One-dimensional eigenfunctions from their perturbation series for regular and singular perturbations

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Some properties of the eigenfunction perturbation series $\Psi(\lambda,x)=\Sigma_{m=0}^{\infty}\psi_m(x)\lambda^m$ for the self-adjoint eigenproblem $H\Psi=E\Psi$ with $H=H_0+\lambda V$ are studied. It is shown that both regular and singular perturbations V of the unperturbed Hamiltonian H_0 can generate partial-sum sequences $\{\Psi_n=\Sigma_{m=0}^{n}\psi_m\lambda^m\}_{n=0}^{\infty}$ that converge in the norm of the Hilbert space in question and are nonuniformly bounded. This latter property is, for a given value of λ, characterized by an increasing separation between the tail of Ψ_n on the large $|x|$ region and that of Ψ as $n\to\infty$, and causes the divergence of expectation value sequences $\{\langle\Psi_n,S\Psi_n\rangle\}_{n=0}^{\infty}$ with some symmetric operators S. As model examples we consider one-dimensional operators H_0 for which the perturbation V can be regular or singular and the eigenfunction series are obtained from the standard perturbation theory. The use of summability methods to get approximating sequences of wave functions with a correct convergence is explored. The results show that, independently of the regular or singular nature of V, a summability method (such as the Padé one) can yield approximations R_n from the Ψ_n's that are L_2 convergent and uniformly bounded, and hence correct physical quantities can be obtained from such R_n's. [S1050-2947(99)09406-8]

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I. INTRODUCTION

The two main ways to compute the bound states Ψ and eigenvalues E of the time-independent Schrödinger equation $H\Psi=E\Psi$ are the variational method and perturbation theory [1]. For many problems of interest the convergence of variational wave functions $\Phi_n(x)=\Sigma_{m=1}^{n}c_{nm}\varphi_m(x)$ in the usual norm of the Hilbert space $L_2(R^N)$ is guaranteed by a completeness argument of the basis set $\{\varphi_m\}_{m=1}^{\infty}$ in a suitable Hilbert space [2,3]. However, it was shown recently [4] that the sequence $\{\Phi_n\}_{n=1}^{\infty}$ may have an inherent property that generates an incorrect convergence of expectation values $S(\Phi_n)=\langle\Phi_n,S\Phi_n\rangle$ with some symmetric operators S. This property (which we will call the *nonuniform* boundedness property) is connected with the capability of Φ_n to reproduce the tail of Ψ on the large $|x|$ region in the limit $n\to\infty$, is independent of rounding errors, and is compatible with several convergence properties of $\{\Phi_n\}_{n=1}^{\infty}$ and some basis set properties [4]. In this work we show that perturbation methods can yield approximating sequences of the true wave functions with the nonuniform boundedness property.

In Sec. II we define the concepts of L_2 convergence and uniform and nonuniform boundedness properties of an approximating sequence $\{\Psi_n\}$ and give a summary of their role in the calculation of some expectation values; practical criteria to determine when $\{\Psi_n\}$ is either uniform or nonuniformly bounded are also given. In Sec. III we study the L_2 convergence and the boundedness properties of some—as called by Kato [5]—formal eigenfunction perturbation series

$$\Psi(\lambda,x)=\sum_{m=0}^{\infty}\psi_m(x)\lambda^m \tag{1.1}$$

for the self-adjoint eigenproblem $H(\lambda)\Psi(\lambda,x)=E(\lambda)\Psi(\lambda,x)$ with $H(\lambda)=H_0+\lambda V$, H_0 being the unperturbed Hamiltonian. The study of formal perturbation series is motivated by the fact that analytic perturbation theory [5] provides a classification of perturbations V of a given H_0 for which such series converge; namely, if V is a regular perturbation of H_0, then, for small $|\lambda|$, $E(\lambda)$ is a complex analytic function and the series (1.1) converges to $\Psi(\lambda,x)$ in the L_2 norm. Nevertheless, in Sec. III A it is shown by means of examples that the sequence $\{\Psi_n\}$ of partial-sum functions $\Psi_n=\Sigma_{m=0}^{n}\psi_m\lambda^m$ can be nonuniformly bounded and therefore the expectation value sequence $\{S(\Psi_n)\}_{n=0}^{\infty}$ may not converge to the correct value $S(\Psi)$. An example is included that shows how the Rayleigh-Schrödinger perturbation theory [6] can yield Fourier expansions of the mth-order term ψ_m that are nonuniformly bounded even if V is regular.

The well-known fact that almost every *nonregular* (or singular) perturbation V of H_0 generates eigenvalue perturbation series with a zero convergence radius has motivated the development of several methods to compute the correct eigenvalues $E(\lambda)$ from the coefficients of its divergent perturbation series [7–13] while the main results of the corresponding eigenfunctions series (1.1) only exhibit the asymptotic nature of such series [5,14,15]. The results of Sec. III B show that the partial-sum sequence $\{\Psi_n\}$ from the series (1.1) can be L_2 convergent but nouniformly bounded for all $\lambda\neq 0$ for which the Hamiltonian H has bound state eigenfunctions $\Psi(\lambda,x)$. This suggests that the eigenfunction series (1.1) from singular V's may be characterized by the nonuniform boundedness of their corresponding sequences $\{\Psi_n\}$ rather than by their L_2 convergence.

Section IV is devoted to exploring some methods that, independently of the regular or singular character of V, can yield approximating sequences of wave functions with a correct convergence toward the true Ψ. In Sec. II we show that

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if $\{\Psi_n\}$ is L_2 convergent, then for each Ψ_n there is a bounded region Ω_n in x space such that a $\{S(\chi_{\Omega_n}\Psi_n)\}_{n=0}^{\infty}$ converges correctly for several operators S, $\chi_\Omega(x)$ being 1 on Ω and 0 otherwise, despite the fact that $\{\Psi_n\}$ may be nonuniformly bounded, and in Sec. IV A we propose a procedure to estimate Ω_n. In Sec. IV B we apply the Padé method to the series (1.1) to show that summability methods can yield approximating wave functions $R_n(\lambda,x)$ with a correct convergence toward the true Ψ even when the corresponding partial-sum sequence $\{\Psi_n\}$ has a wrong L_2 convergence and is nonuniformly bounded. Section V is devoted to some concluding remarks.

II. BASIC CONCEPTS AND RESULTS

Hereafter L_2 denotes the Hilbert space $L_2(0,\infty)$ or $L_2(-\infty,\infty)$ and $\langle\cdot,\cdot\rangle$ and $\|\cdot\|$ denote its inner product and norm. The expectation value $\langle f,Sf\rangle$ of a symmetric operator S is denoted by $S(f)$ and throughout we shall consider that each wave function $f(x)$ is continuous and has a fast decay $[x^k(f)=\langle f,x^kf\rangle<\infty$ for all $k\geqslant 0]$.

The two features of a sequence $\{\Psi_n\}_{n=0}^{\infty}$ of wave functions that we shall consider are (i) the L_2 *convergence* (when $\|\Psi_n-\Psi\|\to 0$ as $n\to\infty$) and (ii) the *boundedness property* which involves the following concepts. Let Ω denote a bounded region of x space and let Ω^c be its complement. We say that $\{\Psi_n\}$ is *uniformly bounded* (UB) if there is at least one rapidly decaying and positive function ψ_B such that the inequality $|\Psi_n|\leqslant\psi_B$ holds in a region Ω^c for $n\geqslant n_0$ where Ω^c is independent of n; otherwise $\{\Psi_n\}$ is *nonuniformly bounded* (NUB). The motivation to consider these properties is their role in the correct calculation of the true Ψ's and expectation values $S(\Psi)$ as follows from the next results [16] (examples with Fourier and Ritz expansions that exhibit graphically or numerically the concepts and results of this section are given in [4]). The first result is given by *Proposition 1*: If $\{\Psi_n\}$ converges to Ψ in the L_2 norm and is UB, then

$$\lim_{n\to\infty} x^k(\Psi_n)=x^k(\Psi) \quad \text{for all } k\geqslant 0. \tag{2.1}$$

Intuitively, this result is possible only if $\{\Psi_n\}$ tends ''correctly'' to Ψ on the whole x space; thus we say that $\{\Psi_n\}$ has a correct *global* convergence towards the true Ψ if it is L_2 convergent and UB. If $\{\Psi_n\}$ is L_2 convergent but NUB, the L_2 convergence still guarantees certain correct *local* convergence. To see this consider an arbitrary bounded region Ω and let $\chi_\Omega(x)=1$ for $x\in\Omega$ and $\chi_\Omega=0$ otherwise. If $\{\Psi_n\}$ is L_2 convergent, then the equation

$$\lim_{n\to\infty} S(\chi_\Omega\Psi_n)=S(\chi_\Omega\Psi) \tag{2.2}$$

holds for any operator $S=s(x)$ defined by a function $s(x)$ that is continuous on the whole x space. This includes any $s(x)=e^{-(x-a)^2/2\sigma^2}$ with small σ which can be used to measure the fit of Ψ_n to Ψ on $\Omega_{a\sigma}=[a-\sigma,a+\sigma]$ through the error $\Delta^{(n)}S=|S(\chi_{\Omega_{a\sigma}}\Psi_n)-S(\chi_{\Omega_{a\sigma}}\Psi)|$. Since $\Delta^{(n)}S$ vanishes as $n\to\infty$, we can say that $\{\Psi_n\}$ tends correctly to Ψ on $\Omega_{a\sigma}$ while its convergence on $\Omega_{a\sigma}^c$ may be completely wrong as occurs with the NUB sequences $\{\Psi_n\}$ for which the part of Ψ_n in the large $|x|$ region (a part that will subsequently be referred to as the *asymptotic tail* of Ψ_n) moves a way from that of Ψ as $n\to\infty$ (see Fig. 5) in such a way that the sequence $\{x^k(\Psi_n)\}_n$ diverges with a large k. Fortunately, since the Ω of Eq. (2.2) is arbitrary, for each Ψ_n there exists a bounded region Ω_n (which we call the *reliability region* of Ψ_n) that satisfies $\Omega_n\subset\Omega_{n+1}$ and such that the equation

$$\lim_{n\to\infty} S(\chi_{\Omega_n}\Psi_n)=S(\Psi) \tag{2.3}$$

holds for many operators S including $S=x^k$ if k is large. Thus the L_2 convergence is indeed a criterion to guarantee the correct calculation of many expectation values $S(\Psi)$ and the true Ψ by means of a sequence $\{\chi_{\Omega_n}\Psi_n\}$ obtained properly from a L_2 convergent one $\{\Psi_n\}$.

Since a formal study of the boundedness property of a sequence $\{\Psi_n\}$ is not an easy task even if each Ψ_n and the true Ψ are known in a closed form, we shall use two criteria to test the *nonuniform* boundedness property. The first one is a geometric characterization of the fact that a NUB sequence $\{\Psi_n\}$ cannot be bounded uniformly by *any* fast decay function. *Proposition 2* [16]: If ψ_B is a fast decay bound of each Ψ_n and the true Ψ on an unbounded region Ω^c and the quantity $\max_{x\in\Omega^c}(\Psi_n/\psi_B)$ diverges as n does, then the asymptotic tail of Ψ_n moves away from that of ψ_B on Ω^c as $n\to\infty$ and hence $\{\Psi_n\}$ is NUB. The second criterion follows from proposition 1. *Corollary 1*: If $\{\Psi_n\}$ converges to Ψ in the L_2 norm but $\{x^k(\Psi_n)\}$ does not converge to $x^k(\Psi)$ for any $k>0$, then $\{\Psi_n\}$ is NUB. Finally, for the uniform boundedness property we have *Corollary 2*: if the Ψ_n's have the monotonic property $|\Psi_{n+1}|\leqslant|\Psi_n|$ on an unbounded region Ω^c independent of n, then $\{\Psi_n\}_{n=j+1}^{\infty}$ is bounded by Ψ_j on Ω^c, and therefore $\{\Psi_n\}$ is UB (see, e.g., Fig. 1).

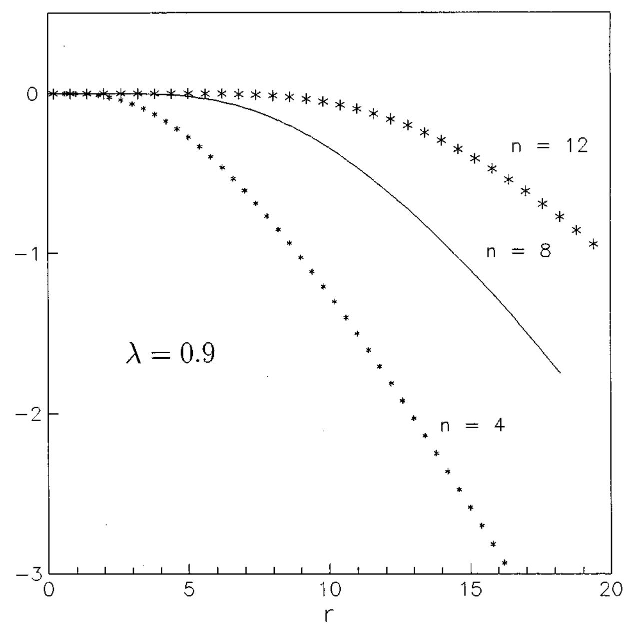

FIG. 1. Graph of $\log_{10}\Psi_n/\Psi$ vs x of example 1. In this figure and the following ones Ψ stands for the exact state of the example in question and R_n is the functional Padé approximant (4.4) of the unnormalized partial sum Ψ_n.

Remark. The results of this section do not depend on the normalization of the wave functions. In fact, from the inequality

$$|x^k(\Psi_n)-x^k(\Psi)|\leq\|\Psi_n-\Psi\|\{[x^{2k}(\Psi_n)]^{1/2}+[x^{2k}(\Psi)]^{1/2}\},$$

it follows that the L_2 convergence ($\|\Psi_n-\Psi\|\to 0$) and the boundedness of the sequence $\{x^{2k}(\Psi_n)\}_n$ are sufficient to guarantee that Eq. (2.1) holds true. Of course, L_2 convergence implies that the norm $\|\Psi_n\|=x^0(\Psi_n)^{1/2}$ tends to $\|\Psi\|$ as $n\to\infty$ and the boundedness of the set $\{x^{2k}(\Psi_n)\}_n$ holds for any $k>0$ when the sequence $\{\Psi_n\}$ is UB, but the wave functions need not be normalized. The motivation to consider unnormalized functions lies in the fact that the partial sums $\Psi_n=\Sigma_{m=0}^n\psi_m\lambda^m$ of the series $\Psi=\Sigma_{m=0}^\infty\psi_m\lambda^m$ are in general unnormalized even if Ψ is normalized. Furthermore, since $\|\Psi_n\|$ may diverge as n increases, we consider it pertinent to study graphically the boundedness property of the Ψ_n's by plotting the ratios Ψ_n/Ψ vs x without the effects generated by a possible incorrect convergence of the normalization factor $\|\Psi_n\|$. Accordingly, we report the values of $x^0(\Psi_n)$ and for $k>0$ the ratios $x^k(\Psi_n)/x^0(\Psi_n)$, these latter ones being the standard *expectation values* of the operators x^k, although, abusing the language, in this article we call ''expectation value'' the quantity $S(f)$ even if f is unnormalized.

III. FORMAL PERTURBATION SERIES

The sequences $\{\Psi_n\}$ to be studied are defined by the partial sums

$$\Psi_n(\lambda,x)=\sum_{m=0}^{n}\psi_m(x)\lambda^m \tag{3.1}$$

of the eigenfunction perturbation series

$$\Psi(\lambda,x)=\sum_{m=0}^{\infty}\psi_m(x)\lambda^m, \tag{3.2}$$

where the infinite series will be referred to as the Ψ series and $\Psi(\lambda,x)$ is a solution of the self-adjoint eigenproblem in L_2,

$$H(\lambda)\Psi(\lambda,x)=E(\lambda)\Psi(\lambda,x), \tag{3.3}$$

where for simplicity we consider $H(\lambda)=H_0+\lambda V(x)$ and as usual the zero-order eigenproblem is $H_0\psi_0=E_0\psi_0$.

In order to expose the main ideas we shall study the so-called *formal* Ψ series of Kato [5], which are obtained by a direct substitution of Eq. (3.2) and the corresponding E series

$$E(\lambda)=\sum_{m=0}^{\infty}E_m\lambda^m \tag{3.4}$$

into Eq. (3.3). We consider formal series because, as we shall see below, their convergence properties are known for several perturbations V of interest while rigorous results for other kinds of Ψ and E series are scarce. In Sec. V we consider other kinds of Ψ series.

The convergence of formal E series is understood in the usual sense of analytic complex functions while a Ψ series is

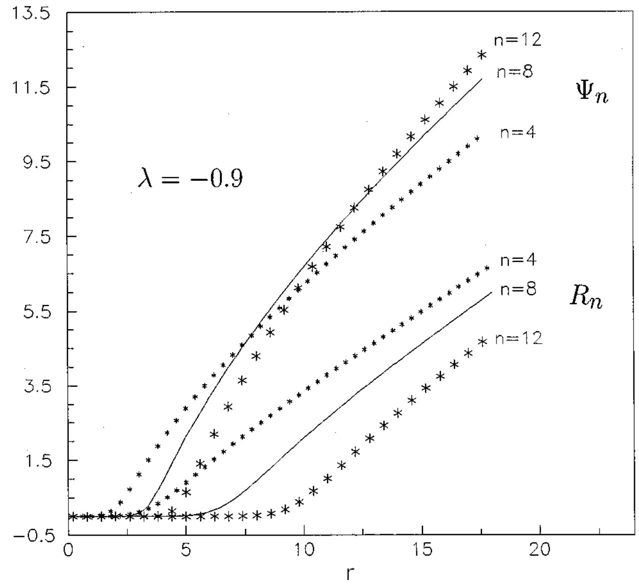

FIG. 2. Graph of $\log_{10}\Psi_n/\Psi$ and $\log_{10}R_n/\Psi$ vs x of example 1.

said to be convergent or having a nonzero convergence radius λ_Ψ if the partial-sum sequence $\{\Psi_n\}$ is L_2 convergent with $|\lambda|<\lambda_\Psi$, that is, if

$$\lim_{n\to\infty}\|\Psi_n-\Psi\|=0 \quad \text{holds for } |\lambda|<\lambda_\Psi. \tag{3.5}$$

According to analytic perturbation theory [5] the two kinds of perturbations V for which the formal E and ψ series have a nonzero convergence radius are (i) the V's *bounded by* H_0 (when $\|V\psi\|\leq a\|\psi\|+b\|H_0\psi\|$ holds with ψ-independent a,b) and (ii) the V's *form bounded by* H_0 (when $|\langle V\psi,\psi\rangle|\leq a'\|\psi\|^2+b'\langle\psi,H_0\psi\rangle$ holds with ψ-independent a',b'). V is referred to as a *regular* perturbation of H_0 if it is bounded or relatively form bounded by H_0; otherwise V is called a *singular* perturbation of H_0. The perturbation theory results for regular V's can be summarized by *Proposition 3*: If V is regular, then the E and Ψ series have a nonzero convergence radius, while it is known that almost all the singular V's generate formal E series with zero convergence radius. In Secs. III A and III B we shall examine the convergence and boundedness properties of formal Ψ series associated with regular and singular V's. We use the notation $\partial_x=\partial/\partial x$ and $\partial_\lambda=\partial/\partial\lambda$.

A. Regular-V Ψ series

Example 1. Consider the $1s$ hydrogen Hamiltonian $H_0=-\frac{1}{2}\partial_x^2-x^{-1}$ and let $H=H_0+\lambda x^{-1}$ on $L_2(0,\infty)$ with $\langle f,g\rangle=\int_0^\infty f^*g\,dx$. It can be shown that $V=x^{-1}$ is bounded by H_0 [18] and therefore the (unnormalized) $1s$ eigenstate $\Psi(\lambda,x)=xe^{-(1-\lambda)x}$ has a L_2 convergent formal Ψ series with convergence radius λ_Ψ (<1). The coefficients ψ_m of the Ψ series are given by $m!\psi_m=\partial_\lambda^m\Psi|_{\lambda=0}$. Figures 1 and 2 show the graph of the ratios Ψ_n/Ψ with $\lambda=\pm 0.9$; as expected we observe a correct local convergence of $\{\Psi_n\}$ on the interval $[0,7]$ of the x axis but on $[10,\infty)$ there is a marked difference between the figures. For $\lambda=0.9$ the asymptotic tail of Ψ_n tends to that of Ψ as n increases and

TABLE I. Expectation values $x^k(\Psi_n)$ from the Ψ_n's of example 1. The quantities $x^0(\Psi_n)=\|\Psi_n\|^2$ and the ratios $x^k(\Psi_n)/x^0(\Psi_n)$ with $k\geqslant 2$ are reported. In this table and the following ones the notation 9.06[−6] (1.4[4]) means 9.06×10^{-6} (1.4×10^4).

n	x^0	x^2	x^3	x^4
		$\lambda=0.9$		
4	1.59[1]	1.8[1]	9.9[1]	5.9[2]
8	5.75[1]	4.5[1]	3.6[2]	3.2[3]
12	1.08[2]	7.9[1]	8.5[2]	9.9[3]
Ex[a]	2.50[2]	3.0[2]	7.5[3]	2.3[5]
		$\lambda=-0.9$		
4	4.0[−1]	3.5[1]	2.4[2]	1.8[3]
8	3.8[−1]	9.5[1]	1.0[3]	1.2[4]
12	2.9[−1]	1.8[2]	2.7[3]	4.1[4]
Ex[a]	3.6	8.3[−1]	1.1	1.7

[a]Exact values from the (unnormalized) exact $\Psi=xe^{-(1-\lambda)x}$.

$\Psi_{n+1}<\Psi_n$ holds on $[10,\infty)$ whereas for $\lambda=-0.9$ there is an increasing separation between the tails. Hence the positive-λ sequence $\{\Psi_n\}$ is UB (Corollary 2) and the negative-λ one $\{\Psi_n\}$ is NUB (Proposition 2), the first result being supported by the correct convergence of positive-λ sequences $\{x^k(\Psi_n)\}_n$ reported in Table I while the second one is confirmed by the divergence of negative-λ sequences $\{x^k(\Psi_n)\}_n$ with $k\geqslant 2$ reported in the same table (Corollary 1).

Example 2. Consider the harmonic oscillator operator $H_0=\frac{1}{2}(-\partial_x^2+x^2)$ and let $H=H_0+\lambda x^2$ on $L_2(-\infty,\infty)$, $\langle f,g\rangle=\int_{-\infty}^{\infty}f^*g\,dx$. It is easy to see that $V=x^2$ is form bounded by H_0 and hence a regular perturbation so that the formal Ψ series of the (normalized) ground state, $\Psi(\lambda,x)=\pi^{-1/4}\exp[-(1+2\lambda)^{1/2}x^2/2]$, has a nonzero convergence radius $\lambda_\Psi(<0.5)$. The coefficients ψ_m are given by $m!\,\psi_m=\partial_\lambda^m\Psi|_{\lambda=0}$. The convergence properties of the sequence $\{\Psi_n\}$ are similar to those in example 1. Figures 3 and 4 show the ratio Ψ_n/Ψ with $\lambda=\pm 0.4$ and we observe a correct local convergence on [0,4] while the behavior of the asymptotic tails indicates that the negative- (positive-) λ sequence $\{\Psi_n\}$ is UB (NUB), a result confirmed by the correct (incorrect) convergence of large-k sequences $\{x^k(\Psi_n)\}_n$ reported in Table II.

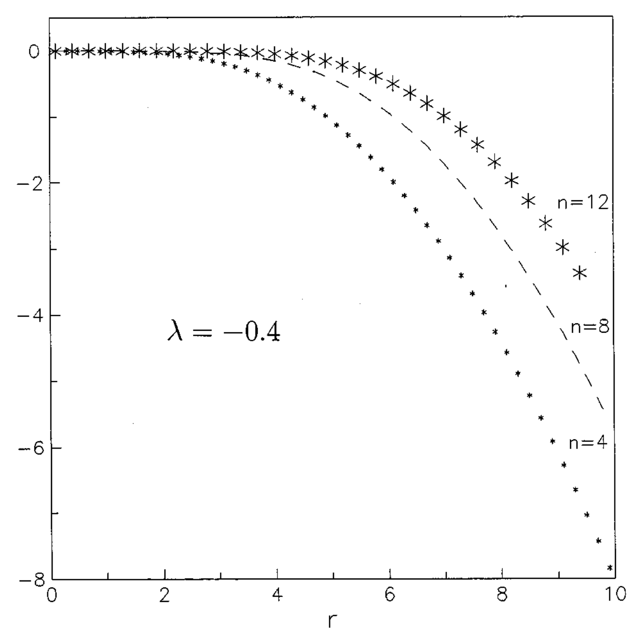

FIG. 3. Graph of $\log_{10}\Psi_n/\Psi$ vs x of example 2.

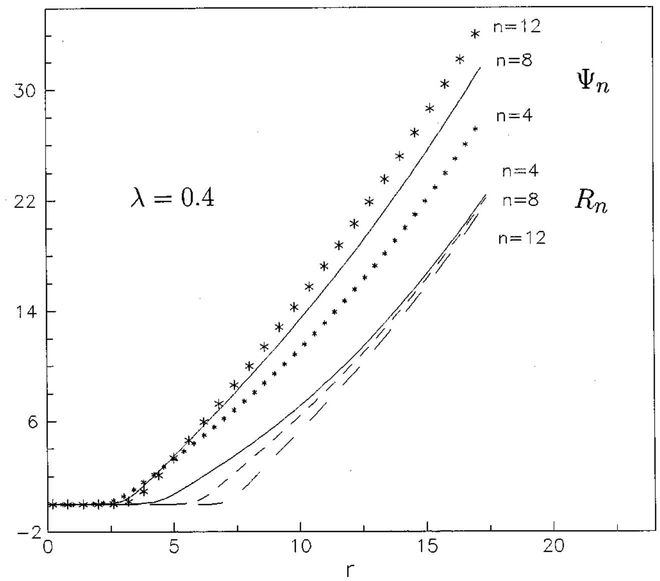

FIG. 4. Graph of $\log_{10}\Psi_n/\Psi$ and $\log_{10}R_n/\Psi$ vs x of example 2.

Suppose that the eigenproblem $H_0\psi_0=E_0\psi_0$ has only nondegenerate eigenvalues $E_0^{(i)}$ and their eigenfunctions $\psi_0^{(i)}$ are normalized ($i=0,1,\ldots$). If the set $\{\psi_0^{(i)}\}_{i=0}^{\infty}$ constitutes a complete basis of the Hilbert space L_2 in question, the Rayleigh-Schrödinger perturbation theory (RSPT) provides the following Fourier series for the first-order term ψ_1 of the ground state Ψ series:

TABLE II. Expectation values $x^k(\Psi_n)$ from the Ψ_n's of example 2. The ratios $x^k(\Psi_n)/x^0(\Psi_n)$ are reported.

n	x^2	x^{10}	x^{24}	x^{30}
		$\lambda=-0.4$		
4	0.977	5.42[2]	2.4[10]	1.6[14]
12	1.106	1.41[3]	4.4[11]	6.7[15]
20	1.117	1.61[3]	9.3[11]	2.0[16]
Ex[a]	1.118	1.65[3]	1.2[12]	3.3[16]
		$\lambda=0.4$		
4	0.3817	17.9	1.6[9]	1.4[13]
12	0.3730	7.52	1.7[9]	4.8[13]
20	0.3727	6.84	3.4[8]	1.8[13]
Ex[a]	0.3727	6.79	2.3[6]	2.3[9]
		$\lambda=0.6$		
4	0.42	2.91[2]	5.6[10]	5.1[14]
12	0.59	1.08[4]	4.2[13]	1.2[18]
20	2.24	2.45[5]	4.6[15]	2.4[20]
Ex[a]	0.34	4.11[0]	6.8[5]	5.1[8]

[a]Exact values from the (normalized) $\Psi=\pi^{-1/4}\exp[-(1+2\lambda)^{1/2}x^2/2]$.

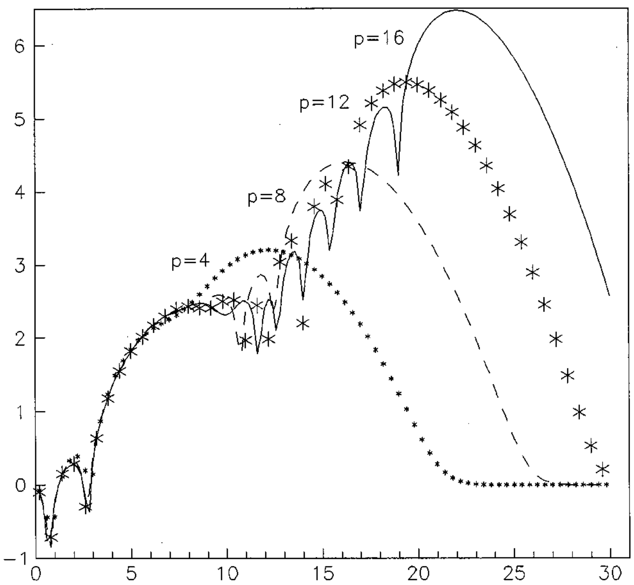

FIG. 5. Graph of $\log_{10}|\psi_{1p}^F/e^{-x}|$ vs x with Fourier ψ_{1p}^F's of example 3 with $\lambda=0.1$.

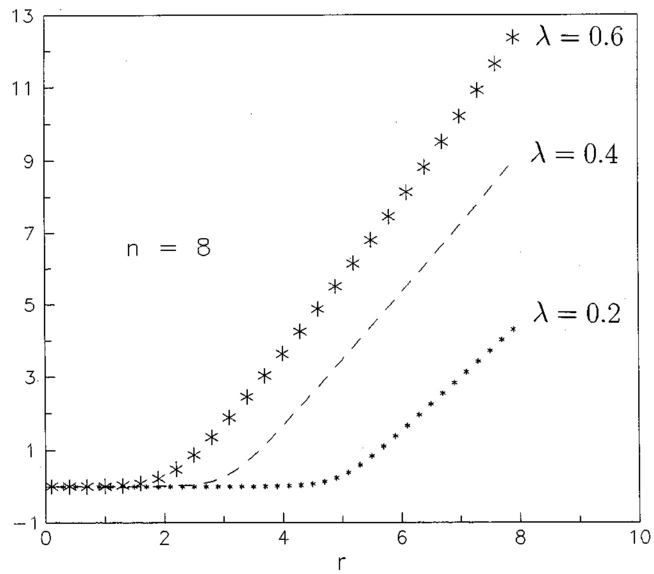

FIG. 6. Graph of $\log_{10}\Psi_n(\lambda,x)/\Psi$ vs x for example 2 with increasing values of λ.

$$\psi_1(x)=\sum_{i=1}^{\infty} \psi_0^{(i)}\langle \psi_0^{(i)},V\psi_0^{(0)}\rangle/(E_0^{(0)}-E_0^{(i)}). \quad (3.6)$$

The completeness of $\{\psi_0^{(i)}\}_{i=0}^{\infty}$ guarantees that the finite Fourier series

$$\psi_{1p}^F(x)=\sum_{i=1}^{p} \psi_0^{(i)}\langle \psi_0^{(i)},V\psi_0^{(0)}\rangle/(E_0^{(0)}-E_0^{(i)}) \quad (3.7)$$

tends to ψ_1 in the L_2 norm as $p\to\infty$, but the sequence $\{\psi_{1p}^F\}_{p=1}^{\infty}$ may be NUB. This is illustrated by the following example.

Example 3. Consider the harmoniclike Hamiltonian $H_0 = -\frac{1}{2}\partial_x^2+\epsilon x^2$ with $\epsilon=10^{-2}$ and let $H=H_0+\lambda x^{-1}$ on $L_2(0,\infty)$ with the eigenstate boundary condition $\Psi|_{x=0}=0$ for all λ. $V=x^{-1}$ is form bounded by H_0 [19] and therefore the formal ground state Ψ series has a nonzero radius of convergence while the completeness of the set $\{\psi_0^{(i)}\}_{i=0}^{\infty}$ [3] guarantees that the ground state sequence $\{\psi_{1p}^F\}_p$ converges to ψ_1. To show that $\{\psi_{1p}^F\}_p$ is NUB we shall use (in the absence of a closed-form expression of ψ_1) a bound ψ_B of ψ_1 and each ψ_{1p}^F in order to exhibit the increasing separation between their asymptotic tails as p increases (proposition 2). Since Ψ and each $\psi_0^{(i)}$ decay like $\exp[-x^2(\epsilon/2)^{1/2}]$, every mth-order term of the Ψ series also does and therefore $\psi_B = e^{-x}$ is a fast-decay bound of ψ_1 and ψ_{1p}^F. Figure 5 shows the increasing separation between the tails of ψ_{1p}^F and ψ_B as p increases; hence the same result holds between those of ψ_1 and ψ_{1p}^F and $\{\psi_{1p}^F\}$ is NUB.

Remark 1. Examples 1 and 2 show that the boundedness property of $\{\Psi_n\}$ can change suddenly from UB to NUB when λ varies continuously within the convergence interval $[-\lambda_\Psi,\lambda_\Psi]$ of the Ψ series. This *discontinuity* of the boundedness property is worthy and motivates the use of the following concept (which is independent of the L_2 convergence) to characterize better such a property. We say that the sequence $\{\Psi_n\}$ from a Ψ series has the *uniform boundedness set* Δ^{UB} if it is UB for $\lambda\in\Delta^{\mathrm{UB}}$; in a similar way we define the *nonuniform boundedness set* Δ^{NUB} of $\{\Psi_n\}$.

Remark 2. If the sequence $\{\Psi_n(\lambda,x)\}$ from a Ψ series has a nonempty Δ^{NUB} and λ_1 and λ_2 are in Δ^{NUB}, we can say that the nouniform boundedness of $\{\Psi_n(\lambda_1,x)\}$ is stronger than that of $\{\Psi_n(\lambda_2,x)\}$ when the separation rate between the asymptotic tails of $\Psi_n(\lambda_1,x)$ and $\Psi(\lambda_1,x)$ is faster than that between the tails of $\Psi_n(\lambda_2,x)$ and $\Psi(\lambda_2,x)$ as n increases. To illustrate this consider the ratios Ψ_n/Ψ plotted in Fig. 6 with $\Psi_n(\lambda,x)$'s from example 2 with $n=8$ and $\lambda=0.2$, 0.4, 0.6; we observe that the tail of Ψ_n moves away from that of Ψ as λ increases and similar results are obtained with other n values; thus larger positive λ values yield a stronger nonuniform boundednes. This suggests that (i) $\Delta^{\mathrm{NUB}}=(0,\infty)$ and (ii) the sequence $\{x^k(\Psi_n)\}_n$ with $k\geqslant 0$ has a worse convergence or diverges as λ is made larger in Δ^{NUB}. As expected, Table II shows that $\{x^k(\Psi_n)\}_n$ diverges from $k\geqslant 2$ with $\lambda=0.6$ whereas $\{x^2(\Psi_n)\}_n$ with $\lambda=0.4$ converges correctly. The numerical evidence (see Fig. 3 and Table II) also suggests that $\{\Psi_n\}$ is L_2 convergent and UB for λ in $(-0.5,0]$, so that $\{\Psi_n\}$ has a correct global convergence for $\lambda\in\Delta^{\mathrm{UB}}=(-0.5,0]$ (see proposition 1). Similar results from example 1 suggest that the 1s Ψ series yields a sequence $\{\Psi_n\}$ having $\Delta^{\mathrm{UB}}=[0,1)$ and $\Delta^{\mathrm{NUB}}=(-\infty,0)$, $\{\Psi_n\}$ being, apparently, L_2 convergent for all λ in Δ^{UB} (see Figs. 1 and 2 and Table I).

Remark 3. We have considered the ground state of example 2 for which there is a one-to-one correspondence between the excited states of the unperturbed Hamiltonian H_0 and those of $H(\lambda)$. Numerical results from the first excited states of example 2 are similar to those of the ground state, so that the corresponding excited Ψ series yield sequences $\{\Psi_n\}$ with $\Delta^{\mathrm{NUB}}=(0,\infty)$ and $\Delta^{\mathrm{UB}}=(-0.5,0]$.

B. Singular-V Ψ series

It is well known that almost all singular perturbations V of a given Hamiltonian H_0 generate formal E series of eigen-

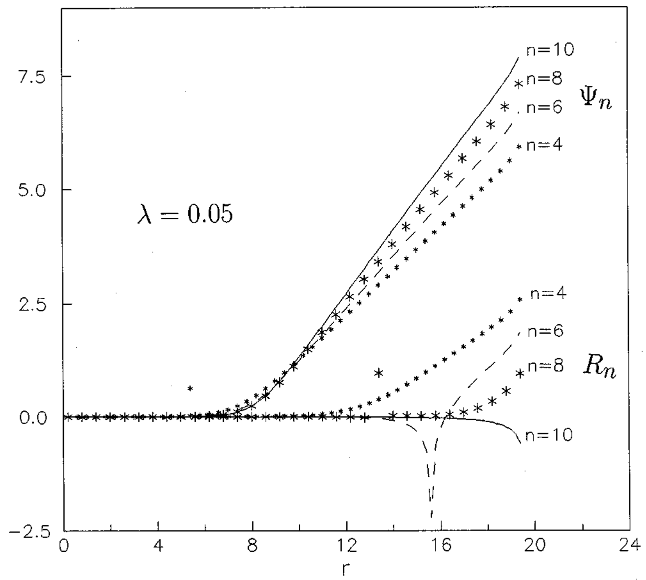

FIG. 7. Graph of $\log_{10}|\Psi_n/\Psi_D|$ and $\log_{10}|R_n/\Psi_D|$ vs x of example 4. In this figure and the following ones Ψ_D is a normalized Dirichlet approximation of Ψ.

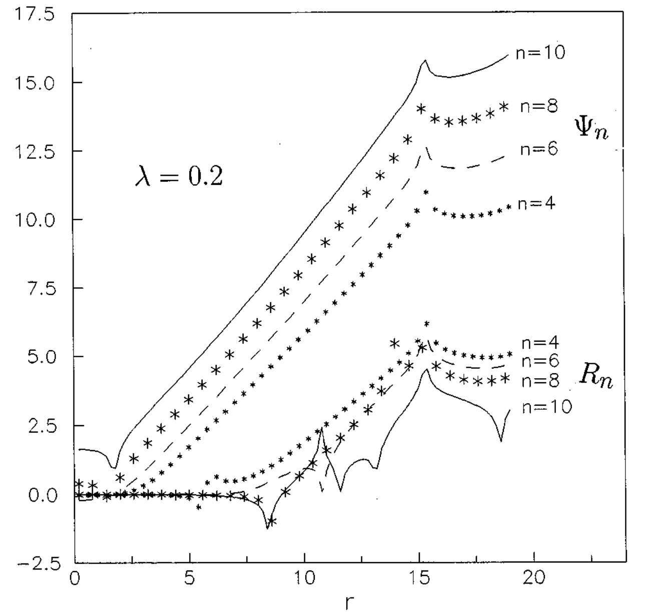

FIG. 8. Graph of $\log_{10}|\Psi_n/\Psi_D|$ and $\log_{10}|R_n/\Psi_D|$ vs x of example 4.

values $E(\lambda)$ with a zero convergence radius while only for some singular V's was it shown that the Ψ series is an asymptotic expansion of the true Ψ up to a particular power of λ [5,14,15], a weak result to assess the correct calculation of the Ψ's or expectation values $S(\Psi)$. Let us examine the convergence properties of some Ψ series associated with singular V's.

Example 4. Consider the 1*s* hydrogen Hamiltonian $H_0 = -2^{-1}\partial_x^2 - x^{-1}$ and let $H = H_0 + \lambda x$ on $L_2(0,\infty)$ with $\lambda \geq 0$, where $V = x$ is a singular perturbation of H_0. The true 1*s* eigenfunction $\Psi(\lambda,x)$ is approximated by a (normalized) Dirichlet-type function $\Psi_D(\lambda,x)$ [20,21], and the Ψ series is obtained from the zeroth-order solutions $E_0 = -1/2$, $\psi_0 = xe^{-x}$. Figure 7 [22] shows the ratio Ψ_n/Ψ_D for $\lambda = 0.05$ and we observe a correct but local convergence of $\{\Psi_n\}$ on $[0,8]$ whereas there is an increasing separation between the asymptotic tails of Ψ_n and Ψ_D as $n \to \infty$; hence $\{\Psi_n\}$ is NUB. Larger λ values yield a faster increasing separation between the asymptotic tails and a worse local convergence as follows from the graph of Ψ_n/Ψ_D with $\lambda = 0.2$ plotted in Fig. 8 and the faster divergence of the sequences $\{x^k(\Psi_n)\}_n$ reported in Table III with $k \geq 0$. This suggests that $\Delta^{\mathrm{NUB}} = (0,\infty)$.

Example 5. Let $H_0 = \frac{1}{2}(-\partial_x^2 + x^2)$ and let $H = H_0 + \lambda x^4$ on $L_2(-\infty,\infty)$ with $\lambda \geq 0$. This is a well-known singular-V problem for which the correct calculation of the true energy $E(\lambda)$ from the formal E series has been a subject extensively studied in the past [7,9,13]. The true ground state Ψ is approximated by a (normalized) Dirichlet wave function Ψ_D [23], and the Ψ series is obtained from the zeroth-order solutions $E_0 = 1/2$, $\psi_0 = \pi^{-1/4}e^{-x^2/2}$. The ratio Ψ_n/Ψ_D plotted in Figs. 9 and 10 with $\lambda = 0.01, 0.05$ shows the correct local convergence of $\{\Psi_n\}$ and the increasing separation between the asymptotic tails of Ψ_n and Ψ_D, so that $\{\Psi_n\}$ is NUB. As occurs with example 4, larger λ values yield a worse local convergence and a stronger nonuniform boundedness; this suggests that $\Delta^{\mathrm{NUB}} = (0,\infty)$.

IV. CORRECT CALCULATION OF Ψ'S AND EXPECTATION VALUES

Having examined the convergence properties of some sequences $\{\Psi_n\}$ from formal Ψ series the question is now how to obtain a correct approximation toward the true Ψ and expectation values $S(\Psi)$ when $\{\Psi_n\}$ does *not* have a correct *global* convergence. In this section we shall attempt to an-

TABLE III. Expectation values $x^k(\Psi_n)$ from the Ψ_n's of example 4. The quantities $x^0(\Psi_n) = \|\Psi_n\|^2$ and the ratios $x^k(\Psi_n)/x^0(\Psi_n)$ with $k \geq 1$ are reported.

n	x^0	x^1	x^2	x^3
		$\lambda = 0.05$		
4	0.2356	1.387	2.525	5.686
6	0.2355	1.386	2.521	5.680
8	0.2355	1.386	2.529	5.827
10	0.2356	1.390	2.616	7.490
Ex[a]		1.385	2.514	5.616
		$\lambda = 0.2$		
4	1.5[0]	7.3[0]	6.3[1]	6.0[2]
6	2.4[2]	1.1[1]	1.8[2]	1.6[3]
8	1.3[5]	1.4[1]	2.0[2]	3.0[3]
10	1.7[8]	1.7[1]	2.9[2]	5.3[3]
Ex[a]		1.2	1.9	3.49
		$\lambda = 1.0$		
4	7.8[5]	8.1	7.0[1]	6.5[2]
6	8.2[10]	1.1[1]	1.2[2]	1.5[3]
8	2.6[16]	1.4[1]	1.9[2]	2.9[3]
10	2.0[22]	1.7[1]	2.9[2]	5.1[3]
Ex[a]		0.9	1.0	1.4

[a]Exact values from a normalized Dirichlet wave function [21].

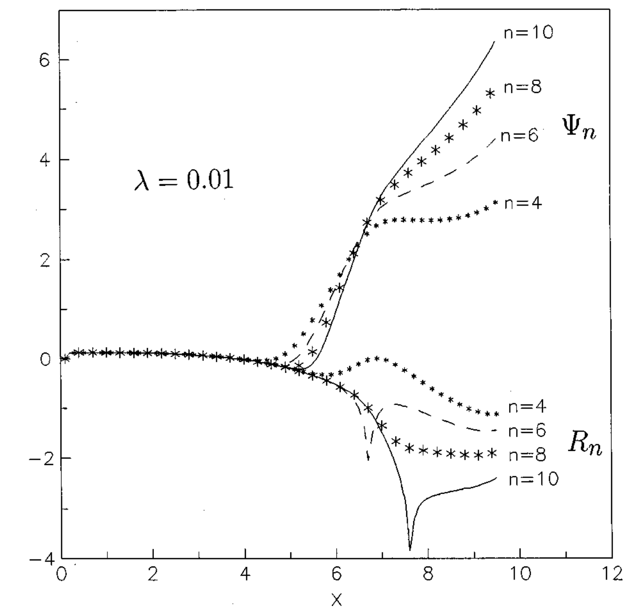

FIG. 9. Graph of $\log_{10}|\Psi_n/\Psi_D|$ and $\log_{10}|R_n/\Psi_D|$ vs x of example 5.

swer this question with the NUB sequences of examples above.

A. Reliability region of the NUB sequence $\{\psi_{1p}^F\}_p$ from RSPT

The Fourier sequence $\{\psi_{1p}^F\}_{p=1}^{\infty}$ of the first-order term $\psi_{m=1}$ of example 3 is NUB but according to the results of Sec. II its L_2 convergence guarantees that each ψ_{1p}^F is reliable on a region $[0,x_{1p}]$ which can be estimated as follows. An arrangement of the terms of ψ_{1p}^F, Eq. (3.7), yields $\psi_{1p}^F = x\exp[-x^2(\epsilon/2)^{1/2}]\phi_{1p}(x)$ with $\phi_{1p}=\phi_{1pq}|_{q=2p-1}$ and ϕ_{1pq} given by

$$\phi_{1pq}=\sum_{j=1}^{q} c_{1pj}x^{j-1}, \tag{4.1}$$

TABLE IV. Convergence of the sequence $\{\phi_{1pq}(x)\}_{q=5}^{2p-1}$ with $p=8$ [Eq. (4.1)] for some x values, example 3 with $\lambda=0.1$. The last row reports approximated x_{1p}'s for which each p fixed sequence $\{\phi_{1pq}(x)\}_{q=5}^{2p-1}$ satisfies Eq. (4.2) with $\delta=0.001$.

q	$x=2$	$x=4$	$x=6$	$x=8$	$x=10$
5	-1.104	-3.643	$-3.3[1]$	$-1.3[2]$	$-3.4[2]$
7	-1.000	3.020	4.3[1]	3.0[2]	1.3[3]
9	-1.009	0.603	$-1.9[1]$	$-3.2[2]$	$-2.4[3]$
11	-1.009	1.069	7.9	1.6[2]	2.1[3]
13	-1.009	1.025	2.2	$-2.3[1]$	$-6.0[2]$
15	-1.009	1.027	2.6	3.4	6.7
	p	4	8	12	16
	x_{1p}	1.2	2.8	4.9	6.1

whose c_{1pj}'s are p dependent. Table IV shows that for $p=8$ and $x=2,4$ the numerical sequence $\{\phi_{pq}(x)\}_{q=1}^{2p-1}$ has the property that $\Delta\phi_{1pq}(x)=|\phi_{1p,q-1}(x)/\phi_{1pq}(x)-1|$ decreases monotonically as $q\to 2p-1$ whereas with $x=6,8,10$, $\Delta\phi_{1pq}(x)$ does not exhibit a convergence pattern as $q\to 2p-1$. A survey of the ratio ψ_{1p}^F/e^{-x} plotted in Figs. 5 and 11 shows that the values $x=2,4$ belong to the interval on which $\psi_{1,p=8}^F$ exhibits a converged behavior while the others x's are in the interval on which the tail of $\psi_{1,p=8}^F$ is clearly wrong. This suggests the use of the convergence pattern of $\{\Delta\phi_{pq}(x)\}_{q=1}^{2p-1}$ to estimate x_{1p} by

$$x_{1p}=\sup_{x\geq 0}\{x:\Delta\phi_{1pq}(x)<\delta \text{ with } q=2p-1\}. \tag{4.2}$$

Table IV shows the x_{1p}'s estimated with $\delta=10^{-3}$ for some p's [24]. The goodness of $[0,x_{1p}]$ to be the reliability region of ψ_{1p}^F is supported by the following facts: (i) The increment of x_{1p} as p increases is congruent with the fact that the L_2 convergence of $\{\psi_{1p}^F\}_{p=1}^{\infty}$ toward ψ_1 guarantees that the reli-

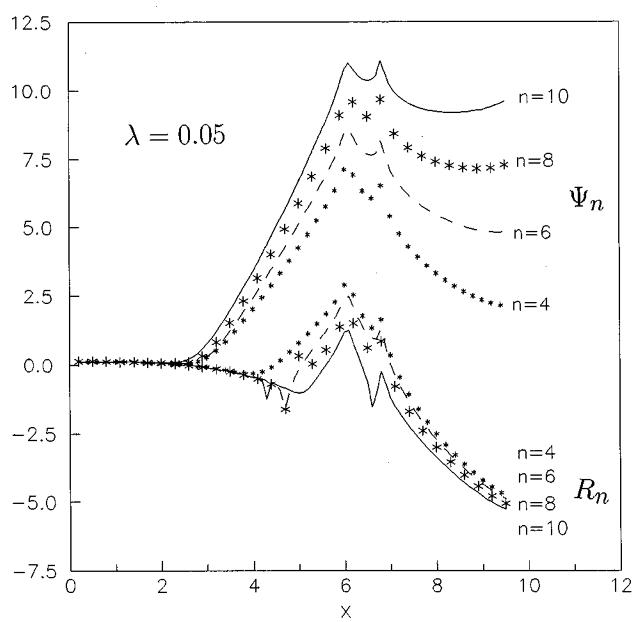

FIG. 10. Graph of $\log_{10}|\Psi_n/\Psi_D|$ and $\log_{10}|R_n/\Psi_D|$ vs x of example 5.

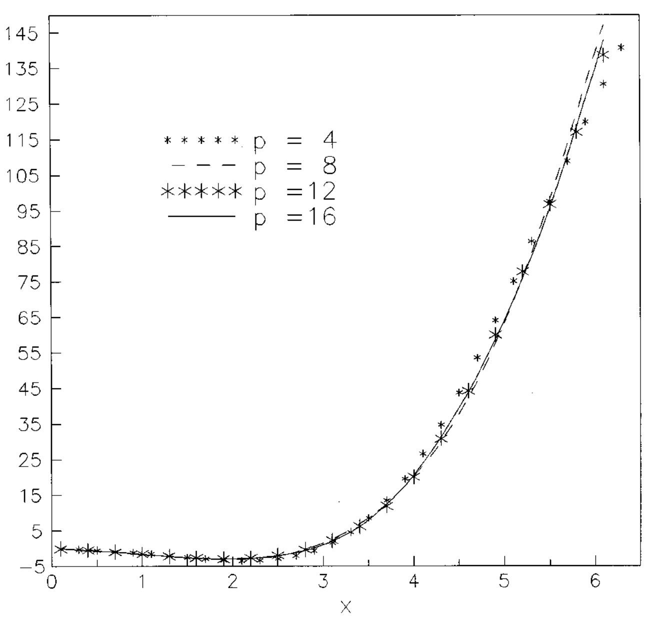

FIG. 11. Graph of ψ_{1p}^F/e^{-x} vs x with Fourier ψ_{1p}^F's of example 3 with $\lambda=0.1$.

TABLE V. Local expectation values $x^k(\chi_{p'}\psi^F_{1p}) = \int_0^{x_{1p'}} |\psi^F_{1p}|^2 x^k\, dx$ and expectation values $x^k(\psi^F_{1p})$ (for which $x_{1p'}=\infty$) from the Fourier expansion ψ^F_{1p} for example 3 with $\epsilon = 10^{-2}$ and $\lambda = 0.1$. The quantities $x^0(\chi_{p'}\psi^F_{1p}) = \|\chi_{p'}\psi^F_{1p}\|^2$ and the ratios $x^k(\chi_{p'}\psi^F_{1p})/x^0(\chi_{p'}\psi^F_{1p})$ with $k \geq 2$ are reported.

p	x^0	x^2	x^8	x^9
		$x_{1,p'=8}=2.8$		
4	1.346	14.09	4.02[5]	2.45[6]
8	1.371	13.76	4.73[5]	2.94[6]
12	1.374	13.64	4.68[5]	2.92[6]
16	1.375	13.64	4.66[5]	2.90[6]
		$x_{1,p'=12}=4.9$		
4	1.346	15.27	1.05[6]	8.70[6]
8	1.371	14.45	7.10[5]	5.00[6]
12	1.374	14.38	6.89[5]	4.78[6]
16	1.375	14.37	6.83[5]	4.72[6]
		$x_{1,p'=16}=6.1$		
4	1.346	15.27	1.06[6]	8.76[6]
8	1.371	14.48	9.40[5]	8.36[6]
12	1.374	14.39	7.27[5]	5.34[6]
16	1.375	14.37	6.99[5]	4.95[6]
		$x_{1,p'}=\infty$		
4	1.346	15.27	1.1[6]	8.8[6]
8	1.371	14.48	9.5[5]	8.6[6]
12	1.374	14.40	9.8[5]	9.9[6]
16	1.375	14.37	1.0[6]	1.1[7]

ablity region of each ψ^F_{1p} increases as $p \to \infty$, (ii) a survey of Figs. 5 and 11 shows that $[0,x_{1p}]$ agrees well with the region on which ψ^F_{1p} exhibits a converged behavior as p increases, and (iii) in agreement with Eqs. (2.2) and (2.3) the ''local'' sequences $\{x^k(\chi_{p'}\psi^F_{1p})\}_p$ reported in Table V, where $\chi_{p'}(x)=1$ for $x \in [0,x_{1p'}]$ and $\chi_{p'}=0$ otherwise, are decreasing and therefore convergent whereas the complete-integral sequences $\{x^k(\psi^F_{1p})\}_p$ reported in the same table are monotonically increasing with large k as expected from the nonuniform boundedness of $\{\psi^F_{1p}\}_p$. The same procedure can be applied to estimate the reliability region $[0,x_{mp_m}]$ of the Fourier expansions $\psi^F_{mp_m}$ with p_m terms of the mth-order coefficients ψ_m. Thus, if $\chi_{mp_m}=1$ on $[0,x_{mp_m}]$ and $\chi_{mp_m}=0$ otherwise, the right-hand term of the expression

$$\Psi(\lambda,x) \sim \psi_0(x) + \sum_{m=1}^{\infty} \chi_{mp_m}\psi^F_{mp_m}(x)\lambda^m \tag{4.3}$$

only considers the reliable part of each finite Fourier expansion $\psi^F_{mp_m}$ and tends to Ψ in the L_2 norm as the p_m's are made larger. Of course, if the partial sums from Eq. (4.3) constitute a UB sequence, then such partial sums can be used to compute expectation values or to obtain a correct global convergence toward Ψ; otherwise we have to combine Eq. (4.3) with a summability method as is done below.

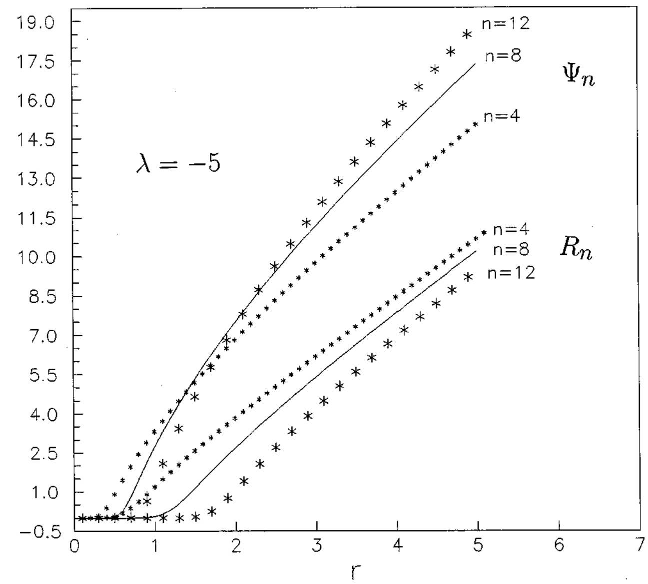

FIG. 12. Graph of $\log_{10}\Psi_n/\Psi$ and $\log_{10}R_n/\Psi$ vs x of example 1.

B. Functional Padé-approximant sequences $\{R_n\}$ from NUB sequences $\{\Psi_n\}$

Examples 1 and 2 showed that regular perturbations V of a given Hamiltonian H_0 can generate sequences $\{\Psi_n\}$ with a nonempty set $\Delta^{\rm NUB}$ and therefore with an incorrect global convergence toward the true Ψ despite its L_2 convergence for small λ in $\Delta^{\rm NUB}$. If $\{\Psi_n\}$ is L_2 convergent, we can, at least in principle, find the reliability region of each Ψ_n to compute Ψ or the expectation values $S(\Psi)$ as was done above but a more convenient way may be the use of a summability method that takes advantage of the fact that Ψ_n is a power series of λ. For instance, Ψ_n can be approximated by the functional Padé approximant [25]

$$R_n(\lambda,x) = \left[\sum_{k=0}^{n} a_k(x)\lambda^k\right] \Bigg/ \left[1+\sum_{k=1}^{n} b_k(x)\lambda^k\right], \tag{4.4}$$

and the question is then to determine if the sequence $\{R_n(\lambda,x)\}_n$ converges in some sense to Ψ (in particular if it is L_2 convergent) and is UB. This is not an easy task if we consider that, under the assumption that $\Psi(\lambda,x_0)$ is λ analytic in the usual sense of complex functions, the strongest property that the x_0-fixed sequence $\{R_n(\lambda,x_0)\}$ may have is given by the Padé conjecture; namely, there exists a subsequence of $\{R_n(\lambda,x_0)\}$ that converges uniformly to $\Psi(\lambda,x_0)$ on certain bounded sets of λ space [8]. In our case $\Psi(\lambda,x_0)$ may not be an analytic function for some x_0's or potentials V and the convergence of its formal Ψ series has been established rigorously only in the L_2 sense [Eq. (3.4)] for regular V. Since a rigorous proof of, for example, the L_2 convergence and the uniform boundednes of $\{R_n(\lambda,x)\}_n$ is a formidable mathematical problem, we shall examine numerically the convergence and boundedness properties of the sequences $\{R_n(\lambda,x)\}$ associated with the examples of Sec. III.

Consider the $1s$ sequence $\{\Psi_n\}$ of example 1 which is NUB for $\lambda \in \Delta^{\rm NUB} = (-\infty,0)$. Figure 2 shows the graph of Ψ_n/Ψ and the corresponding ratios R_n/Ψ with $\lambda = -0.9$.

TABLE VI. Padé approximants $r_n^{(k)}(\lambda)$ [Eq. (4.6)] and expectation values $x^k(\Psi_n)$ from the Ψ_n's of example 1. The quantities $r^{(0)}(\lambda)$, $x_n^{(0)}(\Psi_n)$ and the ratios $r_n^{(k)}(\lambda)/r_n^{(0)}(\lambda)$, $x^k(\Psi_n)/x^0(\Psi_n)$ with $k\geqslant 2$ are reported.

n	x^0	x^2	x^3	x^4
		$\lambda=-0.9$		
		$r_n^{(k)}(\lambda)$		
4	3.723	1.327	3.306	1.18[1]
8	3.645	0.8313	1.098	1.768
12	3.645	0.8310	1.093	1.727
Ex[a]	3.645	0.8310	1.093	1.727
n	x^0	x^1	x^2	x^3
		$\lambda=-5.0$		
		$x^k(\Psi_n)$		
4	8.9[5]	5.6	3.4[1]	2.3[2]
8	8.2[11]	9.7	9.8[1]	1.0[3]
12	5.6[17]	1.4[1]	1.9[2]	2.8[3]
Ex[a]	1.157[1]	2.5[−1]	8.333	3.472
		$r_n^{(k)}(\lambda)$		
4	1.208	3.360	1.1[1]	3.7[1]
8	1.157[1]	2.50[−1]	1.195	1.1[1]
12	1.157[1]	2.50[−1]	8.333	3.472
Ex[a]	1.157[1]	2.50[−1]	8.333	3.472

[a]Exact values from the (unnormalized) exact $\Psi=xe^{-(1-\lambda)x}$.

TABLE VII. Padé approximants $r_n^{(k)}(\lambda)$ [Eq. (4.6)] and $q_n^{(k)}(\lambda)$ [Eq. (4.8)] from the Ψ series and their partial sums Ψ_n's, respectively, of example 2. The quantities $r^{(0)}(\lambda)$, $q_n^{(0)}(\lambda)$ and the ratios $r_n^{(k)}(\lambda)/r_n^{(0)}(\lambda)$, $q_n^{(k)}(\lambda)/q_n^{(0)}(\lambda)$ with $k\geqslant 2$ are reported.

n	x^2	x^{10}	x^{24}	x^{30}
		$\lambda=0.6$		
		$r_n^{(k)}(\lambda)$		
4	0.3371	4.248	8.073[6]	2.97[10]
12	0.3371	4.114	6.809[5]	5.110[8]
20	0.3371	4.114	6.809[5]	5.106[8]
Ex[a]	0.3371	4.114	6.809[5]	5.106[8]
n	x^0	x^2	x^6	x^8
		$\lambda=5.0$		
		$r_n^{(k)}(\lambda)$		
6	0.5581	0.1516	4.630[−2]	6.642[−2]
12	0.5493	0.1508	5.132[−2]	5.431[−2]
18	0.5491	0.1508	5.139[−2]	5.424[−2]
Ex[a]		0.1508	5.139[−2]	5.424[−2]
		$q_n^{(k)}(\lambda)$		
6	1.182	1.643	2.4[1]	1.6[2]
12	1.073	1.502	3.6[1]	3.2[2]
18	1.045	1.432	4.7[1]	5.0[2]
Ex[a]		0.1508	5.139[−2]	5.424[−2]

[a]Exact values from $\Psi=\pi^{-1/4}\exp[-(1+2\lambda)^{1/2}x^2/2]$.

The results are surprising: (i) $\{R_n\}$ converges uniformly to Ψ on finite intervals $[0,x_0]$ and (ii) $\{R_n\}$ is UB, because the R_n's have the monotonic property $R_{n+1}\leqslant R_n$ on $[5,\infty)$ (Corollary 2). To these results we can add the following. It is known that Padé approximants can accelerate the convergence rate of many power series and extend their convergence radius and the R_n's are not the exception. Figures 2 and 12 show the ratios Ψ_n/Ψ and R_n/Ψ with $\lambda=-0.9$, -5 and we observe that the convergence rate of $\{R_n\}$ on a finite interval $[0,x_0]$ is faster than that of its corresponding sequence $\{\Psi_n\}$. On the other hand, the formal Ψ series has a convergence radius λ_Ψ less than 1 because $H(\lambda)$ has no bound eigenstate with $\lambda\geqslant 1$, but Fig. 12 shows that $\{R_n\}$ converges correctly on a finite interval $[0,x_0]$ and is UB with $|\lambda=-5|>\lambda_\Psi$. The correct *global* convergence of $\{R_n\}$ should be reflected by a correct convergence of expectation value sequences $\{S(R_n)\}$. In principle $S(R_n)$ can be computed by numerical quadrature but this procedure may require large computational resources to get $R_n(\lambda,x)$ on a dense x mesh. Instead one can compute Padé approximants of the λ series of $S(\Psi)$; for example, from the series

$$x^k(\Psi)=\sum_{m=0}^{\infty} x_m^{(k)}\lambda^m, \tag{4.5a}$$

where

$$x_m^{(k)}=\sum_{l=0}^{m} \langle \psi_l, x^k\psi_{m-l}\rangle, \tag{4.5b}$$

we get the Padé approximants [25]

$$r_n^{(k)}(\lambda)=\left[\sum_{l=0}^{n} a_{kl}\lambda^l\right]\Bigg/\left[1+\sum_{l=1}^{n} b_{kl}\lambda^l\right]. \tag{4.6}$$

As expected, Table VI shows that the sequences $\{r_n^{(k)}(\lambda)\}_n$ converge to their correct limits with $\lambda=-0.9,-5$ in Δ^{NUB} whereas the corresponding sequences $\{x^k(\Psi_n)\}_n$ diverge from $k=2$ with a rate that increases as λ goes from -0.9 to -5 (see also Table I).

For example 2 we have $\Delta^{\mathrm{NUB}}=(0,\infty)$ but, as occurs with example 1, Fig. 4 shows that the sequence $\{R_n\}$ with $\lambda=0.4$ converges correctly on a finite interval $[0,7]$ and is UB whereas the corresponding sequence $\{\Psi_n\}$ has a slower convergence on $[0,7]$ and is NUB. Similar results are obtained with larger λ's which can be greater than the convergence radius λ_Ψ (<0.5) of the formal Ψ series. For example, a comparison between the moments $x^k(\Psi_n)$ and their Padé approximants $r_n^{(k)}(\lambda)$ reported in Tables II and VII with $\lambda=0.6,5$ shows the correct convergence of $\{r_n^{(k)}(\lambda)\}_n$ whereas $\{x^k(\Psi_n)\}_n$ diverges rapidly from $k=2$. It should be noticed that Ψ_n yields the series

$$x^k(\Psi_n)=\sum_{m=0}^{n} x_m^{(k)}\lambda^m+\sum_{m=n+1}^{2n} x_{nm}^{(k)}\lambda^m, \tag{4.7}$$

where only the $x_m^{(k)}$'s are given by Eq. (4.5b) and whose Padé approximant

TABLE VIII. Padé approximants $r_n^{(k)}(\lambda)$ [Eq. (4.6)] corresponding to the expectation values $x^k(\Psi_n)$ of Table III for the 1s state of example 4. The quantities $r_n^{(0)}(\lambda)$ and the ratios $r_n^{(k)}(\lambda)/r_n^{(0)}(\lambda)$ with $k\geqslant 1$ are reported.

n	x^0	x^1	x^2	x^3
		$\lambda=0.05$		
4	0.23551	1.3849	2.5147	5.6177
6	0.23551	1.3848	2.5143	5.6162
8	0.23550	1.3848	2.5142	5.6162
10	0.23550	1.3848	2.5142	5.6162
Ex[a]		1.3848	2.5142	5.6162
		$\lambda=0.2$		
4	0.2139	1.2110	1.885	3.537
6	0.2134	1.2059	1.869	3.499
8	0.2134	1.2049	1.866	3.493
10	0.2134	1.2047	1.865	3.491
Ex[a]		1.2046	1.865	3.491
		$\lambda=1.0$		
4	0.1876	0.987	1.21	1.66
6	0.1838	0.943	1.10	1.47
8	0.1823	0.923	1.06	1.41
10	0.1817	0.913	1.04	1.38
Ex[a]		0.900	1.02	1.36

[a]Exact values from a normalized Dirichlet wave function [21].

$$q_n^{(k)}(\lambda)=\left[\sum_{l=0}^{n} c_{kl}\lambda^l\right]\bigg/\left[1+\sum_{l=1}^{n} d_{kl}\lambda^l\right] \tag{4.8}$$

diverges as $n\to\infty$ with a large k and $\lambda\in\Delta^{\mathrm{NUB}}$. This is illustrated by results reported in Table VII which shows that $\{r_n^{(k)}(\lambda)\}_n$ converges correctly with $\lambda=5\in\Delta^{\mathrm{NUB}}$ whereas the corresponding sequence $\{q_n^{(k)}(\lambda)\}_n$ diverges with $k\geqslant 6$.

Results from the V-singular examples 4 and 5 showed that the ground state sequences $\{\Psi_n\}$ have the set $\Delta^{\mathrm{NUB}}=(0,\infty)$ that (excepting $\lambda=0$) agrees with the set of λ's for which $H(\lambda)$ has bounded states and therefore $\Delta^{\mathrm{UB}}=\{0\}$, a result that may reflect the fact that the corresponding E series have a zero convergence radius. Fortunately, the corresponding functional Padé approximants $\{R_n\}$ behave like those from examples 1 and 2. In fact, Figs. 7–10 show that the sequences $\{R_n\}$ converge correctly on finite intervals and are UB. As expected, these results are reflected by the correct convergence of Padé approximants $r_n^{(k)}(\lambda)$ for the 1s eigenstate of example 4 reported in Table VIII with $\lambda=0.05,0.2,1.0$ whereas their corresponding $x^k(\Psi_n)$'s diverge rapidly except for $x^0(\Psi_n)$ with $\lambda=0.05$ as Table III shows.

V. SUMMARY AND DISCUSSION

Several criteria for studying the quality of approximating wave functions such as information theory criteria [26] and metrics in the Hilbert space $L_2(R^N)$ [27] have been proposed but they have the deficiency of being insensitive to the nonuniform boundedness problem. Examples 1–5 and the results reported in [4] show that the boundedness property of a sequence of wave functions $\{\Phi_n\}_{n=1}^{\infty}$ can be determined by monitoring the ratio Φ_n/ψ_B with a ψ_B properly chosen or by means of the convergence of sequences $\{x^k(\Phi_n)\}_{n=1}^{\infty}$ for large values of k (see Proposition 2 and Corollaries 1 and 2). According to Proposition 1 the L_2 convergence criterion and the uniform boundedness yield a suitable way to determine the quality of the *global* convergence of $\{\Phi_n\}_{n=1}^{\infty}$: the L_2 convergence guarantees a correct *local* approximation toward the true wave function Ψ on bounded regions Ω_n that increase as n does while the uniform boundedness guarantees that the error of Φ_n on the complementary region Ω_n^c remains bounded and, therefore, vanishes as $n\to\infty$. Convergence in the norm of $L_2(R^N)$ can be replaced by other criteria but it has the feature of being a weak condition to be satisfied by sequences $\{\Phi_n\}$ from variational procedures [2,3] or some perturbation series [5] in $L_2(R^N)$ with $N>1$, while the boundedness property can be studied with a suitable one-dimensional function as was done in [17] with the one-electron density for the lithium atom problem.

We dealt with formal Ψ series because analytic perturbation theory provides a suitable classification of perturbations to characterize some properties of the E and Ψ series [5,7]. Examples 1–3 showed that a regular perturbation V of a given Hamiltonian H_0 can generate NUB sequences $\{\Psi_n\}$, Eq. (3.1), despite its L_2 convergence for small λ's. An interesting result is that the boundedness property of sequences $\{\Psi_n\}$ may be a discontinuous function of λ when it varies continuously within the set of λ values for which the Hamiltonian $H(\lambda)=H_0+\lambda V$ has bound states (remark 1). It is known that almost every singular perturbation V generates E series with a zero convergence radius [5,7] while the main and practically unique result about the corresponding Ψ series is that it is an asymptotic power series expansion of the true Ψ up to a particular power of λ [5,14,15]. Examples 4 and 5 show that the sequences $\{\Psi_n\}$ can be L_2 convergent but even for small λ they are NUB; that is, they have $\Delta^{\mathrm{UB}}=\{0\}$. This result may be connected with the singular character of V or considered as an inherent property of Ψ series with E series having a zero convergence radius. In fact, if this were not the case, then the sequence $\{\Psi_n\}$ for the anharmonic oscillator would have a correct global convergence with at least small λ's, a result that, intuitively, is incongruent with the zero convergence radius of its E series.

Several methods to compute E series without the divergence problems of formal perturbation series (such as multiple-scale perturbation theory [28] or the Ricatti method [29,30]) have been proposed but studies of the new Ψ series are scarce. It is clear that the study of the L_2 convergence and the boundedness property of the corresponding partial-sum sequences $\{\Psi_n\}$ can yield valuable information about the success of such procedures to compute the true Ψ. For example, a numerical calculation shows that the Riccati method [30] provides sequences $\{\Psi_n\}$ for the ground and first excited states of examples 1 and 2 that are UB and L_2 convergent for all λ for which $H(\lambda)$ has bound states; that is, such a method yields partial-sum sequences $\{\Psi_n\}$ with an *empty* set Δ^{NUB} and a correct global convergence whereas for the formal sequences $\{\Psi_n\}$ the set Δ^{UB} is bounded by the small convergence radius of the formal Ψ series and Δ^{NUB} is the semi-infinite interval $(-\infty,0)$ or $(0,\infty)$ (remark 2).

The so-called perturbation theory without a wave function provides the coefficients of formal E series and other expectation values like $x^k(\Psi)$ without an explicit calculation of the corresponding formal Ψ series [31] but such a procedure may hide the incorrect global convergence of the sequence $\{\Psi_n\}$, Eq. (3.1), and, therefore, lead to wrong results or conclusions. For example, since the coefficients $x_m^{(k)}$ of $x^k(\Psi)$ [Eq. (4.5a)] are uniquely determined by those of the Ψ series through Eq. (4.5b), the partial-sum sequence $\{x^k(\Psi_n)\}_n$ will be divergent with a large k if $\{\Psi_n\}$ is NUB, independently of the regular or singular character of the perturbation V.

We considered that for the examples studied here the functional Padé approximant sequences $\{R_n\}$, Eq. (4.4), are L_2 convergent and uniformly bounded with small λ's by considering the tendency of the first R_n's although in strict mathematical terms such properties should be determined with an analysis of the whole set $\{R_n\}_{n=1}^{\infty}$ as Corollary 2 requires. To test numerically these properties with large λ and n values one has to be careful with the loss of precision caused by the rapid growth of the coefficients $|\psi_m(x)|$ as m increases with each x value, in particular with the Ψ_n's from singular V's whose coefficients increase as rapidly as those of the corresponding E series, because such a precision loss may hide the true properties of $\{R_n\}_{n=1}^{\infty}$. This latter problem may be solved partly by scaling or using other summability methods [7–13]. In principle any summability method applied to the formal E series to get the true energy $E(\lambda)$ can also be applied to the Ψ series [32]. Although the correct global convergence of the sequence $\{R_n\}$ or approximating wave functions provided by other summability methods may fail, the study of their local convergence and boundedness property can yield useful, reliable physical information compatible with their accuracy in some bounded region Ω as was done with the NUB sequence $\{\psi_{1p}^F\}$ of Sec. IV A. A study of the problem of determining the reliability region of an approximating wave function that includes a careful analysis of the criterion proposed in Sec. IV A for Fourier sequences will be given in a forthcoming work.

In this work and the previous one [4] we have considered the nonuniform boundedness of variational wave functions and eigenfunction perturbation series separately but there is no reason to expect that the combination of these approaches called ''variation-perturbation theory'' [1] does not yield nonuniformly bounded sequences of approximating wave functions. To date, the unique approach that in rigorous mathematical terms solves the nonuniform boundedness problem is the Dirichlet wave functions approach which, in simple terms, consists of the following. The exact Dirichlet wave functions Ψ_Ω for the eigenproblem $H\Psi = E\Psi$ in $L_2(R^N)$ are the eigensolutions of the corresponding eigenproblem $H_\Omega\Psi_\Omega = E_\Omega\Psi_\Omega$ on a *bounded* region Ω of R^N with the condition $\Psi_\Omega = 0$ on the boundary $\partial\Omega$ of Ω, H_Ω being the self-adjoint Hamiltonian defined on $L_2(\Omega)$ by the boundary condition on $\partial\Omega$. The Ψ_Ω's and their numerical approximations $\Psi_{\Omega,n}$ obtained from standard numerical methods (which include variational and finite difference methods) converge to the bound state eigenfunctions Ψ as $\Omega \to R^N$ [33,34] and in a natural way such functions are UB [17,20]. If we take into account that many *singular* perturbations V of a Hamiltonian H_0 in $L_2(R^N)$ are *regular* perturbations of the corresponding Hamiltonian $H_{0,\Omega}$ defined by Dirichlet boundary conditions on $\partial\Omega$ [35], it seems reasonable to expect that variation-perturbation theory combined with the Dirichlet approach can also yield approximating wave functions with a correct global convergence. This will be studied in a forthcoming work.

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[18] Let $\|\cdot\|_{R^3}$ denote the norm of $L_2(R^3)$ and let r be the usual norm of $\overline{r}\in R^3$. It is known ([5], p. 302) that for every $\delta\in(0,1)$ there is a C_δ such that

$$\|r^{-1}u\|_{R^3}\leqslant C_\delta\|u\|_{R^3}+\delta\|2^{-1}\Delta u\|_{R^3}$$

holds for $u\in D(\Delta)$, the domain of the Laplacian in R^3, and hence if $H_0=2^{-1}\Delta-r^{-1}$, it follows that

$$\|r^{-1}u\|_{R^3}\leqslant(1-\delta)^{-1}(C_\delta\|u\|_{R^3}+\delta\|H_0u\|_{R^3})$$

holds for $u\in D(\Delta)$ ([5], p. 190) so that λr^{-1} is bounded by H_0 and therefore the 1s state $\Psi(\lambda,\overline{r})$ of $H(\lambda)=H_0+\lambda r^{-1}$ has a convergent formal perturbation series. The results of example 1 correspond to the radial part of $\Psi(\lambda,\overline{r})$.

[19] This follows from the inequality $|\langle x^{-1}u,u\rangle|\leqslant C_\delta\|u\|^2+\delta\langle\partial_x u,\partial_x u\rangle$ for $u\in C_0^\infty(0,\infty)$ with a positive small δ ([5], p. 343) and the positiveness of $\langle x^2u,u\rangle$. The integrals $\langle\psi_0^{(i)},x^{-1}\psi_0^{(0)}\rangle$ were computed with the formulas reported for the basis functions $r^ke^{-r^2/2}$ in B. Klahn and J. D. Morgan III, J. Chem. Phys. **81**, 410 (1984), Appendix C.

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[21] For example 4 we use $\Psi_D=\Sigma_{k=1}^{N_D}c_ke^{-\alpha x}(R_D-x)x^k$ where the c_k's are obtained variationally and α,R_D,N_D are chosen properly to obtain an accurate approximation of the true Ψ.

[22] Calculations for Figs. 7–10 were were done with a 32-digit precision machine; the others were done with a 16-digit machine. The cusps observed in Figs. 5 and 7–10 are due to the zeros of wave functions.

[23] For example 5 we used $\Psi_D=\Sigma_{k=1}^{N_D}c_ke^{-\alpha x^2}(R_D^2-x^2)x^{2k-2}$.

[24] The estimation (4.2) does not assume that $\{\psi_{1p}^F\}$ converges point by point or in another sense.

[25] The Padé approximants computed in the present article for a given power series $f(\lambda)=\Sigma_{m=0}^\infty f_m\lambda^m$ are the rational functions

$$F_n(\lambda)=\left[\sum_{k=0}^n a_k\lambda^k\right]\Bigg/\left[1+\sum_{k=1}^n b_k\lambda^k\right],$$

where the a_k's and b_k's are defined by the $2n+1$ equations $F_n(0)=f(0)$ and $\partial_\lambda^kF_n(\lambda)|_{\lambda=0}=\partial_\lambda^kf(\lambda)|_{\lambda=0}$ for $k=1,\ldots,2n$. The computer program used to solve these equations was obtained from W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in FORTRAN*, 2nd ed. (Cambridge University Press, New York, 1992), p. 196. This program was also applied to the partial sum $\Psi_n(\lambda,x_j)$ to compute the functional Padé approximant $R_n(\lambda,x_j)$ for a given set of x_j's.

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[35] For example, if H_0 is the harmonic oscillator Hamiltonian on $L_2(-\infty,\infty)$, then $V=x^4$ is a singular pertubation of H_0 while V is a regular perturbation of the corresponding Dirichlet Hamiltonian $H_{0,R}$ on $L_2(-R,R)$ because V is a bounded operator on $L_2(-R,R)$.