|[I - g\wedge_N H\wedge_N]^{-1} <\phi| \\ &= <\phi|[I - gH_N]^{-1}|\phi>, \end{aligned} \tag{33}$$

where H_N is the projection of H on to the N-dimensional space spanned by the vectors $\{|\phi>, H|\phi>, H^2|\phi>, \ldots, H^{N-1}|\phi>\}$. In general one takes $|\phi>$ to be a suitable trial vector. However experience shows that it is convenient to take it the unperturbed eigenstate $|\phi>$ of equation (1).

Moreover, the power of the Padé Approximants is wider than the strict application of the above theorem to the resolvent. In fact, any Hermitian symmetric operator is suitable for the application of the Padé approximants method. It suffices to prove that a Hermitian operator is symmetric to capitalize on the exponential speed of convergence of its constructed Padé Approximants.

Seemingly unconnected PA have been constructed from different perturbation methods. Thus PA have been constructed from the RS perturbation expansion of the mean value R_{nn} of the symmetrized resolvent of H ([11],[19]). Also PA has been introduced into the BW perturbation theory ([20],[21],[22],[23],[24]). A separate PA treatment of the phase shifts and the introduction of the arctangent of the mean value of the resolvent R_{nn} has been carried out ([11],[18]). All the methods existing in the literature lacked a general formulation of the theory of PA in non-relativistic quantum mechanics.

Recently, it has been shown [9] that PA for RS and BW perturbation methods are related. In fact one of them bears a certain reciprocal relation to the other. Thus, we are left with the inclusion in a unified treatment of the scattering phase shifts. The obvious candidate for that is the level shift operator $X = VF$ of equation (12). This is so since as we have seen with a proper choice of the arbitrary operator D, we may reproduce the RS perturbation method, the BW series of the bound state perturbation theory and - one should emphasize - the scattering phase shift in the limit of infinite enclosure (see equation 30). It rests to show that X, being Hermitian, is symmetric.

This is easy to show. For we have from equation (24)

$$X = V + V\frac{I - \Lambda_n}{E - H_0}X \tag{24}$$

so we can solve for X and get

$$X = \left[I - V\frac{I - \Lambda_n}{E - H_0}\right]^{-1} V \tag{33}$$

If V is a positive potential one may write:

$$\begin{aligned}
X &= \left[I - V^{\frac{1}{2}}V^{\frac{1}{2}}\frac{I - \Lambda_n}{E - H_0}\right]^{-1} V^{\frac{1}{2}}V^{\frac{1}{2}} \\
&= \left[V^{\frac{1}{2}}(V^{-\frac{1}{2}} - V^{\frac{1}{2}}\frac{I - \Lambda_n}{E - H_0}\right]^{-1} V^{\frac{1}{2}}V^{\frac{1}{2}} \\
&= \left[V^{-\frac{1}{2}} - V^{\frac{1}{2}}\frac{I - \Lambda_n}{E - H_0}\right]^{-1} V^{-\frac{1}{2}}V^{\frac{1}{2}}V^{\frac{1}{2}} \\
&= \left[\left(I - V^{\frac{1}{2}}\frac{I - \Lambda_n}{E - H_0}V^{\frac{1}{2}}\right) V^{-\frac{1}{2}}\right]^{-1} V^{\frac{1}{2}} \\
&= V^{\frac{1}{2}}\left[I - V^{\frac{1}{2}}\frac{I - \Lambda_n}{E - H_0}V^{\frac{1}{2}}\right]^{-1} V^{\frac{1}{2}} \qquad \text{(33a)}
\end{aligned}$$

which shows that X is symmetric, and being Hermitian, all the prerequisites for the application of PA are satisfied. The restriction of positivity of the potential, may be removed and the method extends to the case of changing sign potential by the introduction of Padé Approximants in the distorted wave theory [25].

Hence it is established that all of the aforementioned PA constructions are special cases of a general PA built from the series expansion of a single operator which is the level shift operator.

REFERENCES

1. E.P. Wigner, Math.u.naturw.Anz.Ungar. Akad.Wiss. **53**, 475 (1935).
2. L. Brillouin, J. Phys. radium **4**, 1 (1993).
3. R.J. Eden and N.C. Francis, Phys. Rev. **97**, 1366 (1955).
4. H. Tanaka, Progr. Theoret. Phys. Japan **13**, 497 (1955).
5. N. Fukuda, Phys. Rev. **103**, 420 (1956).
6. K.M. Watson, Phys. Rev. **103**, 489 (1956).
7. W.B. Riesenfeld and K.M. Watson, Phys. Rev. **104**, No. 2, 492 (1956).
8. M.L. Goldberger and K.M. Watson, *Collision Theory*, Robert E. Krieger Publishing Company, New York (1975).
9. A.B. Khalil, J. Math. Phys. vol. 33, No. 2, 639 (1992).
10. For a more detailed discussion of this point, see reference 6.
11. D. Bessis and M. Villani, J. Math. Phys., **16**, 462 (1975).
12. For a detailed example see reference (9) equations (12)-(15).
13. See for example chapter 9 in P.M. Morse and H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill Book Company, (1953).
14. M. Fukuda and R.G. Newton, Phys. Rev. **103**, 1558 (1956).

15. B.S. Dewitt, Phys. Rev. **103**, 1565 (1956).

16. A.B. Khalil, General formulation of the Padé approximation to the perturbation series....., (to appear).

17. J.L. Basdevant, *Strong Interaction Physics and the Padé Approximation in Quantum Field Theory*, In Padé Approximants, (P.R. Graves-Morris, ed.), Institute of Physics, London (1973), pp. 77-100.

18. D. Bessis, L. Epele and M. Villani, J. Math. Phys., **15**, 2071 (1974).

19. G.A. Baker, Jr. Essentials of Padé Approximants, Academic, New York, (1975).

20. R.C. Young, L.C. Biedenharn and E. Feenberg, Phys. Rev. **106**, 1151 (1957).

21. B.G. Giraud, Phys. Rev. C, 17, 800 (1978).

22. B.G. Giraud and G. Turchetti, Lett. Nuovo Cimento, **21**, 605 (1978).

23. G. Turchetti, F. Ortolani and C. Sagretti, Nuovo Cimento A, **44**, 211 (1978).

24. N. Barnsley and G. Truchetti, comput. Phys. commun., **22**, 325 (1981).

25. B. Giraud, A.B. Khalil, and P. Moussa, Phys. Rev. C. **14**, 1679 (1976).

MATHEMATICS DEPARTMENT, FACULTY OF SCIENCE, CAIRO UNIVERSITY, GIZA, EGYPT

Date received June 19, 1995