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SOME APPLICATIONS OF PADÉ APPROXIMANTS TO QUANTUM FIELD THEORY MODELS*

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1. **Introduction.** We recall that a power series

$$P(z) = c_0 + c_1 z \cdots \tag{1}$$

is a series of Stieltjes iff $D(0, n)$ and $D(1, n) > 0$ [10] where

$$D(m, n) = \det \begin{bmatrix} c_m & \cdots & c_{m+n} \\ \vdots & \ddots & \\ c_{m+n} & & c_{m+2n} \end{bmatrix}. \tag{2}$$

Let $P(z)$ be a series of Stieltjes, then it may be represented as

$$g(z) = \int_{-\infty}^{\infty} \frac{d\sigma(x)}{1 - zx} \tag{3}$$

with $d\sigma(x) \geqq 0$ and $c_n = \int_{-\infty}^{\infty} x^n \, d\sigma(x)$. The problem of constructing $\sigma(x)$ from a knowledge of the c_n is the Hamburger moment problem while the requirement $d\sigma(x) = 0$ for $x < 0$ defines the Stieltjes moment problem. The moment problems are either determinate ($\sigma(x)$ unique) or indeterminate (infinitely many $\sigma(x)$'s). Note that the determinateness of the Hamburger moment problem implies the determinateness of the Stieltjes moment problem but that the converse is not true.

The $[n/n + j](z)$ Padé approximant to $P(z)$ is $P_n(z)/Q_{n+j}(z)$ where $P_n(z)$ is a polynomial of degree n and $Q_{n+j}(z)$ is a polynomial of degree $n + j$ in z. If the Stieltjes moment problem is determinate then $[n/n + j](z)$ converges as $n \to \infty$ to the unique function $g(z)$ for z in the cut plane $z \notin [0, \infty)$ and gives one an approximate method of constructing $\sigma(x)$ via the Stieltjes inversion formula which expresses $\sigma(x)$ in terms of $g(z)$.

In Sec. 2 we review the close connection between Padé approximants applied to series of Stieltjes and the theory of positive symmetric operators in a Hilbert space. This will allow us to (1) establish useful

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criteria for the self-adjointness of a symmetric operator in terms of the determinateness of a Hamburger moment problem and (2) to obtain a method of approximating such operators related to the $[n/n + 1]$ Padé approximant.

In Sec. 3 we indicate how these results may be applied to a quantum field theory model to give (1) a simple proof of the self-adjointness of the Hamiltonian and (2) a method of solving the Hamiltonian eigenvalue problem using the $[n/n + 1]$ Padé approximant.

2. **Vectors of Uniqueness.** Let $\mathcal{H}$ be a complex Hilbert space. We denote the inner product and norm in $\mathcal{H}$ by (f, g) and $\|f\| = (f, f)^{1/2}$ respectively. A linear operator on $\mathcal{H}$ with domain $\mathfrak{D}(A)$ and range $\mathcal{R}(A)$ is symmetric iff (i) $(f, Ag) = (Af, g)$ for all $f, g \in \mathfrak{D}(A)$ and (ii) $\mathfrak{D}(A)$ is dense in $\mathcal{H}$ (i.e., given $g \in \mathcal{H}$ and $\epsilon > 0$ one can find an $f \in \mathfrak{D}(A)$ such that $\|g - f\| < \epsilon$). A symmetric operator is said to be strictly positive if $(f, Af) > a\|f\|^2$ for some $a > 0$ and all $f \neq 0$ in $\mathfrak{D}(A)$. For any densely defined operator A one may define a unique adjoint operator mapping g to A^+g by the requirement that $(A^+g, f) = (g, Af)$ for fixed g and all $f \in \mathfrak{D}(A)$. The symmetry of A implies that in general $A \subseteq A^{++} \subseteq A^+$ where $A \subseteq B$ (read as B extends A or A is a restriction of B) means that $\mathfrak{D}(A) \subseteq \mathfrak{D}(B)$ and $Af = Bf$ for $f \in \mathfrak{D}(A)$. A is said to be self-adjoint (s.a.) if $A = A^+$ and essentially self-adjoint (e.s.a.) if $A^{++} = A^+$. A basic criteria for these properties to hold is given by the theorem,

THEOREM 1. *Let A be a strictly positive symmetric operator in a Hilbert space $\mathcal{H}$. Then A is e.s.a. iff $\mathcal{R}(A)$ is dense in $\mathcal{H}$ and s.a. iff $\mathcal{R}(A) = \mathcal{H}$.*

For proof see [3].

We wish to use the theory of Padé approximants applied to series of Stieltjes to examine the problem of when A is e.s.a. and to obtain approximations to A. To this end it is convenient to define some special classes of vectors which we call C^∞ vectors and vectors of uniqueness for A.

DEFINITION. *A vector $f \in C^\infty(A) = \bigcap_{n=1}^{\infty} \mathfrak{D}(A^n)$ is a C^∞ vector for A.*

Given f a C^∞ vector for a symmetric operator A one may construct the linear subspace $\mathcal{L}_f(A) =$ linear span $\{A^n f \mid n = 0, 1, \cdots\}$ and its completion $\mathcal{H}_f = \mathrm{Cl}(\mathcal{L}_f)$ a Hilbert subspace of $\mathcal{H}$. If the vectors $A^n f$, $n = 0, 1, 2, \cdots$ are not linearly independent then $\dim \mathcal{L}_f = m < \infty$, $\mathcal{H}_f = \mathcal{L}_f$ and $A \mid \mathcal{L}_f$ the restriction of A to the subspace $\mathcal{L}_f$ is an $m \times m$ symmetric matrix. A complete knowledge of $A \mid \mathcal{L}_f$ is then trivially obtained from the standard theory of matrices acting in a finite dimensional Hilbert space. If on the other hand the vectors $A^n f$, $n = 0, 1, \cdots$ are linearly independent then $\dim \mathcal{L}_f = \infty$ and the situation is more subtle. We may then orthonormalize the vectors $A^n f$ by means of the Gram-Schmidt orthogonalization procedure. One obtains the set of orthogonal vectors $\{f_n\}$ with $f_0 = f$, $f_1 = (A - a_0)f$ and

$$f_{n+1} = (A - a_n)f_n - b_{n-1}^2 f_{n-1} = q_{n+1}(A)f, \quad n = 1, 2, \cdots,$$

where $z^{n+1}q_{n+1}(z^{-1})$ is the denominator of the $[n + 1/n]$ Padé approximant and an orthonormal basis $\{e_n = f_n/\|f_n\|\}$ for $\mathcal{H}_f$. With respect to this basis $A \mid \mathcal{L}_f$ is represented as an infinite tridiagonal Jacobi matrix

$$J = \begin{bmatrix} a_0 & b_0 & & & 0 \\ b_0 & a_1 & b_1 & & \\ & b_1 & \ddots & \ddots & \\ 0 & & \ddots & \ddots & \end{bmatrix} \tag{4}$$

with $a_n = (e_n, Ae_n)$, $b_n = (e_n, Ae_{n+1}) = \|f_{n+1}\|/\|f_n\| > 0$ and

$$Ae_n = Je_n = b_{n-1}e_{n-1} + a_n e_n + b_n e_{n+1}. \tag{5}$$

The e.s.a. of $A \mid \mathcal{L}_f$ or J is related to the determinateness of the moment problem associated with the sequence $c_n = (f, A^n f)$, $n = 0, 1, \cdots$.

THEOREM 2. *Let A be symmetric and strictly positive and let $f \in C^\infty(A)$ with $\dim \mathcal{L}_f(A) = \infty$. Then associated with the pair A, f is a series of Stieltjes with coefficients $c_n = (f, A^n f)$. Furthermore the operator $A \mid \mathcal{L}_f$ on $\mathcal{H}_f$ is e.s.a. iff the associated Hamburger moment problem is determinate.*

PROOF. To show that the c_n are the coefficients of a series of Stieltjes it suffices to show that $D(0, n)$ and $D(1, n)$ are positive for all n. $D(0, n) > 0$ follows from the symmetry of A and the linear independence of $f, Af, \cdots, A^n f$ since by adding appropriate linear combinations of rows and columns one obtains $D(0, n) = \prod_{k=0}^{n} \|f_k\|^2$. Similarly one obtains $D(1, n) = D(0, n) \prod_{k=0}^{n} \lambda_k$ where $\{\lambda_k\}$ is the set of eigenvalues of the $n + 1 \times n + 1$ matrix obtained by truncating the matrix J. The positivity of each λ_k follows from the positivity of A. For the proof of the relation between e.s.a. and the determinateness of the moment problem see [1] and [5].

The C^∞ vectors associated with a determinate Hamburger moment problem are thus of special interest to us. We call them *vectors of uniqueness.*

DEFINITION. *Let f be a C^∞ vector for a symmetric operator A. Then f is a vector of uniqueness for A if $A \mid \mathcal{L}_f$ is e.s.a.*

A useful criteria for f to be a vector of uniqueness is given by the following theorem.

THEOREM 3. *If $\sum_{n=0}^{\infty} b_n^{-1/2} = \infty$ or $\sum_{n=1}^{\infty} c_n^{-1/2n} = \infty$ then f is a vector of uniqueness for the strictly positive symmetric operator A.*

The two conditions are closely related. In fact the divergence of the second series implies the divergence of the first series. For a proof see [5].

Theorems 2 and 3 provide one with information about A on only a subspace of the original Hilbert space unless $\mathcal{H}_f = \mathcal{H}$. In general one has only $\mathcal{H}_f \subset \mathcal{H}$ but with sufficiently many vectors of uniqueness one may conclude that A itself is e.s.a. For details we refer the reader to [5], [8] and [9].

The construction of the J matrix in Equation (4) provides one with a natural method of approximating A. If we introduce the projection operators P_n which project onto the subspace spanned by the vectors $f, Af, \cdots, A^n f$ then the operator $A_n = P_n A P_n$ is represented by the truncated J matrix with only $n + 1$ non-zero rows and columns. The resolvent of A_n may thus be calculated using ordinary matrix methods and is closely related to the Padé approximant to the series (1) with coefficients $c_n = (f, A^n f)$.

THEOREM 4. *Let f be a C^∞ vector for the strictly positive symmetric operator A. Then $(f, (1 - zA_n)^{-1} f) = [n/n + 1](z)$. Moreover if f is a vector of uniqueness for A then $[n/n + 1](z)$ converges to $(f, (1 - z(A \mid \mathcal{L}_f)^+)^{-1} f)$ for $z \notin [0, \infty)$.*

For a proof of this see [4].

We will also need the following special case of Theorem 4 which uses the monotonic character of the Padé approximate for real negative z.

THEOREM 5. *Let $1 + A$ be s.a. and strictly positive. If f is a vector of uniqueness for A then $(f, (1 + A_n)^{-1} f) = [n/n + 1](-1)$ converges monotonically from below to $(f, (1 + A)^{-1} f)$.*

3. **Applications.** The results of Sec. 2 have been recently applied to some quantum field theory models in the constructive field theory programme of Glimm and Jaffe [2]. Theorem 3 has been used to give

a simple proof of the self-adjointness of the spatially cut off Hamiltonian for scalar bosons with a quartic interaction in two-dimensional space-time (the $(\phi^4)_2$ theory) [6] while Theorem 4 has been used to solve the vacuum eigenvalue problem in the $(\phi^{2m})_2$, $m = 2, 3$ theory [7]. We do not want to digress here into a description of quantum field theory. Instead we will illustrate the essential ideas of these applications by turning to a simple one degree of freedom model of quantum mechanics: the anharmonic oscillator.

This model is a nonrelativistic description of one particle moving in one spatial dimension under the influence of a potential which is a quartic polynomial in the position variable. The Hilbert space is $L^2(R^1) = \{f(x) \mid \int_{-\infty}^{\infty} |f(x)|^2 \, dx < \infty\}$ the Lebesgue square integrable functions of one real variable. The Hamiltonian is $H = H_0 + \lambda V$ with $\lambda > 0$,

$$H_0 = \frac{1}{2}\left(- \frac{d^2}{dx^2} + x^2 - 1 \right),$$

and $V = x^4$. The "free" Hamiltonian H_0 describes the harmonic oscillator and has a complete set of orthonormal eigenvectors $\phi_n = h_n(x)e^{-x^2/2}$, $n = 0, 1, \cdots$ where $h_n(x)$ is, apart from normalization, the Hermite polynomial of degree n and $H_0\phi_n = n\phi_n$.

It is convenient to introduce the annihilation and creation operators $a = (x + d/dx)/2^{1/2}$ and $a^* = (x - d/dx)/2^{1/2}$. One then has

$$\begin{aligned} a\phi_n &= n^{1/2}\phi_{n-1} \\ a^*\phi_n &= (n+1)^{1/2}\phi_{n+1} \\ H_0 &= a^*a \\ V &= (a + a^*)^4/4. \end{aligned} \tag{6}$$

We now show that H is e.s.a. on the domain $\mathfrak{D}$ = linear span $\{\phi_n \mid n = 0, 1, \cdots\}$. Since H is strictly positive it follows from Theorem 1 that it suffices to show that

$$(\psi, H\phi) = 0 \tag{7}$$

for all $\phi \in \mathfrak{D}$ implies that $\psi = 0$. Expanding ψ in terms of the ϕ_n's, $\psi = \sum_{n=0}^{\infty} d_n\phi_n$, $d_n = (\phi_n, \Psi)$, defining $\psi_n = d_{4n}\phi_{4n} + d_{4n+1}\phi_{4n+1} + d_{4n+2}\phi_{4n+2} + d_{4n+3}\phi_{4n+3}$ and putting $\phi = \psi_n$ in (7) one has

$$\begin{aligned} &(\psi_n, H\psi_n) + \lambda(\psi_{n+1}, V\psi_n) \\ &\qquad + \lambda(\psi_{n-1}, V\psi_n) = 0, n = 0, 1, \cdots. \end{aligned} \tag{8}$$

We will assume that $\|\psi_n\| \neq 0$, $n = 0, 1, 2, \cdots$ and obtain a contradiction. If one defines

$$(9) \qquad \begin{aligned} a_n &= (\psi_n, H\psi_n)/\|\psi_n\|^2 \\ b_n &= -\lambda(\psi_{n+1}, V\psi_n)/\|\psi_n\| \, \|\psi_{n+1}\|. \end{aligned}$$

Eq. (8) becomes

$$(10) \qquad a_n\|\psi_n\| - b_{n-1}\|\psi_{n-1}\| - b_n\|\psi_{n+1}\| = 0, n = 0, 1, \cdots$$

which is just the equation $(\chi, Je_n) = 0$ with J given by Equation (4) and $\chi = \sum_0^\infty (-1)^n\|\psi_n\|e_n$.

One may now use the fact that V is of the fourth power in the operators a and a^* to get the estimate that $b_n <$ const n^2. From Theorem 3 one has that J is e.s.a. which implies using Theorem 1 that $\chi = 0$ and hence that $\psi = 0$.

Turning now to the eigenvalue problem for H we let $E(\lambda)$ be the smallest eigenvalue and $\psi(\lambda)$ the corresponding eigenvector. We write $\psi(\lambda) = \phi_0 + \chi(\lambda)$ where $\chi(\lambda) = P\psi(\lambda)$ and P projects onto the subspace orthogonal to ϕ_0. The eigenvalue problem may be recast in the following form.

$$(11) \qquad \chi(\lambda) = \lambda H_0^{-1/2}(1 + A(E(\lambda)))^{-1}f$$

where $E(\lambda)$ satisfies the equation

$$(12) \qquad E = \lambda(\phi_0, V\phi_0) - \lambda^2(f, (1 + A(E))^{-1}f)$$

with $f = H_0^{-1/2}PV\phi_0$ and $A(E) = H_0^{-1/2}P(\lambda V - E)PH_0^{-1/2}$. Equation (12) is just the Brillouin-Wigner implicit formula for the eigenvalue.

The following facts are verifiable and in fact needed in order to justify the manipulations needed to derive (11) and (12).

(1) $1 + A(E)$ is strictly positive for $E \leqq E(\lambda) + \epsilon$ for some $\epsilon > 0$. This follows from the fact that $E(\lambda)$ is the least eigenvalue of H and is isolated.

(2) f is a vector of uniqueness for $A(E)$. This follows from Theorem 3 and the estimate $\|A^n(E)f\| = (c_{2n})^{1/2} < (\text{const.})^n n!$ which is again due to the quartic nature of the perturbation V.

One is now in a position to obtain approximate solutions to the eigenvalue problem using Theorem 5. In (12) one replaces $A(E)$ by $A_n(E)$ and solves for E to get an approximate eigenvalue $E_n(\lambda)$. From the monotonic behaviour of A as a function of E and the monotonic properties of the $[n/n + 1]$ Padé approximate it follows that $E_n(\lambda)$ converges monotonically from above to $E(\lambda)$. The approximate eigenvector is then obtained by replacing $A(E(\lambda))$ in (11) by $A_n(E_n(\lambda))$to obtain $\chi_n(\lambda)$. It follows that $\|\chi_n(\lambda) - \chi(\lambda)\| \to 0$ as $n \to \infty$.

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