Summation of perturbation series of eigenvalues and eigenfunctions of anharmonic oscillators

Marco A. Núñez*

Departamento de Física, Universidad Autónoma Metropolitana, Iztapalapa, Apartado Postal 55-534, CP 09340 México, Distrito Federal, Mexico

A perturbation approach to compute the bound states of the Schrödinger equation $H\Psi = E\Psi$ with $H^0 + \lambda V$ and $\Psi|_{x=\pm\infty} = 0$ is studied. The approach involves solving the corresponding Dirichlet problem $H_R\Psi_R = E_R\Psi_R$ on a finite interval $[-R,R]$ by the Rayleigh-Schrödinger perturbation theory (RSPT). The method is based on the fact that E_R, Ψ_R converge to E, Ψ as $R \to \infty$. The model problems to study the summability properties of the RSPT series $E_R = \Sigma_{k=0}^{\infty} E_R^{(k)}\lambda^k$ are the anharmonic oscillators $H = p^2 + x^2 + \lambda x^{2M}$, with $M = 2,3,4$ for which the RSPT produces strongly divergent series $E = \Sigma_{k=0}^{\infty} E^{(k)}\lambda^k$. The summation of the latter series with large λ for the octic case is considered as an extremely challenging summation problem, in part, since it was rigorously proven that the Padé approximants cannot converge and the two-point Padé approximants, which combine information of the renormalized weak coupling and strong coupling expansions, give relatively good results. The calculations of this work show that the ordinary Padé approximants from the sole un-normalized E_R series for the octic oscillator give accurate results with small or large λ. The coefficients $E_R^{(k)}$ are calculated with the eigenvalue series of an operator H_{Rn}, whose resolvent converges to that of H_R as $n \to \infty$. The Padé approximants of the RSPT eigenfunction series $\Psi_R = \Sigma_{k=0}^{\infty} \psi_R^{(k)}\lambda^k$ also provide accurate results for the octic oscillator.

I. INTRODUCTION

The Rayleigh-Schrödinger perturbation theory (RSPT) is one of the main methods to solve the quantum eigenproblem $H\Psi = E\Psi$, $\Psi|_{x=\pm\infty} = 0$, when H can be partitioned into an unperturbed Hamiltonian H^0 with known eigenvalues and eigenfunctions and a perturbation V, $H = H^0 + \lambda V$ [1–7]. The RSPT yields formal series in powers of the coupling parameter λ,

$$E(\lambda) \sim \sum_{k=0}^{\infty} E^{(k)}\lambda^k. \qquad (1.1)$$

There is an extensive literature on the summation of this series [2,5–20]. The Padé approximants have become a standard tool to sum the slowly convergent or divergent series [14–20], and recently nonlinear sequence transformations have been used for the summation of strongly divergent series [9–12]. The Series (1.1) is called weak coupling expansion since it is an expansion around $\lambda = 0$, but if such a series has to be summed in the strong coupling regime the problem encountered is that the summation methods only work for small or at the most moderately large λ [8,11–13].

The main approach to compute the eigenvalues in the strong coupling regime has been the substitution of the Hamiltonian H by means of the normalization techniques [7,14,21–25] or the variational perturbation methods [26] which produce an equivalent Hamiltonian H^* with a better eigenvalue series. The method studied in this work, which will be referred to as the Dirichlet wave functions approach (DWFA), belongs to this class of methods. It involves solving the eigenproblem $H_R\Psi_R = E_R\Psi_R$ for $|x| \leq R(<\infty)$,

where $H_R = H_R^0 + \lambda V$ is the operator defined by the Dirichlet boundary conditions $\Psi_R|_{x=\pm R} = 0$. The basis of the DWFA is that the eigensolutions E_R, Ψ_R converge to E, Ψ as $R \to \infty$ [27–31]. The results of Sec. IV show that the RSPT yields eigenvalue series

$$E_R(\lambda) = \sum_{k=0}^{\infty} E_R^{(k)}\lambda^k, \qquad (1.2)$$

which can be summed more effectively than series (1.1).

Since the seminal work of Bender and Wu [18–20], the anharmonic oscillators $H = p^2 + x^2 + \lambda x^{2M}$ $(M = 1,2,\dots)$ have provided the examples of strongly divergent eigenvalue series because the coefficients $E^{(k)}$ of series (1.1) behave like $([M-1]k)!/k^{1/2}$ as $k \to \infty$. In the quartic and sextic cases, it was proved that the Padé approximants are able to sum series (1.1), but they are numerically useless for large λ [8,15–17]. In the octic case, it was proved rigorously by Graffi and Grecchi [32] that the Padé approximants cannot sum the eigenvalue series. Some renormalization schemes produce eigenvalue series that can be summed by Padé approximants or nonlinear sequence transformations if λ is small [12], but the summation in the strong coupling regime is considered a challenging problem [8,11–13].

The transformation of a Hamiltonian H into an equivalent H^* having advantageous properties in the troublesome strong coupling regime can pose some problems, e.g., the renormalization schemes of Symanzik [15] or Vinette and Čížek [21,22] produce eigenvalue series for the anharmonic oscillators which converge for large λ, but the eigensolutions of the zero-order problem are unknown. There are alternative approaches for the computation of the coefficients of the corresponding eigenvalue series [23–26], but the problem is open in general. The DWFA yields one way to compute the coefficients of series (1.1) when the eigenstates of H^0 are unknown, a rigorous proof is given in Ref. [33].

*Electronic address: manp@xanum.uam.mx

The zero-order Dirichlet problem is solvable in some cases [34], but in general its eigensolutions are unknown. This problem is solved with the substitution of the operator H_R by its projection $H_{Rn} = H_{Rn}^0 + \lambda V_{Rn}$ on the space generated by a suitable orthonormal set $\{\varphi_{Rm}\}_{m=1}^n$. The eigenvalues of H_{Rn} are obtained with a formal series

$$E_{Rn}(\lambda) = \sum_{k=0}^{\infty} E_{Rn}^{(k)} \lambda^k, \qquad (1.3)$$

whose coefficients $E_{Rn}^{(k)}$ converge to those of series (1.2) as $n \to \infty$. Hence the properties of series (1.2), (1.3) are essentially the same for large n, and the coefficients $E^{(k)}$ of the series (1.1) can be estimated by $E_{Rn}^{(k)}$'s with large R, n. The results given by the ordinary Padé approximants for the octic oscillator show that series (1.2), (1.3) have good numerical properties.

A dual approach was studied by Čížek *et al.* [13], who showed that the normalization scheme of Vinette and Čížek [20,21] provides both the weak coupling and the strong coupling expansions [10] which can be summed simultaneously with the expectation of obtaining better results than a summation method that uses information from one expansion. This expectation is supported by the results given by the two-point Padé approximants for the octic anharmonic oscillator [13], which is considered as an extremely challenging summation problem for large λ [8,11–13]. In Sec. IV, it is shown that the ordinary Padé approximants from the sole un-normalized and weak coupling series (1.3) give eigenvalues as accurate as those reported in Ref. [13] for the octic oscillator, a result that emphasizes the good summability properties of series (1.2), (1.3).

There are relatively few works that consider perturbation calculations of the eigenfunctions [1,2,35–42]. Recent approaches such as multiple scale perturbation theory [37,38], optimized perturbation theory [39,40] give good estimations of the eigenfunctions for the quartic anharmonic oscillator, but in general the calculation of the true Ψ, is not easy even if the eigenvalue series (1.1) is well behaved. Variational or perturbation methods can yield wave functions Ψ_n that converge in the norm to the true Ψ whereas the expectation value $\langle \Psi_n, x^{2M} \Psi_n \rangle$ diverges with some M [42–44] as $n \to \infty$. The set of Dirichlet wave functions $\{\Psi_R\}_{R>0}$ converges in norm [27,28] and is uniformly bounded [29,30] so that the calculation of Ψ_R with large R yields an accurate estimation of Ψ. The results of Sec. V show that the DWFA produces eigenfunction series with properties as good as those of the eigenvalue series (1.2), (1.3).

II. FORMAL RESULTS

Consider the Hamiltonian $H(\lambda) = H^0 + \lambda V$ with $H^0 = p^2 + V^0$, where V^0, V are continuous functions of x. If the eigenfunctions Ψ^{j0} of H^0 form a complete basis of the space $L_2(-\infty, \infty)$, which will be denoted by L_2, the RSPT produces *formal* series of the ith eigenvalue $E^i(\lambda)$ and eigenfunction $\Psi^i(\lambda, x)$ of $H(\lambda)$,

$$E^i(\lambda) \sim \sum_{k=0}^{\infty} E^{ik} \lambda^k,$$

$$\Psi^i(\lambda, x) \sim \sum_{k=0}^{\infty} \psi^{ik}(x) \lambda^k. \qquad (2.1)$$

These series will be referred to as E^i series and Ψ^i series, respectively. The main result about the convergence of these series can be summarized as follows [1,2]. Let $\mathcal{H}$ be a Hilbert space with norm $\|.\|_{\mathcal{H}}$ and $T(\lambda) = T_0 + \lambda V$ be a self-adjoint operator in $\mathcal{H}$. If there are constants $a, b \geq 0$ such that

$$\|Vu\|_{\mathcal{H}} \leq a\|u\|_{\mathcal{H}} + b\|T_0 u\|_{\mathcal{H}}$$

holds for "all" u, then the eigenvalues and eigenfunctions of $T(\lambda)$ can be represented by analytic functions in the neighborhood of $\lambda = 0$. In this case, V is referred to as a *regular* perturbation of T_0, otherwise V is called *singular* perturbation of T_0. The models of singularly perturbed Hamiltonians are the anharmonic oscillators $H = H^0 + \lambda x^{2M}$ with $H^0 = p^2 + x^2$ and $M = 2, 3, \ldots$ [18–20]. In this case, the E^i series is asymptotic as $\lambda \to 0$ [1,2,8], but this property does not guarantee that the eigenvalue $E^i(\lambda)$ can be obtained from the coefficients E^{ik} because different functions may have the same asymptotic series. If E^{ik}'s satisfy a "modified strong asymptotic condition of order q,"

$$\left| E^i(\lambda) - \sum_{k=0}^{n} E^{ik} \lambda^k \right| \leq C \sigma^{n+1} [q(n+1)]! |\lambda|^{n+1}, \quad (2.2)$$

then $E^i(\lambda)$ is uniquely determined by the set $\{E^{ik}\}_{k=0}^{\infty}$ [2,8,45]. This condition is satisfied by the E^i series of the anharmonic oscillators [2,8,45], but for the general Hamiltonian $H = p^2 + V^0 + \lambda V$ the correctness of Eq. (2.2) is an open question.

The basis of the DWFA is the solution of the equation

$$H_R(\lambda) \Psi_R^i(\lambda, x) = E_R^i(\lambda) \Psi_R^i(\lambda, x) \qquad (2.3)$$

with $|x| \leq R$, $H_R(\lambda)$ being the Hamiltonian defined by the Dirichlet boundary conditions $\Psi_R^i = 0$ at $x = \pm R$. If the lower part of the spectrum of $H(\lambda)$ consists of isolated eigenvalues $E^0(\lambda) < E^1(\lambda) < \cdots$, the eigenstates of $H_R(\lambda)$ converge to those of $H(\lambda)$ as R increases,

$$\lim_{R \to \infty} \| \Psi_R^i(\lambda, x) - \Psi^i(\lambda, x) \| = 0,$$

$$\lim_{R \to \infty} E_R^i(\lambda) = E^i(\lambda), \qquad (2.4)$$

where we define $\Psi_R^i \equiv 0$ for $|x| \geq |R|$ and $\|.\|$ denotes the norm of L_2 [27,28]. This result together with the *uniform boundedness* of the set $\{\Psi_R^i\}_{R>0}$ guarantees the correct convergence of Ψ_R^i toward Ψ^i as $R \to \infty$ [29,30]. Numerical results [31] suggest that the convergence rate of Ψ_R^i can be characterized by the relationship

$$\| \Psi_R^i - \Psi^i \| \sim 10 \| \chi_R \Psi^i - \Psi^i \|,$$

where $\chi_R(x)=1$ for $|x|\leqslant R$ and $\chi_R=0$ otherwise. Thus, for practical purposes the calculation of $E_R^i(\lambda)$, $\Psi_R^i(\lambda,x)$ on a suitable interval $[-R,R]$ provides accurate estimations of $E^i(\lambda)$, $\Psi^i(\lambda,x)$. Additionally, the eigenvalues obey the variational inequality [29,30]

$$E^i(\lambda)\leqslant E_R^i(\lambda)\leqslant E_{R'}^i(\lambda) \quad \text{for } R'<R. \tag{2.5}$$

Let L_2^R denote the Hilbert space $L_2(-R,R)$ and let $\langle,\rangle_R$, $\|.\|_R$ be its inner product and norm. From a theoretical point of view there are some advantages in solving Eq. (2.3) by RSPT. The basic premise of the RSPT is that the eigenfunctions of the zero-order operator $H_R^0\equiv H_R(0)$ form a complete basis of L_2^R. This premise holds true because the resolvent of $H_R(\lambda)$ is a *compact* operator in L_2^R for any pair λ, R when V^0, V are continuous. In contrast, the operator H^0 in L_2 with $V^0=-e^{-|x|}$ has a finite number of bounded eigenstates and the RSPT is not applicable. In the context of perturbation methods, the remarkable feature of the DWFA is that the *singular* perturbations V of H^0 are *regular* perturbations of H_R^0. In fact, if V is continuous it satisfies

$$\|Vu\|_R\leqslant a_R\|u\|_R+b_R\|H_R^0u\|_R$$

with $a_R=\max_{|x|\leqslant R}|V|$, $b_R=0$; that is, V is a *bounded* operator in L_2^R. Hence the analytic perturbation theory [1,2] guarantees that both the E_R^i and Ψ_R^i series,

$$E_R^i(\lambda)=\sum_{k=0}^{\infty} E_R^{ik}\lambda^k,$$

$$\Psi_R^i(\lambda,x)=\sum_{k=0}^{\infty} \psi_R^{ik}(x)\lambda^k, \tag{2.6}$$

converge for small λ. In contrast, the eigenvalue $E_R^i(\lambda)$ may not be uniquely determined by the set $\{E^{ik}\}_{k=0}^{\infty}$ when it does not satisfy Eq. (2.2).

The exact solution of the zero-order Dirichlet problem,

$$H_R^0\Psi_R^{j0}(x)=E_R^{j0}\Psi_R^{j0}(x), \tag{2.7}$$

$\Psi_R^{j0}(x=\pm R)=0$, is known in some cases [34] but in general this problem has to be solved numerically. In this work, the Dirichlet problem (2.3) is replaced by an n-dimensional problem,

$$H_{Rn}(\lambda)\Phi_{Rn}^i(\lambda,x)=E_{Rn}^i(\lambda)\Phi_{Rn}^i(\lambda,x), \tag{2.8}$$

where $H_{Rn}(\lambda)$ is given by

$$H_{Rn}(\lambda)=H_{Rn}^0+\lambda V_{Rn} \tag{2.9}$$

with $H_{Rn}^0\equiv P_{Rn}H_R^0P_{Rn}$, $V_{Rn}\equiv P_{Rn}VP_{Rn}$, where $P_{Rn}=\sum_{m=1}^n|\varphi_{Rm}\rangle\langle\varphi_{Rm}|$ is the projection operator on the n dimensional space generated by the first n-elements of an orthonormal basis $\{\varphi_{Rm}(x)\}_{m=1}^{\infty}$ of L_2^R which satisfies the boundary condition $\varphi_{Rm}(\pm R)=0$. The main idea behind this procedure is that for large n the eigenstates $E_{Rn}^i(\lambda)$, $\Phi_{Rn}^i(\lambda,x)$ of H_{Rn} are essentially equal to those, $E_R^i(\lambda)$,

$\Psi_R^i(\lambda,x)$, of H_R because the resolvent operator of $H_{Rn}(\lambda)$ converges to that of $H_R(\lambda)$ in the operator's norm as $n\to\infty$ [27,28]; hence we get

$$\lim_{n\to\infty}\|\Phi_{Rn}^i(\lambda,x)-\Psi_R^i(\lambda,x)\|_R=0,$$

$$\lim_{n\to\infty}E_{Rn}^i(\lambda)=E_R^i(\lambda). \tag{2.10}$$

In particular, for $\lambda=0$ the eigensolutions of the zero-order problem,

$$H_{Rn}^0\Phi_{Rn}^{j0}(x)=E_{Rn}^{j0}\Phi_{Rn}^{j0}(x), \tag{2.11}$$

converge to those of H_R^0,

$$\lim_{n\to\infty}\|\Phi_{Rn}^{j0}(x)-\Psi_R^{j0}(x)\|_R=0,$$

$$\lim_{n\to\infty}E_{Rn}^{j0}=E_R^{j0}. \tag{2.12}$$

The application of the RSPT to Eq. (2.8) yields the formal series

$$E_{Rn}^i(\lambda)=\sum_{k=0}^{\infty} E_{Rn}^{ik}\lambda^k,$$

$$\Phi_{Rn}^i(\lambda,x)=\sum_{k=0}^{\infty} \phi_{Rn}^{ik}(x)\lambda^k, \tag{2.13}$$

whose convergence is guaranteed for small λ since the perturbation V_{Rn} is a bounded operator on L_2^R.

III. RELATIONSHIP BETWEEN SERIES

Let us consider the relationship between the formal series (2.1) and (2.6). According to the RSPT in order to compute series (2.6), one has to solve the zero-order problem (2.7) for all $j=1,2,\ldots$, with normalized Ψ_R^{j0}'s. Let $E_R^{i,k=0}\equiv E_R^{j=i,0}$ and $\psi_R^{i,k=0}\equiv\Psi_R^{j=i,0}$. Since Ψ_R^{j0}'s form an orthonormal basis of L_2^R, every eigenfunction series coefficient ψ_R^{ik} has the Fourier series

$$\psi_R^{ik}=\sum_{j=1}^{\infty} c_j^{ik}\Psi_R^{j0}, \quad k=0,1,\ldots, \tag{3.1a}$$

where $c_j^{i,k=0}=\delta_{ij}$ and $c_{j=i}^{ik}=0$ for $k\geqslant 1$. The remainder c_j^{ik}'s are calculated together with the eigenvalue series coefficients E_R^{ik} with the formulas

$$E_R^{ik}=V_{j=i}^{i,k-1},$$

$$c_{j(\neq i)}^{ik}=(S_j^{ik}-V_j^{i,k-1})/(E_R^{j0}-E_R^{i0}), \tag{3.1b}$$

where the quantities

$$S_j^{ik}=\sum_{k'=0}^{k-1} E_R^{i,k-k'}c_j^{ik'},$$

$$V_j^{i,k-1} = \sum_{j'=1}^{\infty} c_{j'}^{i,k-1} \langle \Psi_R^{j0}, V\Psi_R^{j'0} \rangle_R \qquad (3.1c)$$

are obtained from the Fourier series

$$V\psi_R^{i,k-1} = \sum_{j=1}^{\infty} V_j^{i,k-1} \Psi_R^{j0},$$

$$S^{ik} \equiv \sum_{k'=0}^{k-1} E_R^{i,k-k'} \psi_R^{ik'} = \sum_{j=1}^{\infty} S_j^{ik} \Psi_R^{j0}. \qquad (3.1d)$$

The computation of coefficients E^{ik}, $\psi^{ik}(x)$ of series (2.1) is carried out with formulas (3.1a)–(3.1d) where E_R^{i0}, ψ_R^{i0}, $\langle \Psi_R^{j0}, V\Psi_R^{j'0} \rangle_R$ are replaced by E^{i0}, ψ^{i0}, $\langle \Psi^{j0}, V\Psi^{j'0} \rangle$, respectively. The convergence of the first three quantities toward the latter three as $R \to \infty$ leads to the convergence of the coefficients of series (2.6) toward those of series (2.1).

The convergence of E_R^{i0}, Ψ_R^{j0} to E^{i0}, Ψ^{j0} follows from Eq. (2.4) with $\lambda = 0$, but the *sole* convergence of Ψ_R^{j0} toward Ψ^{j0} in the L_2 norm [Eq. (2.4)] does *not* guarantee the correctness of equation

$$\lim_{R \to \infty} \langle \Psi_R^{j0}, V\Psi_R^{j'0} \rangle_R = \langle \Psi^{j0}, V\Psi^{j'0} \rangle \qquad (3.2)$$

for $V = x^{2M}$. The examples of wave functions Ψ_n that converge in the L_2 norm to the correct Ψ, whereas the expectation value $\langle \Psi_n, x^{2M}\Psi_n \rangle$ diverges for some power operator x^{2M} as $n \to \infty$, are given in Refs. [42–44]. The additional condition to guarantee the convergence of $\langle \Psi_n, x^{2M}\Psi_n \rangle$ is the *uniform boundedness* of the set $\{\Psi_n\}_{n=1}^{\infty}$ in the x space (see Refs. [42,44] or Sec. V for details). The set of Dirichlet eigenfunctions $\{\Psi_R^j(\lambda,x)\}_{R>0}$ is uniformly bounded by the asymptotic form of the corresponding $\Psi^j(\lambda,x)$ for $\lambda \geq 0$ [29,30] and therefore Eq. (3.2) holds true. Thus we have the equations

$$\lim_{R \to \infty} E_R^{ik} = E^{ik},$$

$$\lim_{R \to \infty} \psi_R^{ik}(x) = \psi^{ik}(x), \quad k = 0,1, \ldots . \qquad (3.3)$$

There is a similar result between series (2.6) and (2.13). The coefficients E_{Rn}^{ik}, $\phi_{Rn}^{ik}(x)$ are computed with formulas (3.1a)–(3.1d), where E_R^{i0}, ψ_R^{i0}, $\langle \Psi_R^{j0}, V\Psi_R^{j'0} \rangle_R$ are replaced by E_{Rn}^{i0}, ϕ_R^{i0}, $\langle \Phi_{Rn}^{j0}, V\Phi_{Rn}^{j'0} \rangle_R$, respectively. Since V is a bounded operator in L_2^R, the sole convergence of the sequence $\{\Phi_{Rn}^{j0}\}_{n=1}^{\infty}$ in the L_2^R norm [Eq. (2.12)] guarantees the convergence of $\langle \Phi_{Rn}^{j0}, V\Phi_{Rn}^{j'0} \rangle_R$,

$$\lim_{n \to \infty} \langle \Phi_{Rn}^{j0}, V\Phi_{Rn}^{j'0} \rangle_R = \langle \Psi_R^{j0}, V\Psi_R^{j'0} \rangle_R.$$

This result and the convergence of E_{Rn}^{j0}, Φ_{Rn}^{j0} to E_R^{j0}, Ψ_R^{j0} [Eq. (2.12)] lead to the convergence of the coefficients of the E_{Rn}^i and Ψ_{Rn}^{ik} series,

$$\lim_{n \to \infty} E_{Rn}^{ik} = E_R^{ik},$$

$$\lim_{n \to \infty} \phi_{Rn}^{ik}(x) = \psi_R^{ik}(x), \quad k = 0,1, \ldots . \qquad (3.4)$$

The solution of the n-dimensional problem (2.8) by RSPT has some advantages. The zero-order problem (2.11) can be solved completely since it has a finite number of solutions E_{Rn}^{j0}, Φ_{Rn}^{j0} which can be computed with the standard numerical software. Since there are just n functions Φ_{Rn}^{j0}, the infinite series (3.1a)–(3.1d) are replaced by the finite ones and, therefore, the coefficients E_{Rn}^{ik}, ϕ_{Rn}^{ik} can be computed up to the desired order k. It could be expected that it is necessary to carry out calculations with large n to get accurate estimations of $E_R^i(\lambda)$, and $\Psi_R^i(\lambda,x)$ but the numerical results given below show that this is not the case for anharmonic oscillators when a trigonometric basis is used.

The Eqs. (3.3) and (3.4) are independent of the singular or regular character of the perturbation V, a proof of such equations with tools of functional analysis is given in Ref. [33]. If λ_{ERin}, λ_{ERi}, and λ_{Ei} denote the convergence radii of the E_{Rn}^i, E_R^i, and E^i series, respectively, we can surmise the following result:

$$\lim_{n \to \infty} \lambda_{ERin} = \lambda_{ERi},$$

$$\lim_{R \to \infty} \lambda_{ERi} = \lambda_{Ei}. \qquad (3.5)$$

If V is a singular perturbation, we have $\lambda_{ERin}, \lambda_{ERi} \to \lambda_{Ei} = 0$ as $n, R \to \infty$, although the continuity of $V(x)$ guarantees that λ_{ERin}, λ_{ERi} are nonzero for any R since V is a bounded operator in L_2^R. In this case, the sequences $\{E_{Rn}^{iK}(\lambda)\}_{K=0}^{\infty}$, $\{E_R^{iK}(\lambda)\}_{K=0}^{\infty}$ of the partial sums

$$E_{Rn}^{iK}(\lambda) = \sum_{k=0}^{K} E_{Rn}^{ik} \lambda^k,$$

$$E_R^{iK}(\lambda) = \sum_{k=0}^{K} E_R^{ik} \lambda^k \qquad (3.6)$$

converge to $E_{Rn}^i(\lambda)$ and $E_R^i(\lambda)$ for $|\lambda| < \lambda_{ERin}$ and $|\lambda| < \lambda_{ERi}$, respectively.

IV. SUMMATION OF EIGENVALUE SERIES

To begin consider the calculation of the ground state for the quartic oscillator $H = p^2 + x^2 + \lambda x^4$ with the trigonometric basis

$$\varphi_{Rm} = \frac{\sin(m\pi x/R)}{\sqrt{R}} \quad m = 1,2, \ldots . \qquad (4.1)$$

The set $\{\varphi_m\}_{m=1}^{n=30}$ produces accurate estimations E_{Rn}^{i0}, Φ_{Rn}^{i0} of the first eigensolutions E_R^{i0}, Ψ_R^{i0} of H_R^0 (2.7) with several R values, larger sets $\{\varphi_m\}_{m=1}^{n}$ yield the same results. Table I reports some coefficients E_{Rn}^{ik} for $R = 1$, 2.1, 2.5, 5, 10. The

TABLE I. Coefficients $E_{R,n=30}^{ik}$ for the ground state of $H=p^2+x^2+\lambda x^4$. In this table and the following ones, the notation $[m]$ means $\times 10^m$.

k	E_{1n}^{ik}	$E_{2.1n}^{ik}$	$E_{2.5n}^{ik}$	E_{5n}^{ik}	E_{10n}^{ik}
0	3[0]	1[0]	1[0]	1[0]	1[0]
5	1[−10]	1[0]	2[0]	2[2]	2[2]
10	5[−21]	2[−3]	−1[1]	−4[7]	−5[7]
15	3[−31]	−2[−4]	−9[1]	3[13]	1[14]
20	3[−41]	−7[−5]	8[2]	−4[19]	−1[21]
25	2[−51]	−1[−5]	1[4]	5[25]	6[28]
30	2[−61]	−3[−7]	−1[5]	−6[31]	−8[36]
35	2[−71]	3[−7]	−2[6]	7[37]	2[45]
40	1[−81]	9[−8]	1[7]	−8[43]	−1[54]

coefficients with $R=1$ behave like $E_{Rn}^{ik} \sim 10^{-2k-1}$, and this suggests that the E_{Rn}^{i} series has the convergence radius $\lambda_{ERin} \sim 10$. However, $|E_{Rn}^{ik}|$ increases rapidly as R goes from 2.1 to 10 and k is increased. Table II reports the ratio E_{Rn}^{ik}/E^{ik} with the coefficient E^{ik} of the E^{i} series and we see that E_{Rn}^{ik} tends to E^{ik} as R increases. This confirms the convergence of the coefficients E_{Rn}^{ik}, E_{R}^{ik} toward E^{ik} as n,R increase [Eqs. (3.3) and (3.4)] and supports the expectation that the convergence radii λ_{ERin}, λ_{ERi} tend to that λ_{Ei} of the E^{i} series [Eq. (3.5)]. The quartic anharmonic oscillator has $\lambda_{Ei}=0$ [15,18] and therefore $\lambda_{ERin}, \lambda_{ERi} \rightarrow 0$ as $R,n \rightarrow \infty$, although the analytic perturbation theory guarantees that λ_{ERin}, λ_{ERi} are nonzero.

To estimate the eigenvalue $E^{i}(\lambda)$ with the Dirichlet values $E_{Rn}^{i}(\lambda)$, these have to be estimated with a large R. The above results show that the E_{Rn}^{i} and E_{R}^{i} series diverge with large λ, R so that, apparently, there is no advantage in computing such series. However, we can take the following approach. Instead of making calculations with large R to compute $E^{i}(\lambda)$ for any λ, we fix λ and compute the largest R for which the partial-sum sequence $\{E_{Rn}^{iK}(\lambda)\}_{K=0}^{\infty}$ converges. This R value depends on λ, i, n, and will be denoted by $R_{\lambda in}$. The values $E_{Rn}^{iK}(\lambda=1)$ reported in Table III show that $\{E_{Rn}^{iK}\}_{K=0}^{\infty}$ converges with $R \leqslant 2.0$, hence $R_{\lambda in}=2.0$. Table IV reports exact eigenvalues $E_{R}^{i}(\lambda)$ calculated variationally and shows their convergence toward $E^{i}(\lambda)$ as R increases. Ac-

TABLE II. Ratio E_{Rn}^{ik}/E^{ik} between E_{Rn}^{ik}'s of Table I and the coefficients E^{ik} of the corresponding E^{i} series.

k	E_{1n}^{ik}	$E_{2.1n}^{ik}$	$E_{2.5n}^{ik}$	E_{5n}^{ik}	E_{10n}^{ik}
0	3[0]	1	1	1	1
5	5[−13]	2[−4]	1[−2]	1	1
10	−9[−29]	−3[−11]	2[−7]	9[−1]	1
15	3[−45]	−2[−18]	−8[−13]	3[−1]	1
20	−2[−62]	5[−26]	−6[−19]	3[−2]	1
25	3[−80]	−2[−34]	2[−25]	7[−4]	1
30	−3[−98]	4[−44]	1[−32]	7[−6]	1
35	8[−117]	1[−52]	−1[−39]	3[−8]	1
40	−1[−135]	−7[−62]	−1[−47]	7[−11]	1

TABLE III. Partial sums $E_{R,n=30}^{iK}(\lambda=1)$ for the ground state of $H=p^2+x^2+\lambda x^4$.

K	$E_{2.0\,n}^{iK}$	$E_{2.2\,n}^{iK}$	$E_{2.3\,n}^{iK}$
0	1.075	1.035	1.024
10	1.398	1.399	1.394
20	1.398	1.389	1.169
30	1.398	1.394	2.357
40	1.398	1.393	−1.01

cording to this table, eigenvalue $E_{R}^{i}(1)$ has to be estimated with $R \geqslant 2.8$ to get $E^{i}(1)$ with seven exact figures, while the partial-sum sequence $\{E_{Rn}^{iK}(1)\}_{K=0}^{\infty}$ converges for $R \leqslant 2.0$.

An alternative way to compute $E_{R}^{i}(\lambda)$ with a "large" R is the application of summability methods to the E_{Rn}^{i} series. In this work, we use the diagonal Padé approximants

$$E_{Rn}^{iPK}(\lambda) = \left[\sum_{k=0}^{K/2} a_k \lambda^k \right] \bigg/ \left[1 + \sum_{k=1}^{K/2} b_k \lambda^k \right] \qquad (4.2)$$

obtained from the partial sums $E_{Rn}^{iK}(\lambda)$ with $K=2,4,\dots$ [46]. Let $R_{\lambda in}^{P}$ be the largest R for which the Padé sequence $\{E_{Rn}^{iPK}(\lambda)\}_K$ converges to a useful estimation of $E_{R}^{i}(\lambda)$. The following heuristic argument suggests that $R_{\lambda in}^{P}$ is larger than $R_{\lambda in}$. Figure 1 shows a qualitative graph of R vs the convergence radius λ_{ERin} of the E_{Rn}^{i} series with $\lambda_{Ei}=0$ [Eq. (3.5)]. Let λ_{ERin}^{P} denote the maximum λ for which the Padé sequence $\{E_{Rn}^{iPK}(\lambda)\}_K$ converges. If the Padé approximants extend the convergence radius of a series, then λ_{ERin}^{P} is greater than λ_{ERin} for each R and therefore the graph of R vs λ_{ERin}^{P} is qualitatively as Fig. 1 shows. We see that if $\{E_{Rn}^{iK}(\lambda)\}_K$ converges with a given λ, the sequence $\{E_{Rn}^{iPK}(\lambda)\}_K$ also does with a larger R, hence we get

$$R_{\lambda in}^{P} > R_{\lambda in}.$$

Finally, if $R_{\lambda in}^{P}$ is large enough, the sequence $\{E_{Rn}^{iPK}(\lambda)\}_K$ converges to a reliable estimation of $E^{i}(\lambda)$. As we shall see below this is the case for λ from the weak to the strong coupling regime of the quartic, sextic, and octic oscillators. The calculations were done with 32-digit precision.

Following with the ground state of the quartic oscillator, Table V reports the Padé approximants $E_{R,n=30}^{iPK}(\lambda)$ with λ

TABLE IV. Eigenvalues $E_{R}^{i}(\lambda)$ for the ground state of $H=p^2+x^2+\lambda x^4$.

R	$\lambda=0.1$	R	$\lambda=1$
4.5	1.065285509547	2.8	1.392351935104
5.0	1.065285509544	4.0	1.392351641530
9.0	1.065285509544	5.0	1.392351641530
	$\lambda=10$		$\lambda=100$
2.0	2.449174298327	1.5	4.999417547532
2.5	2.449174072118	2.0	4.999417545137
3.0	2.449174072118	2.5	4.999417545137

FIG. 1. Qualitative graph of R vs the convergence radius λ_{ERin} and λ_{ERin}^{P}.

TABLE VI. First and last Padé approximants of sequences $\{E_{R,n=30}^{iPK}(\lambda)\}_{K_{\min}}^{K_{\max}}$ for the ground state of $H = p^2 + x^2 + \lambda x^4$.

K	$\lambda = 100$	K	$\lambda = 500$
	$R = 1.40$		$R = 1.10$
56	4.99941770295	56	8.4616426903
70	4.99941770294	70	8.4616426904
	$R = 1.45$		$R = 1.15$
38	4.99941756608	62	8.461642638
40	4.99941756607	70	8.461642635
	$R = 1.50$		$R = 1.20$
38	4.9994175479	68	8.46164264
40	4.9994175476	76	8.46164269
ex[a]	4.9994175451		8.461642629

[a]Accurate eigenvalues $E^i(\lambda)$.
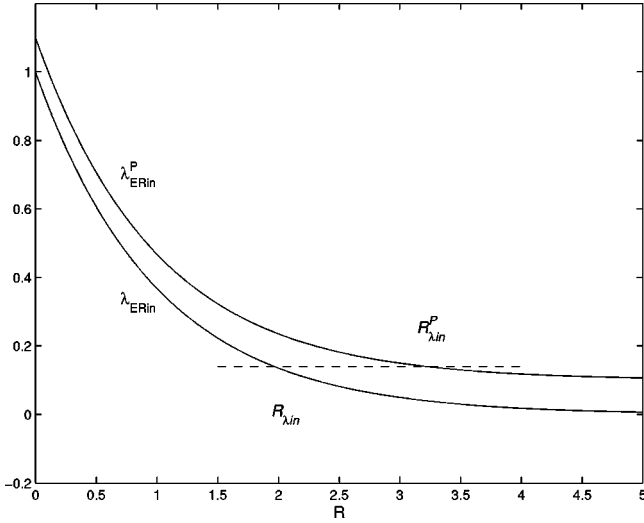
$=0.1$, 1, 100 and increasing R values. In order to exhibit the convergence rate, we report the first and the last elements of a sequence $\{E_{Rn}^{iPK}(\lambda)\}_K$ of approximants, which have the same figures except the last one. The Padé approximants $E^{iPK}(\lambda)$ from the E^i series are reported with ∞. For $\lambda = 0.1$, there is convergence with $R = 5$, 10, ∞ and therefore $R_{\lambda in}^{P} = \infty$. The Padé approximants reported for $\lambda = 1$, 100 show that the convergence rate of $\{E_{Rn}^{iPK}(\lambda)\}_{K=2}^{40}$ is slower as R and λ increase. For $\lambda = 1$, the sequence $\{E_{Rn}^{iPK}(\lambda)\}_{K=2}^{40}$ converges with $R \leq 4.5$, hence we get $R_{\lambda in}^{P} = 4.5$, which is large enough to estimate $E^i(1)$ with 11 exact figures. For $\lambda = 100$ and $R = 1.4$, the sequence $\{E_{Rn}^{iPK}(\lambda)\}_{K=2}^{40}$ converges to an estimation of $E^i(\lambda)$ with six exact figures, whereas the Padé sequence $\{E^{iPK}(\lambda)\}_{K=2}^{40}$ from the E^i series has a null accuracy.

The calculations for $\lambda = 100$, 500 are given in Table VI. We report the first and the last elements of a sequence of $E_{Rn}^{iPK}(\lambda)$'s, which have the same figures except the last one, calculations beyond $K_{\max}$ yield $E_{Rn}^{iPK}(\lambda)$'s which oscillate be-

cause of rounding errors. The convergence pattern allows us to determine the accuracy of $E_{Rn}^{iPK}(\lambda)$'s when they are seen as estimations of $E_R^i(\lambda)$ or $E^i(\lambda)$. For fixed R and λ, $E_{Rn}^{iPK_{\min}}(\lambda)$ and $E_{Rn}^{iPK_{\max}}(\lambda)$ differ in the last figure, hence they coincide with $E_R^i(\lambda)$ except in such a figure. Consider the best $E_{Rn}^{iPK}(\lambda)$'s for each R value and the same λ. As expected, they obey the variational inequality (2.5) as R increases and consequently each value is an upper bound of $E^i(\lambda)$,

$$E^i(\lambda) \leq E_{Rn}^{iPK}(\lambda) \leq E_{R'n}^{iPK}(\lambda) \quad \text{for } R' < R.$$

The convergence pattern allows one to get the accuracy of each $E_{Rn}^{iPK}(\lambda)$ when it is seen as an approximation of $E^i(\lambda)$. For example, $E_{R,n=30}^{iPK}(500)$ with $R = 1.10$, 1.15, 1.20 has seven exact figures of $E^i(500)$, a result confirmed by comparison with the exact $E^i(\lambda)$ given at the bottom of Table VI. These results show that (i) $R_{\lambda ni}^{P}$ is large enough to estimate $E^i(\lambda)$ and (ii) both the E_{Rn}^i and E_R^i series can be summed much more effectively than the E^i series to provide accurate estimations of $E^i(\lambda)$ with λ from the weak to the strong coupling regime.

TABLE V. First and last Padé approximants of the sequences $\{E_{R,n=30}^{iPK}(\lambda)\}_{K_{\min}}^{40}$, $\{E^{iPK}(\lambda)\}_{K_{\min}}^{40}$ for the ground state of $H = p^2 + x^2 + \lambda x^4$. $E^{iPK}(\lambda)$ corresponds to ∞.

K	$\lambda = 0.1$	K	$\lambda = 1$	K	$\lambda = 100$
	$R = 5$		$R = 3.5$		$R = 1.4$
22	1.065285509544	38	1.392351641529	34	4.9994175
40	1.065285509544	40	1.392351641529	40	4.9994177
	$R = 10$		$R = 4.5$		$R = 1.7$
36	1.065285509544	38	1.3923516415	32	4.9992
40	1.065285509544	40	1.3923516415	40	4.9994
	∞		∞		∞
38	1.065285509544	38	1.39235	36	3.33
40	1.065285509544	40	1.39235	40	3.42
ex[a]	1.065285509544		1.392351641530		4.9994175

[a]Accurate eigenvalues $E^i(\lambda)$ from Table IV.

TABLE VII. Padé approximants $E_{R,n=30}^{iPK}(\lambda)$ for the ground state of $H=2^{-1}(p^2+x^2)+\lambda x^4$.

K	$\lambda=1$	K	$\lambda=10^3$
	$R=3.5$		$R=0.9$
66	0.803770651234	50	6.69422085
78	0.803770651234	80	6.69422085
ex[a]	0.803770651234		6.69422085
			6.69426[b]
			6.69422085[c]
			6.69422085[d]

[a]Accurate eigenvalues $E^i(\lambda)$.
[b]Padé approximants from series (4.4), values from Table III of Ref. [13].
[c]Effective characteristic polynomials from series (4.4), values from Table IV of Ref. [13].
[d]Two-point Padé approximants from Table VI of Ref. [13].

Tables VII–IX give a summary of calculations for the ground state of $H=2^{-1}(p^2+x^2)+\lambda V$ with $V=x^4$, x^6, x^8 and $\lambda=1$, 10^3. We report the first and the last elements of a sequence $\{E_{Rn}^{iPK}(\lambda)\}_K$ of Padé approximants, which have the same figures except the last one, and the exact $E^i(\lambda)$ was estimated variationally. The results for the sextic case are interesting because they provide accurate approximations of $E^i(\lambda)$ for small or large λ whereas the Padé approximants from the $E^i(\lambda)$ series have a useless convergence [8,15,17]. The results for the octic oscillator are remarkably accurate and surprising since they show that the Padé approximants are able to sum the E_R^i and E_{Rn}^i series from the weak to the strong coupling regime, whereas Graffi and Grecchi [32] proved rigorously that the Padé approximants cannot sum the corresponding E^i series for any $\lambda>0$.

The RSPT produces weak coupling eigenvalue series which can be summed for small λ. The main approach to solve the problem with large λ has been the substitution of the original Hamiltonian H by another H^* with eigenvalue series having better numerical properties. In this kind of methods, we have the DWFA studied in this work, and the renormalization techniques which can be complemented with summation techniques such as nonlinear transformations

TABLE VIII. Padé approximants $E_{R,n=30}^{iPK}(\lambda)$ for the ground state of $H=2^{-1}(p^2+x^2)+\lambda x^6$.

K	$\lambda=1$	K	$\lambda=10^3$
	$R=2.4$		$R=1.0$
52	0.804965976056	70	3.850869184
72	0.804965976058	90	3.850869184
ex[a]	0.804965976012		3.85086918 2
			3.85080[b]
			3.850869[d]

[a]Accurate eigenvalues $E^i(\lambda)$ from Table IV.
[b]Effective characteristic polynomials, values from Table V of Ref. [13].
[c]Two-point Padé approximants, values from Table VII of Ref. [13].

TABLE IX. Padé approximants $E_{R,n=30}^{iPK}$ for the ground state of $H=2^{-1}(p^2+x^2)+\lambda x^8$.

	$\lambda=1$		$\lambda=10^3$
K	$R=2.1$	K	$R=1.05$
50	0.82068517861	72	2.833101931
68	0.82068517861	80	2.833101931
ex[a]	0.82068517857		2.833101930
			2.8334[b]

[a]Accurate eigenvalues $E^i(\lambda)$.
[b]Two-point Padé approximants from Table VIII of Ref. [13].

[9–12], the effective characteristic polynomials method (ECPM), or the two-point Padé approximants [13]. The n-dimensional version of the DWFA [Eqs. (2.8), (2.9)] is similar to the ECPM since it starts from an orthonormal set $\{\Phi_\nu\}_{\nu=1}^n$ in L_2 to compute the eigenvalues by means of the secular problem $P_n(E)=\det|\langle\Phi_\nu,H\Phi_\mu\rangle-E\delta_{\nu\mu}|=0$, where the original Hamiltonian $H=H^0+\lambda V$ is replaced by an other H^* that leads to an effective characteristic polynomial $P_n^*(E)$ which produces more accurate eigenvalues [13].

As an example of the renormalization techniques, we have the scheme of Čížek and Vrscay [22], which was worked out in detail by Vinette and Čížek [21], and Weniger *et al.* [12]. The scheme uses the variable $\hat{x}=(1-\kappa)^{-1/4}x$ with

$$\lambda\equiv\kappa(1-\kappa)^{-(M+1)/2}B_M^{-1}$$

and $B_M\equiv M(2M-1)!!/2^{M-1}$ to transform the problem $(p^2+x^2+\lambda x^{2M})\Psi^i=E^i\Psi^i$ into the equation

$$\hat{H}(\kappa)\hat{\Psi}^i(\kappa,x)=\hat{E}^i(\kappa)\hat{\Psi}^i(\kappa,x), \qquad (4.3)$$

where $\hat{H}(\kappa)=[\hat{p}^2+\hat{x}^2+\kappa(\hat{x}^{2M}/B_M-\hat{x}^2)]$, $\hat{E}^i(\kappa)=(1-\kappa)^{1/2}E^i(\lambda)$, and $\hat{\Psi}^i(\kappa,\hat{x})\equiv\Psi^i(\lambda,x)$. The coefficients c^{ik} of the formal series

$$\hat{E}^i(\kappa)=\sum_{k=0}^{\infty}c^{ik}\kappa^k \qquad (4.4)$$

grow similarly to the coefficients E^{ik} of the E^i series for the quartic, sextic, and octic cases [12]. However, the results of Ref. [12] show that the $\hat{E}^i$ series can be summed more effectively than the E^i series for small λ. Čížek and co-workers [13] combined the ECPM and the Padé summation to compute the ground state of the quartic oscillator with the E^i and $\hat{E}^i$ series. Table VII reports these values for $\lambda=10^3$, and shows that their accuracy is similar to that of the Padé approximants $E_{Rn}^{iPK}(\lambda)$ [47].

If both the weak coupling and the strong coupling expansions are constructed in terms of a same coupling parameter, we can use summation methods that combine the information from such expansions to produce, at least in principle, better results than a summation technique that uses information from one expansion [48]. This is the case of anharmonic

oscillators. Following Weniger [10], the renormalized Hamiltonian $\hat{H}(\kappa)$ can be partitioned as follows:

$$\hat{H}(\kappa) = (\hat{p}^2 + \hat{x}^{2M}B_M^{-1}) + (1-\kappa)(\hat{x}^2 - \hat{x}^{2M}B_M^{-1}) \quad (4.5)$$

hence $\hat{E}^i(\kappa)$ has the series

$$\hat{E}^i(\kappa) = \sum_{k=0}^{\infty} \Gamma^{ik}(1-\kappa)^k, \quad (4.6)$$

which converges in the neighborhood of $\kappa = 1$, or, equivalently, the series

$$E^i(\lambda) = (1-\kappa)^{-1/2} \sum_{k=0}^{\infty} \Gamma^{ik}(1-\kappa)^k$$

converges for large λ [10], that is, it is a strong coupling expansion of $\hat{E}^i(\kappa)$. This series poses the problem of computing the coefficients Γ^{ik} since the eigenstates of the unperturbed Hamiltonian, $\hat{p}^2 + \hat{x}^{2M}B_M^{-1}$, are unknown. Γ^{ik}'s are given by the divergent series that can be summed with the nonlinear sequence transformations [10]. Čížek *et al.* [13] used these coefficients together with those of the weak coupling expansion (4.4) to sum the series with the two-point Padé approximants. Tables VII–IX report some results from Ref. [13] for $\lambda = 10^3$, and we have a surprising fact that their accuracy is equal to or lower than that of the ordinary Padé approximants $E_{Rn}^{iPK}(\lambda)$ even when the latter were obtained from the (un-normalized) weak coupling E_{Rn}^i series, a result that emphasizes the good properties of the E_{Rn}^i series.

The convergence of the Padé sequence $\{E^{iPK}(\lambda)\}_K$ from the E^i series for the quartic and sextic anharmonic oscillators is guaranteed by the fact that the coefficients E^{ik} are essentially the coefficients of a Stieltjes series

$$f(\lambda) \sim \sum_{q=0}^{\infty} (-1)^q \mu_q \lambda^q,$$

for which there is a unique $\rho(t)$ such that $\mu_q = \int_0^{\infty} t^q d\rho(t)$ [2,8,15]. However, Graffi and Grecchi [32] proved that for high-order oscillators the measure $\rho(t)$ is not unique and, therefore, the sequence $\{E^{iPK}(\lambda)\}_K$ does not converge. The Stieltjes-series argument cannot be applied to prove the convergence of Padé approximants $E_{Rn}^{iPK}(\lambda)$ (4.2) because the sign of the coefficients E_{Rn}^{ik} is not alternant as Table I shows. The convergence may be explained by the Padé conjecture [16] which concerns the convergence of the diagonal Padé approximants to analytic functions, but no proof yet exists. If this conjecture is correct, the approximants $E_{Rn}^{iPK}(\lambda)$ converge uniformly to $E_R^i(\lambda)$ for small λ since the analytic perturbation theory guarantees that $E_R^i(\lambda)$ is an analytic function of λ [49].

The excellent numerical convergence of $\{E_{Rn}^{iPK}\}_K$ for the quartic, sextic, and octic oscillators may be attributed to the smallness of the coefficients E_{Rn}^{ik}. In all the cases studied here, $|E_{Rn}^{ik}|$ with $k \geq 1$ increases monotonically and tends to $|E^{ik}|$ as R increases (see Table I),

$$|E_{R'n}^{ik}| < |E_{Rn}^{ik}| < \cdots < |E^{ik}| \quad \text{for} \quad R' < R. \quad (4.7)$$

This behavior can be attributed to the fact that the matrix elements $V_{Rn}^{jj'} = \langle \Psi_{Rn}^{j0}, V\Psi_{Rn}^{j'0} \rangle_R$ are basically increasing functions of R but convergent to $\langle \Psi^{j0}, V\Psi^{j'0} \rangle$ as $R, n \to \infty$, of course [Eqs. (3.2)–(3.4)]. For instance, in the case $H^0 = p^2$, $V = x^2$, the trigonometric basis yields $V_{Rn}^{jj'} \sim R^2$. According to Eq. (4.7), we can say that the convergence (divergence) rate of the E_{Rn}^i series is faster (slower) than that of the E^i series and, therefore, the E_{Rn}^{ik} series can be summed more effectively than the E^i series, a result that can be extrapolated to the E_R^i series.

V. SUMMATION OF EIGENFUNCTION SERIES

If V is a regular perturbation of H^0, the Ψ^i series converges in the L_2 norm; that is, the sequence $\{\Psi^{iK}(\lambda, x)\}_{K=0}^{\infty}$ of the partial sums

$$\Psi^{iK}(\lambda, x) = \sum_{k=0}^{K} \psi^{ik}(x)\lambda^k \quad (5.1)$$

converge to $\Psi^i(\lambda, x)$ in the norm for small λ, $||\Psi^{iK} - \Psi^i|| \to 0$ [1,2]. This convergence does not guarantee the correct calculation of $\Psi^i(\lambda, x)$ since the set $\{\Psi^{iK}(\lambda, x)\}_{K=0}^{\infty}$ has to be uniformly bounded in the x space. To define such a concept, let us denote the expectation value $\langle f, Sf \rangle$ of a symmetric operator S by $S(f)$ and consider that wave functions $f(x)$ are rapidly decaying when $x^k(f) = \langle f, x^k f \rangle < \infty$ holds for all $k \geq 0$. Let Ω denote a bounded region and Ω^c be its complement. We say that the set $\{\Psi_n\}$ is *uniformly bounded* (UB) if there is one rapidly decaying Ψ_B such that the inequality $|\Psi_n(x)| \leq \Psi_B(x)$ holds on a region Ω^c for large n where Ω^c is independent of n, otherwise $\{\Psi_n\}$ is *nonuniformly bounded* (NUB). If $\{\Psi_n\}_{n=1}^{\infty}$ converges to Ψ in the L_2 norm and is UB, the sequence $\{x^M(\Psi_n)\}_{n=1}^{\infty}$ converges to $x^M(\Psi)$ for all $M \geq 0$. Thus one can say that Ψ_n has a correct *global* convergence on the whole x space as $n \to \infty$, but if $\{\Psi_n\}_{n=1}^{\infty}$ is NUB the sequence $\{x^M(\Psi_n)\}_{n=1}^{\infty}$ does not converges to the correct value for some M [42,44].

The boundedness property is a suitable criterion to characterize sequences $\{\Psi_n\}$ calculated with the variational or perturbation methods. If $\{\varphi_m\}_{m=1}^{\infty}$ is a complete basis set of the Sobolev space $W_{2,1}$, the sequence $\{\Phi_m\}_{m=1}^{\infty}$ of the variational wave functions, $\Phi_n = \Sigma_{m=1}^n c_{nm}\varphi_m$, converges to the correct Ψ in the energy norm [50], but in Ref. [44], it was proved that $\{\Phi_n\}_{n=1}^{\infty}$ can be NUB and yield incorrect expectation values. On the other hand, in Ref. [42], it was shown that the Ψ^i series can yield a NUB sequence of the partial sums $\{\Psi^{iK}\}_{K=0}^{\infty}$ even when V is a regular perturbation of H^0.

If V is a singular perturbation, the main rigorous result about the Ψ^i series is its asymptotic nature [1,2]. This means that $\Psi^i(\lambda, x)$ may not be determined uniquely by the set of coefficients $\psi^{ik}(x)$. Additionally, in Ref. [42] we saw that the Ψ^i series can be characterized by the nonuniform boundedness of the partial-sum sequence $\{\Psi^{iK}(\lambda, x)\}_{K=0}^{\infty}$. These
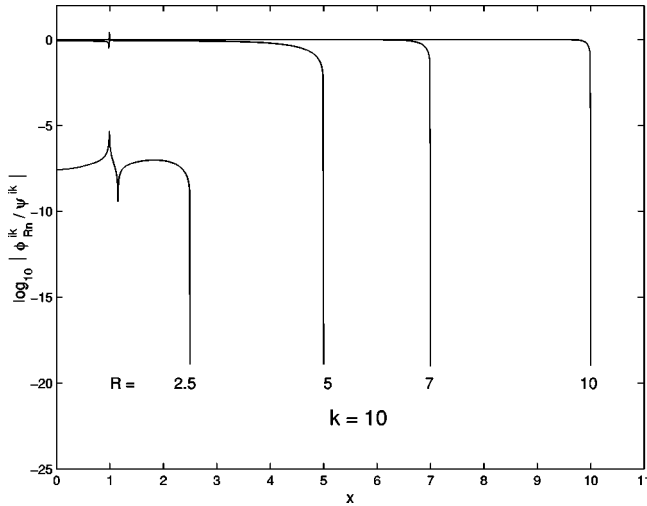
FIG. 2. Graph of x vs $\log_{10}|\phi^{ik}_{R,n=30}/\psi^{ik}|$ with $k=10$ for the ground state of $H=p^2+x^2+\lambda x^4$.

two problems are solved by the DWFA. Since the set of Dirichlet wave functions $\{\Psi^i_R(\lambda,x)\}_{R>0}$ is UB and converges to $\Psi^i(\lambda,x)$ in the L_2 norm [29,30], it is enough to estimate $\Psi^i_R(\lambda,x)$ with "large" R. The computation of $\Psi^i_R(\lambda,x)$ with $|x|\leqslant R$ eliminates the nonuniform boundedness problem since it is a problem on an unbounded region of the x space. On the other hand, since singular perturbations of H^0 such as $V=x^{2M}$ are regular perturbations of H^0_R, the sequence $\{\Psi^{iK}_R(\lambda,x)\}^\infty_{K=0}$ of the partial sums

$$\Psi^{iK}_R(\lambda,x)=\sum_{k=0}^{K}\psi^{ik}_R(x)\lambda^k \qquad (5.2)$$

converge to $\Psi^i_R(\lambda,x)$ in the norm for small λ, $\|\Psi^{iK}_R-\Psi^i_R\|_R\to 0$ [1,2]. Hence the sequence $\{x^M(\Psi^{iK}_R)\}^\infty_{K=0}$ converges to $x^M(\Psi^i_R)$ for $M\geqslant 0$ since x^{2M} is a bounded operator in L^R_2. These results are easily extended to the sequence $\{\Phi^{iK}_{Rn}\}^\infty_{K=0}$ of the partial sums

$$\Phi^{iK}_{Rn}(\lambda,x)=\sum_{k=0}^{K}\phi^{ik}_R(x)\lambda^k \qquad (5.3)$$

from the Φ^i_{Rn} series corresponding to Hamiltonian H_{Rn} (2.9). Let us see some numerical examples.

Consider the ground-state calculation for $H=p^2+x^2+\lambda x^4$ with the basis φ_{Rm} (4.1). Figure 2 shows the graph of x vs $\log_{10}|\phi^{ik}_{Rn}/\psi^{ik}|$ for $k=10$ and $R=2.5, 5, 7, 10$; the observed cusps are due to the zeros of the functions. We see that ϕ^{ik}_{Rn} tends uniformly to ψ^{ik} as R increases and similar results are obtained with other k values. This confirms the convergence of coefficients $\phi^{ik}_{Rn},\psi^{ik}_R$ toward ψ^{ik} as $R,n\to\infty$ [Eqs. (3.3)–(3.4)]. Hence we can expect a poor convergence of both the Φ^i_{Rn} and Ψ^i_R series as R,n increase. Instead of summing these series with large R, we fix λ and estimate the largest R for which the summation of the series yields a useful estimation of $\Psi^i(\lambda,x)$. The following results show that R estimated with eigenvalue calculations can be used.

TABLE X. Functional Padé approximants for the ground state of $H=p^2+x^2+\lambda x^4$. The ratios $\Phi^{iPK}_{Rn}/\sqrt{x^{0K}_{Rn}}$, $\Psi^{iPK}/\sqrt{x^{0K}_{Rn}}$ with $K=40$, $n=30$ are reported, Ψ^{iPK} corresponds to $R=\infty$.

R	$\lambda=1$ $x=0$	$\sqrt{x^{0K}_{Rn}}=1.0165062$ $x=3.5$
4	0.8347097115	5.340719[-8]
∞	0.884708	-1.3[-8]
ex[a]	0.8347097115	5.340717[-8]
	$\lambda=100$	$\sqrt{x^{0K}_{Rn}}=1.118298$
	$x=0$	$x=1$
1.5	1.16709754	0.01979228
∞	1.07	0.09
ex[a]	1.16709758	0.01979230
	1.70 [b]	0.01885 [b]

[a]Accurate eigenfunction $\Psi^i(\lambda,x)$.
[b]Values taken from Table I of Ref. [39].

The Φ^i_{Rn} series are summed by the so-called functional Padé approximants [16]

$$\Phi^{iPK}_{Rn}(\lambda,x)=\left[\sum_{k=0}^{K/2}a^\Phi_k(x)\lambda^k\right]\Bigg/\left[1+\sum_{k=1}^{K/2}b^\Phi_k(x)\lambda^k\right],$$

which are obtained from the partial sums $\Phi^{iK}_{Rn}(\lambda,x)$ with a given x value and $K=2,4,\ldots$ [46]. Table X reports the ratios $\Phi^{iPK}_{Rn}/\sqrt{x^{0K}_{Rn}}$, $\Psi^{iPK}/\sqrt{x^{0K}_{Rn}}$ at some x values for $\lambda=1, 100$ and $n=30$, $K=40$. The normalization constant $\sqrt{x^{0K}_{Rn}}$ is computed by the Padé summation as is explained below; $\Psi^{iPK}(\lambda,x)$ is the Padé approximant from the Ψ^i series and the exact $\Psi^i(\lambda,x)$'s are estimated variationally. We see that $\Phi^{iPK}_{Rn}(\lambda,x)$'s are very accurate, whereas $\Psi^{iPK}(\lambda,x)$'s have a poor or null accuracy. This result is reflected in the graphs of x vs $\log_{10}|\Phi^{iPK}_{Rn}|/\Psi_{as}$, $\log_{10}|\Psi^{iPK}|/\Psi_{as}$ plotted in Fig. 3 for $\lambda=100$ where
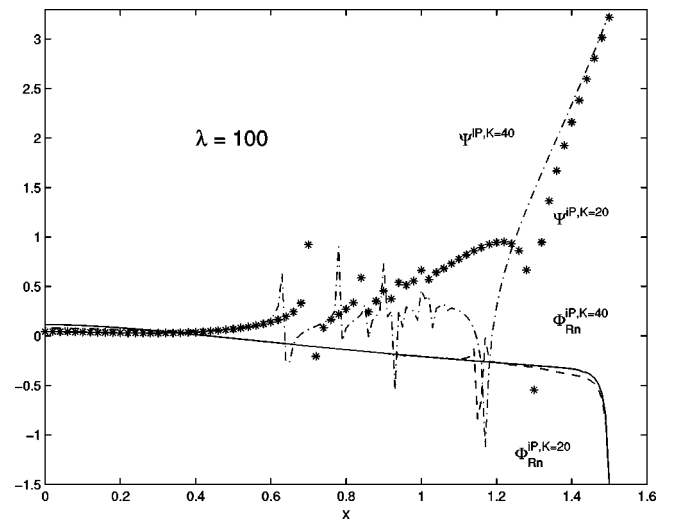

FIG. 3. Graphs of x vs $\log_{10}|\Phi^{iPK}_{Rn}|/\Psi_{as}$ and $\log_{10}|\Psi^{iPK}|/\Psi_{as}$ for the ground state of $H=p^2+x^2+\lambda x^4$ with $R=1.05$, $n=30$.

TABLE XI. Padé approximants $x_{R,n=30}^{MK}$ for the ground state of $H_R = p^2 + x^2 + \lambda x^4$ with $\lambda = 500$, $R = 1.15$, $50 \leq K \leq 60$.

$\langle x^0 \rangle$	$\langle x^2 \rangle$	$\langle x^4 \rangle$
1.280573	4.547445[−2]	5.580462[−3]
ex[a]	4.547445[−2]	5.580462[−3]

[a]Values from the accurate $\Psi^i(\lambda,x)$.

$$\Psi_{as}(\lambda,x) = \exp(-\lambda^{1/2}|x|^3/3)$$

is the asymptotic form of the exact Ψ^i [38]. In agreement with the uniform boundedness of the set $\{\Psi_R^i(\lambda,x)\}_{R>0}$ [29,30], $\Phi_{Rn}^{iPK}(\lambda,x)$ remains bounded by Ψ_{as} as K increases. The "largeness" of $R = 1.05$ guarantees that $\Phi_{Rn}^{iPK}(\lambda,x)$ is an accurate estimation of $\Psi^i(\lambda,x)$ on $[0,R]$ except in a small vicinity of $x = R$ where $\Phi_{Rn}^{iPK}(\lambda,x)$ satisfies the Dirichlet boundary condition.

The convergence of the sequence $\{\Phi_{Rn}^{iPK}(\lambda,x)\}_K$ is reflected by the Padé approximants

$$x_{Rn}^{MK} = \left[\sum_{k=0}^{K/2} a_k^M \lambda^k\right] \Bigg/ \left[1 + \sum_{k=1}^{K/2} b_k^M \lambda^k\right]$$

obtained from the first K terms of the expectation value series

$$x^M(\Phi_{Rn}^i) = \sum_{k=0}^{\infty} \left(\sum_{m=0}^{k} \langle \phi_{Rn}^{i,k-m}, x^M \phi_{Rn}^{im} \rangle_R\right) \lambda^k.$$

Table XI reports $x_{Rn}^{M=0,K} \equiv \|\Phi_{Rn}^{iPK}\|_R^2$ and the ratio x_{Rn}^{MK}/x_{Rn}^{0K} for $M = 2, 4$ and $\lambda = 500$. We see that x_{Rn}^{MK}'s coincide with the values from the exact $\Psi^i(\lambda,x)$ estimated variationally.

The calculations for the ground state of $H = 2^{-1}(p^2 + x^2) + \lambda V$ with $V = x^6, x^8$ and $\lambda = 1, 10^3$ are given in Tables XII and XIII; the exact $\Psi_R^i(\lambda,x)$ and $\Psi^i(\lambda,x)$ are calculated variationally. Table XII shows that $\Phi_{Rn}^{iPK}(\lambda,x)$'s are accurate

TABLE XII. Functional Padé approximants for the ground state of $H = 2^{-1}(p^2 + x^2) + \lambda V$ with $V = x^6$, x^8. The ratio $\Phi_{Rn}^{iPK}/\sqrt{r_{Rn}^{0K}}$ with $K_{min} \leq K \leq 90$ and $n = 30$ is reported.

	$\lambda = 1$	$\lambda = 10^3$
$V = x^6$	$\Phi_{R=2.4,n}^{iP,K \geq 52}$	$\Phi_{R=1.0,n}^{iPK,K \geq 52}$
$x = 0$	0.877379780	1.31546068
	0.877379780[a]	1.31546068[a]
$x = .5$	0.710919869	0.33010483
	0.710919869[a]	0.33010483[a]
$x = 2$	6.40764[−4]	
	6.40768[−4][a]	
$V = x^8$	$\Phi_{R=2.1,n}^{iP,K \geq 44}$	$\Phi_{R=1.05,n}^{iP,K \geq 56}$
$x = 0$	0.885440760	1.2230217
	0.885440760[a]	1.2230217[a]
$x = 1$	0.312207486	2.68[−5]
	0.312207486[a]	2.70[−5][a]

[a]Accurate values of eigenfunction $\Psi^i(\lambda,x)$.

TABLE XIII. Padé approximants $x_{R,n=30}^{MK}$ for the ground state of $H = 2^{-1}(p^2 + x^2) + \lambda V$ with $V = x^6, x^8$. The values $x_{Rn}^{M=0,K}$ and $x_{Rn}^{MK}/x_{Rn}^{0,K}$ with $M = 2, 4$ are reported.

	$\lambda = 1$	$\lambda = 10^3$
$V = x^6$	$r_{R=2.4,n}^{M,K \geq 34}$	$r_{R=1.0,n}^{M,K \geq 46}$
$\langle x^0 \rangle$	1.070075	1.185283
$\langle x^2 \rangle$	0.238707	4.592118[−2]
$\langle x^4 \rangle$	0.150127	5.432953[−3]
$V = x^8$	$r_{R=2.1,n}^{M,K \geq 48}$	$r_{R=1.05,n}^{M,K \geq 46}$
$\langle x^0 \rangle$	1.067079	1.131956
$\langle x^2 \rangle$	0.225647	6.033521[−2]
$\langle x^4 \rangle$	0.130854	9.163312[−3]

estimations of $\Psi^i(\lambda,x)$ except in the vicinity of $x = R$. The graph of x vs the ratio Φ_{Rn}^{iPK}/Ψ_R^i is plotted in Fig. 4 for the octic oscillator with $\lambda = 10^3$. We observe a uniform convergence of $\{\Phi_{Rn}^{iPK}(\lambda,x)\}_K$ toward $\Psi_R^i(\lambda,x)$. Table XIII reports the Padé approximants x_{Rn}^{MK} which coincide with the values from the exact $\Psi^i(\lambda,x)$. These results show that the Padé approximants $\Phi_{Rn}^{iPK}(\lambda,x)$ provide accurate estimations of $\Psi^i(\lambda,x)$ for λ from the weak to the strong coupling regime.

Recent perturbation approaches consider the calculation of eigenfunctions. Table X reports the estimations of $\Psi^i(\lambda,x)$ obtained with the so-called optimized perturbation theory for the ground state of $H = p^2 + x^2 + \lambda x^4$ with $\lambda = 100$ [39,40]. A comparison between these values and the Padé approximants $\Phi_{Rn}^{iPK}(\lambda,x)$ shows that the latter are significantly more accurate. The multiple scale perturbation theory [37,38] was successfully applied to the eigenfunction calculations of the quartic anharmonic oscillator, but its extension to the sextic and octic oscillators is not easy since the method involves the solution of nonlinear operator equations. A renormalization scheme was used in Ref. [41] to estimate the eigenfunctions with a series that converges in
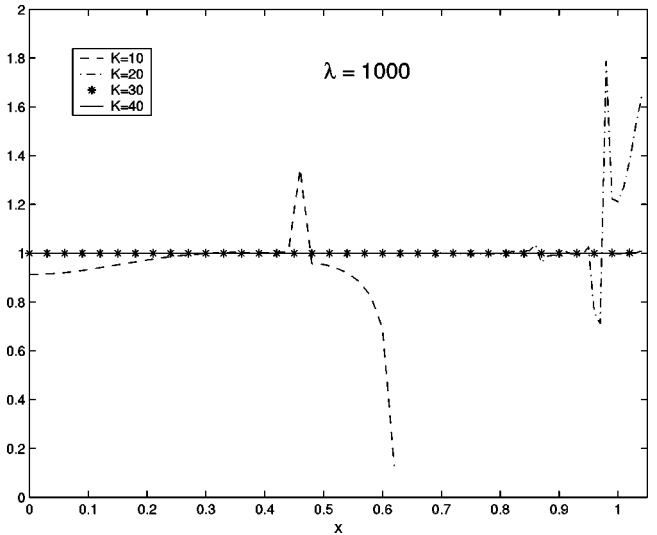

FIG. 4. Graph of x vs Φ_{Rn}^{iPK}/Ψ_R^i for the ground state of $H = 2^{-1}(p^2 + x^2) + \lambda x^8$ with $R = 1.05$, $n = 30$.

the norm, but the boundedness property of the corresponding partial-sum sequence was not investigated.

VI. DISCUSSION

The DWFA has some advantages from a theoretical point of view. The basic premise of the RSPT is the completeness in L_2 of the eigenfunctions of $H^0 = p^2 + V^0$, this excludes potentials such as $V^0 = -e^{-|x|}$, while the RSPT is applicable to the Dirichlet eigenproblem (2.3) because the compactness of the resolvent of H_R^0 guarantees that its eigenfunctions form a complete basis of L_2^R. If V is a singular perturbation, the eigensolutions $E^i(\lambda)$, $\Psi^i(\lambda,x)$ may not be determined uniquely by their formal series. This problem of uniqueness, which was solved for the anharmonic oscillators, is open for a continuous and singular perturbation V. In contrast, such a problem disappears with the DWFA since V is a regular perturbation of H_R^0.

Since the coefficients E_{Rn}^{ik} converge to E_R^{ik} as $n \to \infty$ (3.4), the results obtained with the E_{Rn}^i series can be extrapolated to the E_R^i series. The numerical results show that the E_{Rn}^i series can be summed much more effectively than the E^i series. By simplicity, the E_{Rn}^i series were summed with the ordinary Padé approximants $E_{Rn}^{iPK}(\lambda)$. The Padé conjecture may be an explanation for the convergence of Padé approximants $E_{Rn}^{iPK}(\lambda)$ for small λ, but the excellent numerical results can be attributed to the "smallness" of coefficients E_{Rn}^{ik} [Eq. (4.7)]. It is a surprising result that $E_{Rn}^{iPK}(\lambda)$'s give accurate estimations of $E^i(\lambda)$ for anharmonic oscillators with small or large λ. The results for the octic oscillator are particularly remarkable since in this case the Padé approximants $E^{iPK}(\lambda)$ from the E^i series do not converge for any $\lambda > 0$ [32].

Renormalization methods give a way to compute eigenvalues in the strong coupling regime. The renormalized Hamiltonian $\hat{H}$ (4.3) is interesting because, as was shown by Čížek et al. [13], it produces both the weak coupling and the strong coupling expansions which can be summed simultaneously with the two-point Padé approximants to obtain accurate eigenvalues $E^i(\lambda)$ for small or large λ. It is surprising that the ordinary Padé approximants $E_{Rn}^{iPK}(\lambda)$, which were obtained with a sole weak coupling expansion from the "un-normalized" Hamiltonian H_{Rn}, yield estimations of $E^i(\lambda)$ as accurate as those obtained by Čížek et al. [13]. This result emphasizes the good properties of the E_{Rn}^i and E_R^i series. Of course, such properties can be exploited with other summability methods. For instance, if the DWFA is applied to Hamiltonian $\hat{H}$ (4.3), one can expect that the corresponding two-point approximants will yield better results.

The methods that replace the original Hamiltonian H by an other H^* with better eigenvalue series can lead to a zero-order problem with unknown eigenstates, as occurs with the partition (4.5) of Hamiltonian $\hat{H}$ (4.3), and the DWFA is not an exception. Although the eigenstates of H_R^0 are known in some cases [34], in general such eigenstates have to be estimated numerically. We can apply other methods such as finite-element or finite-difference methods which replace H_R^0

by an n-dimensional version $\tilde{H}_{Rn}^0$, whose eigenstates $\tilde{E}_{Rn}^i$, $\tilde{\Psi}_{Rn}^i$ converge to those of H_R^0 [27,28]. These methods and the RSPT produce $\tilde{E}_{Rn}^i$ and $\tilde{\Psi}_{Rn}^i$ series whose coefficients converge to those of the E_{Rn}^i and Ψ_{Rn}^i series [Eq. (3.4)]. Thus, the DWFA gives a general approach to compute the coefficients of the E^i and Ψ^i series when the eigenstates of the unperturbed Hamiltonian are unknown. For instance, the coefficients of some strong coupling series such as Eq. (4.6), whose calculation has been the subject of several studies [10,22–26], can be computed with the series of the corresponding operator H_{Rn}.

The main result of the Ψ^i series when V is a singular (regular) perturbation is the asymptotic nature (convergence in the L_2 norm) [1,2]. The calculation of the true $\Psi^i(\lambda,x)$ requires a UB partial-sum sequence $\{\Psi^{iK}(\lambda,x)\}_K$, but it can be NUB even if V is regular [42]. The calculation of the Dirichlet eigenfunctions $\Psi_R^i(\lambda,x)$ eliminates the nonuniform boundedness problem. The functional Padé approximants $\Phi_{Rn}^{iPK}(\lambda,x)$, which yield accurate estimations of $\Psi^i(\lambda,x)$ for the sextic and octic oscillators in the strong coupling limit, show the excellent properties of the Ψ_R^i and Ψ_{Rn}^i series. To the best of our knowledge, perturbation calculations of these wave functions have not been reported in the literature.

In principle the equation $H\Psi^i = E^i\Psi^i$ can be solved by means of an n-dimensional problem such as Eq. (2.8). This approach, which is called "variation-perturbation" theory (see, e.g., Ref. [4]), involves solving the n-dimensional problem $(H_n^0 + \lambda V_n)\Phi_n^i = E_n^i\Phi_n^i$ by means of a perturbation method, where $H_n^0 \equiv P_n H^0 P_n$, $V_n \equiv P_n V P_n$, $P_n = \sum_{m=1}^n |\varphi_m\rangle\langle\varphi_m|$, and $\{\varphi_m\}_{m=1}^\infty$ is an orthonormal basis of L_2. Since the operator V_n is bounded in L_2, the formal series

$$E_n^i(\lambda) = \sum_k^\infty E_n^{ik}\lambda^k, \quad \Phi_n^i(\lambda,x) = \sum_k^\infty \phi_n^{ik}\lambda^k$$

have a nonzero convergence radius for any n, but these series or the functions Φ_n^i may have bad numerical properties as $n \to \infty$. Let us consider the convergence arguments behind Eqs. (3.2) and (3.3). The uniform boundedness of the set $\{\Psi_R^{j0}\}_{m=1}^\infty$ and its L_2 convergence guarantee the convergence of $\langle\Psi_R^{j0}, x^{2M}\Psi_R^{j'0}\rangle_R$ to $\langle\Psi^{j0}, x^{2M}\Psi^{j0}\rangle$ as $R \to \infty$. In contrast, the variational sequence $\{\Phi_n^{j0}\}_{n=1}^\infty$ can be NUB and therefore the quantity $\langle\Phi_n^{j0}, V\Phi_n^{j'0}\rangle$ can converge to a wrong limit or diverge $n \to \infty$ even when V is a regular perturbation. In this case, the coefficients E_n^{ik} and, consequently, the E_n^i series itself do not converge as $n \to \infty$. The examples of variational sequences for which $\langle\Phi_n^{j0}, x^{2M}\Phi_n^{j'0}\rangle$ diverge with $2M \geq 6$ are given in Refs. [43,44]. If $\{\Phi_n^{j0}\}_{n=1}^\infty$ is UB, $\{E_n^{ik}\}_{n=1}^\infty$ converges to E^{ik}, a result that can be used to compute the coefficients E^{ik} when the eigenstates of H^0 are unknown, and the properties (good or bad) of both the E_n^i and E^i series will be similar as n increases. On the other hand, the calculation of $\Phi_n^i(\lambda,x)$'s does not guarantee the calculation of the true $\Psi^i(\lambda,x)$ since the set $\{\Phi_n^i(\lambda,x)\}_{n=1}^\infty$, which is a variational sequence itself, may be NUB [44].

The formal results of the DWFA are independent of the basis set $\{\varphi_{Rm}\}_{m=1}^{\infty}$ used to solve the Dirichlet problem (2.3), but the numerical results obtained with the anharmonic oscillators can be attributed in part to the use of the trigonometric basis (4.1). The numerical efficiency of the DWFA depends of the basis set $\{\varphi_{Rm}\}_{m=1}^{\infty}$, which should be chosen according to the problem in question. Recent perturbation methods deal with the one-dimensional eigenfunction calculations [37–40], but their extension to the high-dimensional problems is not trivial. The DWFA provides eigenvalues and eigenfunctions and, from a theoretical point of view, its extension to many particle problems is easy.

VII. SUMMARY

We have observed the following points.

(i) The DWFA converts the singular perturbation problems $H = H^0 + \lambda V$ into the regular ones and, therefore, solves the problems posed by the asymptotic character of the E^i and Ψ^i series when V is a singular perturbation of H^0.

(ii) The DWFA provides a general method to compute the coefficients of the E^i and Ψ^i series [Eqs. (3.3), (3.4)]. This is important when a renormalization technique yields a zero-order problem whose eigenstates are unknown.

(iii) The numerical results show that the convergence properties of the series given by the DWFA turn out to be very good, even for the strongly anharmonic oscillators. This is clearly illustrated by the Padé summation of the series for the un-normalized octic case, which is known to be notoriously difficult and many standard resummation techniques fail in this case.

(iv) To date, the DWFA is the unique approach that, in rigorous mathematical terms, guarantees the calculation of the UB sequences of approximating wave functions and, therefore, the correct calculation of wave functions. Some renormalization schemes convert a singular perturbation problem $H^0 + \lambda V$ into a regular one $\check{H}^0 + \check{\lambda}\check{V}$, but this does not guarantee the correct calculation of the exact eigenfunction $\check{\Psi}^i$ since the $\check{\Psi}^i$ series can be NUB even when it converges in the norm of $L_2(-\infty, \infty)$.

(v) The formal results of this paper consider the general problem $H = p^2 + V^0 + \lambda V$, where V^0, V are continuous functions but some results can be extended to potentials with Coulomb-type singularities as well as to some many particle problems. This will be shown in a forthcoming work.

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