Multiple-turning-point problems and lattice multiscale singular perturbation

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It is shown how the single-turning-point singular-perturbation analysis of Bender and Sharp may be extended to multiple-turning-point problems. The methodology presented emphasizes the importance of combining a function-moments analysis together with high-temperature lattice expansions and associated Padé analysis. This approach has been previously developed by Handy for nonlinear kink and soliton solutions and will be referred to as lattice multiscale singular-perturbation theory (LMSPT). The formalism is developed in the context of one-dimensional polynomial potential systems and highlights recursive moment relations heretofore unappreciated in general. As such, for these kinds of systems, the LMSPT approach offers an alternative to the conventional WKB method; and is extendible to nonlinear systems.

I. GENERAL DISCUSSION

The seminal work by Bender *et al.*[1] on the development of a strong-coupling perturbative quantum field theory fostered a new type of mathematical analysis for understanding many quantum and classical systems requiring singular-perturbation analysis. The subsequent works by Bender *et al.*,[2] Handy,[3] and Bender and Sharp[4] pursued these issues to varying degrees.

This work is a continuation of the general thesis advocated by Handy,[3] wherein it is argued that singular perturbation is intrinsically a Fourier-space problem. The consequence of this general observation is that the singular-perturbation character of a problem disappears when it is represented in terms of an extensive set of dynamical variables. The power moments (i.e., the Taylor expansion coefficients of the Fourier transform) provide such a representation.

There is an important class of problems which serve to dramatize the preceding remarks. Specifically, we address the Schrödinger equation for arbitrary polynomial potential, although the specific example treated will be the harmonic quantum oscillator. An important aspect of this endeavor is that we are able to extend the one-turning-point results of Bender and Sharp[4] to that of multiple turning points.

It is evident that once a configuration-space problem has been transformed into an extensive-dynamical-variable representation space and solved therein, one must be able to transform back to the original space. Considering our moments' perspective, we are obligated to address the century-old problem of function-moments reconstruction.[5] Although such issues are not completely understood, recent work on the formulation of Polya-Padé approximants[6] show them to be very relevant to our multiple-turning-point problems. These are described in Sec. IV.

Let us reconsider the harmonic-oscillator problem[7]

$$-\epsilon^2\psi''+x^2\psi=E\psi \ . \tag{1.1}$$

The singular-perturbation parameter is $\epsilon\equiv\hbar/\sqrt{2m}$. An explicit ϵ-dependent perturbative expansion of this system requires the conventional WKB[7] representation, $\psi(x)=\exp(S/\epsilon)$, where $S(x)$ is assumed expandable in powers of ϵ. Clearly, the ϵ-analytic structure of $\psi(x)$ is not simple.

Let us now apply the integral operation $\int dx\, x^p$ on both sides of (1.1). Denoting by $\mu(p)\equiv\int dx\, x^p\psi(x)$ the pth-order Hamburger power moment, one obtains the recursive relation

$$\mu(p+2)=E\mu(p)+\epsilon^2 p(p-1)\mu(p-2), \quad p\geq 0 \ . \tag{1.2}$$

For simplicity, we will limit our discussion to symmetric solutions only. The extension of the following analysis to the antisymmetric case is immediate. Thus $\mu(p=\text{odd})=0$. It follows that only $\mu(0)$ is required to completely determine all moments; because of the arbitrary choice of normalization we may take $\mu(0)=1$.

Relation (1.2) follows from (1.1) only for physical solutions, since these decay exponentially and have finite moments. Nonetheless, (1.2) together with $\mu(0)=1$ admit general moment solutions which are explicitly polynomial analytic in ϵ^2 and E. In two recent works[8,9] a powerful energy-quantization technique, utilizing relations of the type (1.2), has been developed. Excellent results were obtained for various polynomial potentials, including that of (1.1). In the present work, we will assume that the physical energy value, E, is given. Our interest is in wave-function reconstruction.

Relation (1.2) is consistent with our general assertion that a reformulation of singular-perturbation-type problems in terms of an extensive-dynamical-variables representation will diminish or eliminate the "singular" nature of the configuration-space problem. Specifically, the solutions to (1.2), for fixed E, are trivial analytic functions of ϵ^2 in contrast to that for the wave function $\psi(x)=\exp(S/\epsilon)$.

The zeroth-order limit of the relation (1.2) gives $\mu^{(0)}(p+2)=E\mu^{(0)}(p)$, or

$$\mu^{(0)}(p)=(x_\tau)^p, \quad \text{if } p=\text{even (0,otherwise)}\ , \tag{1.3a}$$

$$x_\tau \equiv \sqrt{E}\ . \tag{1.3b}$$

The configuration-space solution corresponding to (1.3) is

$$\psi^{(0)}(x)=\tfrac{1}{2}[\delta(x+x_\tau)+\delta(x-x_\tau)]\ . \tag{1.4}$$

This is the formal solution to the symbolic, zeroth-order, configuration-space equation

$$x^2\psi^{(0)}(x)=E\psi^{(0)}(x)\ . \tag{1.5}$$

The $\pm x_\tau$ values correspond to the two "turning points." The work in Ref. 4 concerns itself with the monomial system $-\epsilon^2\psi''+x\psi=E\psi$; thus, only one turning point is involved.

It is clear that for the harmonic-quantum-oscillator problem, all of the power moments are known. As such, one can proceed to the reconstruction phase of our program in Sec. IV. In general this is not the case. There will usually be a finite number of undetermined power moments. It is the intent of the following discussion to suggest one possible method of determining these missing power moments. As an example, we once again turn to the system (1.1).

Let us translate the harmonic-oscillator problem in (1.1) by the amount x_τ. Thus for the system

$$-\epsilon^2\psi''+(x+x_\tau)^2\psi=E\psi \tag{1.6}$$

the recursive moment relation is

$$\mu(p+2)=-2x_\tau\mu(p+1)+\epsilon^2 p(p-1)\mu(p-2),\quad p\geq 0\ . \tag{1.7}$$

It is clear that $\mu(0)$ and $\mu(1)$ are now needed in order to determine all other moments. In general, we cannot solve our system by a simple translation [i.e., back to (1.1)]. Assuming $\mu(0)\equiv 1$, how may we solve for $\mu(1)$? One possibility is to find an appropriate lattice-space model for the continuum system. Let us do so for the original problem (1.1). In the following sections we will analyze in greater detail the high-temperature lattice expansion for the system

$$-\epsilon^2\frac{\Delta^{(2)}}{a^2}\psi+(aL)^2\psi=E\psi\ ,$$

$$a\equiv\text{lattice spacing}\ , \tag{1.8}$$

$$\Delta^{(2)}\psi\equiv\psi(L+1)+\psi(L-1)-2\psi(L)\ .$$

By applying Padé analysis[10] to the lattice representation for the continuum power moment, $\mu(p)\to a^{1+p}\times\sum L^p\psi(L)$, we can obtain the continuum-limit values through analytic continuation, $a\to 0$. In this manner all unknown moments may be obtained. It is important to stress that E's quantization is not necessary. For arbitrary E one can determine the associated unknown moments.

The generalization of the preceding harmonic results are immediate. Thus, for $V(x)=\sum_{j=1}^{J} c_j x^j$ (c_0 can be incorporated into E; $J=$even)

$$-\epsilon^2\psi''+\left[\sum_{j=1}^{J} c_j x^j\right]\psi=E\psi\ , \tag{1.9}$$

$$\mu(p+J)=E\mu(p)+\epsilon^2 p(p-1)\mu(p-2)-\sum_{j=1}^{J-1} c_j\mu(P+j)\ . \tag{1.10}$$

Now $\mu(0),\ldots,\mu(J-1)$ are required before all moments may be generated. Clearly, they cannot all be zero; hence, one of them may be normalized to unity. Thus there are $J-1$ unknowns, for arbitrary E. These may be determined through the methods developed in the following sections. It is to be stressed that any complicated ϵ dependence will be explicitly contained in the missing moments. Despite this, we expect that any such possible complicated ϵ dependence will be far less so than that for the configuration-space solution.

Finally, the zeroth-order solution to (1.10) takes on the form

$$\mu^{(0)}(p)=\sum_{j=1}^{N} f_j(x_{\tau;j})^p\ , \tag{1.11}$$

where $x_{\tau;j}$ is a turning-point root of $V(x)=E$. Clearly, the configuration-space representation of (1.11) is

$$\psi^{(0)}(x)=\sum_{j=1}^{N} f_j\delta(x-x_{\tau;j})\ . \tag{1.12}$$

The entire program consisting of using high-temperature lattice expansion methods to recover the unknown moments, and using some prescription for recovering the wave-function solution is designated by lattice multiscale singular-perturbation theory (LMSPT).

II. DEVELOPING A LATTICE-SPACE MODEL

Let us rewrite (1.1) as[11]

$$\psi''+(E-\tfrac{1}{4}x^2)\psi=0\ . \tag{2.1}$$

As is well known, the quantized energies correspond to $E=n+\frac{1}{2}$, $n=$integer.

Consider the following lattice model:

$$\frac{\Delta^{(2)}}{a^2}\psi+\tfrac{1}{4}a^2(L_0{}^2-L^2)\psi=fD(L,L_0)\ , \tag{2.2a}$$

where

$$\Delta^{(2)}\psi=\psi(L+1)+\psi(L-1)-2\psi(L)\ , \tag{2.2b}$$

$$E\equiv\tfrac{1}{4}(aL_0)^2(L_0=\text{an integer})\ , \tag{2.2c}$$

$$D(L,L_0)\equiv\begin{vmatrix}\delta_{L,L_0-1} & -\delta_{L,L_0+1}\\ +\delta_{L,-L_0+1} & -\delta_{L,-L_0-1}\end{vmatrix}\ , \tag{2.2d}$$

$$f=\frac{x_\tau}{12}\quad (x_\tau\equiv 2\sqrt{E}\,)\ . \tag{2.2e}$$

The last relation will be motivated shortly; so too will the necessity for $D(L,L_0)$.

It will be noted that $D(L,L_0)$ is defined on a set of measure zero. Also, in the continuum limit [$a\to 0, L_0\to\infty$, while $E=\frac{1}{4}(aL_0)^2$ is kept fixed], $D(\ )$

vanishes. $D(\ )$'s structure is consistent with our interest in generating symmetric solutions. We will *conjecture* that in the continuum limit, as specified, (2.2a) becomes equivalent to the continuum system (2.1).

If we accept the preceding conjecture, then it must also be that the following system approaches (2.1) in its respective continuum limit:

$$\frac{1}{a^3}\Delta^{(2)}\psi+\tfrac{1}{4}a_f(L_0{}^2-L^2)\psi=\frac{f}{a_f}D(L,L_0)\ . \qquad (2.3)$$

The basic difference between (2.3) and (2.2) is that a_f is kept fixed at some small value, while L_0 is some large integer satisfying $E=\frac{1}{4}(a_fL_0)^2$. The a variable will define the high-temperature expansion parameter a^{-3}. Our goal will be to perform a lattice high-temperature expansion and continue the (2.3) theory from the regime where a^{-3}=small to $a_f{}^{-3}$; afterward, all $a_f\to 0$.

The principal reason for adopting (2.3) is that it will lead to the elimination of all explicit "L_0" dependences. In addition, the fact that the eventual lattice high-temperature expansion will involve $(1/a^3)\Delta^{(2)}\psi$ as the only perturbative term mimics the nature of the ϵ^2 expansion in (1.2).

Let us now assume that the lattice field for (2.3) is expandable at every lattice space point L according to

$$\psi(L)=\sum_{w=0}\left[\frac{1}{a^3}\right]^w\psi^{(w)}(L;a_f)\ . \qquad (2.4)$$

The beauty of (2.3) is that the lattice turning points $L^2=L_0{}^2$ do not complicate the recursive generation of $\psi^{(w)}$. Indeed, at such turning points we have from (2.3)

$$\Delta^{(2)}\psi(\pm L_0)=0\ . \qquad (2.5)$$

Away from these lattice turning points, the recursive generation of (2.4) becomes

$$\psi^{(w)}(L;a_f)=\frac{\Delta^{(2)}\psi^{(w-1)}-(f/a_f)D(L,L_0)\delta_{w,0}}{\frac{1}{4}a_f(L^2-L_0{}^2)}\ ,\qquad L^2\neq L_0{}^2\ , \qquad (2.6a)$$

while from (2.5) we generate

$$\psi^{(w)}(\pm L_0;a_f)=\tfrac{1}{2}[\psi^{(w)}(\pm L_0+1;a_f)+\psi^{(w)}(\pm L_0-1;a_f)]\ . \qquad (2.6b)$$

It is clear that $D(\ )$'s presence is necessary; if it were absent then $\psi^{(0)}=0$. The factor f is determined from the requirement that the system [i.e., the zeroth-order version of (2.3)]

$$\tfrac{1}{4}a_f(L_0{}^2-L^2)\psi^{(0)}=\frac{f}{a_f}D(L,L_0),\quad L^2\neq L_0{}^2\ , \qquad (2.7a)$$

$$\Delta^{(2)}\psi^{(0)}(\pm L_0)=0\ , \qquad (2.7b)$$

yield in the continuum limit [$a_f\to 0, L_0\to\infty$, $E=\frac{1}{4}(a_fL_0)^2$] exactly the same power moments as the zeroth-order continuum theory [Eq. (1.3a) with $x_\tau=2\sqrt{E}$]. This calculation is straightforward and yields relation (2.2e).

One very important property that will allow the numerical determination of the lattice power moments $[a^{1+p}\sum L^p\psi(L)]$ is the fact that the lattice support space for each $\psi^{(w)}(L;a_f)$ is bounded and increases with w. Specifically, for all orders satisfying $w\leq L_0-2$, the lattice support set, S_w, consists of two disjoint subsets, $S_w=S_w^{(+)}\cup S_w^{(-)}$, where

$$S_w^{(\pm)}=\{L\ |\ \tilde{L}\equiv L-(\pm L_0),-(w+1)\leq\tilde{L}\leq w+1\}\ . \qquad (2.8)$$

If L_0 is very large, then for all practical purposes only at comparably large expansion orders will the above sets intersect. We assume that the lower orders contain sufficient information to solve the system. This assumption is supported by the fact that as a_f approaches the continuum limit (and thus $L_0\to\infty$) the configurations $\psi^{(w)}(L;a_f)$ will become more and more $\tilde{L}$ dependent, forgetting their dependence on L_0. This can be seen from (2.6a), which may be written

$$\psi^{(w)}(L_0+\tilde{L};a_f)=\frac{\Delta^{(2)}\psi^{(w-1)}-(f/a_f)D(\tilde{L})\delta_{w,0}}{\tilde{L}(\sqrt{E}+\frac{1}{4}\tilde{L}a_f)}\ ,\qquad \tilde{L}\geq -L_0,\ \tilde{L}\neq 0 \qquad (2.9a)$$

[for $\tilde{L}=0$ use (2.6b)]

$$D(\tilde{L})=\delta_{\tilde{L},-1}-\delta_{\tilde{L},1}\ . \qquad (2.9b)$$

Because we are generating symmetric solutions, we only need $\psi^{(w)}(L;a_f)$ for $L\geq 0$, or equivalently $\tilde{L}\geq -L_0$. Furthermore, we may assume that L_0 is very large, while $w\leq W\ll L_0-2$. Accordingly, for such orders $\psi^{(w)}(0;a_f)=0$.

The structure of (2.9) shows that upon rescaling as

$$\hat{\psi}^{(w)}(\tilde{L};a_f)\equiv a_f\psi^{(w)}(L_0+\tilde{L};a_f)\ , \qquad (2.10)$$

the $a_f\to 0$ limit for the left-hand-side expression becomes

$$\hat{\psi}^{(w)}(\tilde{L};0)=\frac{\Delta^{(2)}\hat{\psi}^{(w-1)}(\tilde{L};0)-fD(\tilde{L})\delta_{w,0}}{\tilde{L}\sqrt{E}}\qquad (\tilde{L}\neq 0,\tilde{L}\geq -L_0)\ , \qquad (2.11a)$$

$$\hat{\psi}^{(w)}(0;0)=\tfrac{1}{2}[\hat{\psi}^{(w)}(1;0)+\hat{\psi}^{(w)}(-1;0)]\ . \qquad (2.11b)$$

We shall examine (2.11) in the following section.

Considering all that has been stated, we may define the lattice power moments

$$\mu(p;a_f)=\begin{cases}2a^{1+p}\sum_{L=0}L^p\psi(L), & p=\text{even}\\ 0, & p=\text{odd}\ .\end{cases} \qquad (2.12)$$

In view of the fact that $\psi^{(w)}$, for $L>0$, is nonzero on a finite set centered at L_0, it is clear that (2.12) implicitly has an L_0 dependence. This fact can complicate any attempt at directly continuing (2.12) into the continuum. For this reason, it becomes convenient to work with "relative moments," as derived below:

$$\mu(p=\text{even};a_f)=2a^{1+p}\sum_{\tilde{L}=-L_0}(L_0+\tilde{L})^p\psi(L_0+\tilde{L})\ , \qquad (2.13)$$

$$\mu(p=\text{even};a_f)$$
$$=2a^{1+p}\sum_{\rho=0}^{p}B\binom{p}{\rho}L_0{}^{p-\rho}\sum_{\tilde{L}=-L_0}\tilde{L}^{\rho}\psi(L_0+\tilde{L}) \tag{2.14}$$
$$=2\sum_{\rho=0}^{p}B\binom{p}{\rho}x_\tau^{p-\rho}\mu_r(\rho;a_f) \tag{2.15}$$

$[B\binom{p}{\rho}=\text{binomial coefficients}]$.

Utilizing the lattice high-temperature expansion $\psi(L)=\sum(1/a^3)^w\psi^{(w)}$, the relative moments have their corresponding lattice high-temperature expansion:

$$\mu_r(\rho;a_f)=a^{1+p}\sum_{\tilde{L}=-L_0}\tilde{L}^{\rho}\psi(L_0+\tilde{L}) \tag{2.16}$$
$$=a^{1+p}\sum_{w=0}^{W}\left[\frac{1}{a^3}\right]^w C_r(\rho;w;a_f)\ , \tag{2.17}$$

where the numerically calculable coefficients are

$$C_r(\rho;w;a_f)\equiv\sum_{\tilde{L}\in S_w^{(+)}}\tilde{L}^{\rho}\psi^{(w)}(\tilde{L};a_f)\ . \tag{2.18}$$

In the following section we will work with $\hat{C}_r(\rho;w;a_f)$ which is defined similarly to (2.18) but using $\hat{\psi}^{(w)}(\tilde{L};a_f)$.

III. FORMING PADÉ APPROXIMANTS FOR THE CONTINUUM LIMIT

It is clear from (2.15) that in order to obtain the continuum moments, $\mu(p=\text{even})$, we must obtain the relative moments $\mu_r(\rho;a_f)$ satisfying

$$\mu(p=\text{even})=2\sum_{\rho=0}^{p}B\binom{p}{\rho}x_\tau{}^{p-\rho}\mu_r(\rho)\ . \tag{3.1}$$

Note that up to any given order p, there are $1+p/2$ even moments and $1+p$ relative moments. Clearly, knowledge of the left-hand side does not allow for a unique set of relative moments, to any finite order. Because of this, once our lattice theory has given us adequate values for the μ_r's, we must use them to calculate the μ's.

It is easy to see that the system corresponding to (2.11) is given by the lattice model

$$\frac{\Delta^{(2)}}{a^3}\psi+\tfrac{1}{4}a_f[(L_0-L)(2L_0)]\psi=\frac{f}{a_f}D(\tilde{L})\ . \tag{3.2}$$

Utilizing $2\sqrt{E}=a_fL_0$, where E is the energy for the harmonic quantum oscillator, the continuum version of (3.2) becomes

$$\psi''-\sqrt{E}\ x\psi=0\ . \tag{3.3}$$

Accordingly, the corresponding recursive moment expression involves the relative moments

$$\sqrt{E}\ \mu_r(p+1)=p(p-1)\mu_r(p-2)\ . \tag{3.4}$$

We can see that $\mu_r(1)=\mu_r(2)=\mu_r(4)=0$; while $\mu_r(3)/\mu_r(0)=2/\sqrt{E}$. Indeed, $\mu_r(p\neq\text{multiple of }3)=0$.

It is found numerically that the lattice high-temperature coefficients, $\hat{C}_r(\rho;w;0)\equiv\sum\tilde{L}^{\rho}\hat{\psi}^{(w)}(\tilde{L};a_f=0)$ are consistent with the above. That is, for $\rho\neq$multiple of 3 we find that $\hat{C}_r(\rho;w;0)=0$ if $\rho-3w<0$. What this means is that the corresponding moment is given by

$$\mu_r(\rho;a_f=0)=\frac{a^{1+\rho}}{a_f}\left[\sum_{0\leq w\leq\rho/3}a^{-3w}\hat{C}(\rho;w;a_f=0)+\sum_{\rho/3<w<\infty}a^{-3w}\hat{C}(\rho;w;0)\right]\ . \tag{3.5}$$

For those $\rho\neq$multiple of 3 we find that all of the $\hat{C}$'s of the rightmost sum are zero; whereas the finite left-hand sum has an $a_f^{\rho>0}$ dependence which makes the entire sum vanish in the continuum limit ($a=a_f$ and $a_f\to 0$). The same seems to be true for the case $\rho=$multiple of "3." We say "seems" because we have only verified things up to order $\rho=4$. For the case $\rho=0$ and 3 we find that the only nonvanishing term ($a_f\to 0$) is $\hat{C}(\rho;\rho/3;0)$; the latter takes on the values $\frac{1}{2}$ and $1/\sqrt{E}$ for $\rho=0$ and 3, respectively. Thus all is consistent with (3.4), particularly when we compare moment ratios.

The main conclusion from the above is that the seemingly insignificant denominator expression $\frac{1}{4}\tilde{L}a_f$ in (2.9a) is very important and needs to be incorporated if the quadratic nature of the harmonic-oscillator problem is to be taken into account. What this means is that the lowest-order corrections to the various coefficients are needed:

$$\hat{C}_r(\rho;w;a_f)=\hat{C}_r(\rho;w;0)+a_f\hat{C}_r^{(1)}(\rho;w)+a_f{}^2\hat{C}_r^{(2)}(\rho;w)+\cdots\ . \tag{3.6}$$

With regard to the first term in this expansion, it should be noted that the system (2.11) alternates between being symmetric and antisymmetric with the evenness or oddness of the expansion order, w, respectively [i.e., $\psi^{(w)}(-\tilde{L})=\text{sgn}\psi^{(w)}(\tilde{L})$, where $\text{sgn}=1,-1$, if $w=\text{even, odd}$]. Because of this one finds that $\hat{C}_r(\rho;w;0)=0$, if $\rho+w=\text{odd}$.

It has been found numerically that the most stable analysis is obtained if one works with the ratios $\mu_r(\rho)/\mu_r(0)$. The coefficients of such an expansion are readily obtainable from a straightforward linear analysis similar to that typically used in obtaining the Padé coefficients for a given expansion,[10]

$$\frac{\mu_r(\rho)}{\mu_r(0)}=a^{\rho}\left[\sum_{w=0}^{W}a^{-3w}R(\rho;w;a_f)+O((a^{-3})^{W+1})\right]\ . \tag{3.7}$$

We explicitly examined the numerical behavior of the various coefficients in (3.7) for $\rho=1$, 2, 3, and 4. The upper limit on the expansion was taken to be of the order $W=45$. It was ascertained that the lowest-order corrections behave as follows:

For $\rho=1$ *and 3*,

$$R(\rho;w;a_f)=\frac{2}{\sqrt{E}}\delta_{\rho,3}\delta_{w,1}+\begin{cases}a_f R^{(1)}(\rho;w) & \text{if } w=\text{even}\,,\\ a_f{}^2R^{(2)}(\rho;w) & \text{if } w=\text{odd}\,.\end{cases} \tag{3.8}$$

For $\rho=2$ *and 4*,

$$R(\rho;w;a_f)=[R(\rho;w)\neq 0]+a_f{}^2R^{(2)}(\rho;w),\quad w=\text{even}\,, \tag{3.9a}$$

$$R(\rho;w;a_f)=a_fR^{(1)}(\rho;w),\quad \text{if } w=\text{odd}\,. \tag{3.9b}$$

Inserting each of the above expansions into (3.7) we obtain the following:

For $\rho=1$ *and 3*,

$$\frac{\mu_r(\rho)}{\mu_r(0)}=a^\rho\left[a^{-3}\left[\frac{2}{\sqrt{E}}\delta_{\rho,3}\right]+a_f\left[\sum_{w=\text{even}}a^{-3w}R^{(1)}(\rho;w)\right]+a_f{}^2\left[\sum_{w=\text{odd}}a^{-3w}R^{(2)}(\rho;w)\right]\right]\,. \tag{3.10}$$

For $\rho=2$ *and 4*,

$$\frac{\mu_r(\rho)}{\mu_r(0)}=a^\rho\left[\sum_{w=\text{even}}a^{-3w}[R(\rho;w)+a_f{}^2R^{(2)}(\rho;w)]+a_f\sum_{w=\text{odd}}a^{-3w}R^{(1)}(\rho;w)\right]\,. \tag{3.11}$$

It will be recognized that the generic form for all of the series expressions appearing in (3.10) and (3.11) take on the form (after setting $a_f=a$) $a^q\sum_w^W a^{-3w}S(w)$, where q is some integer. It is clear that because q is not generally a multiple of 3 we cannot use Padé approximants for such expressions; however, we may do so for the cubed expression

$$a^{3q}\left[\sum_{w=0}^{W}a^{-3w}[S(w)]\right]^3=a^{3q}\left[\sum_{w=0}^{W}a^{-3w}S_3(w)+O((a^{-3})^{W+1})\right] \tag{3.12}$$

$$=a^{3q}\left\{\frac{\sum_{\eta=0}^{T}a^{-3\eta}N(\eta)}{\sum_{\delta=0}^{B}a^{-3\delta}D(\delta)}+O((a^{-3})^{W+1})\right\}\,. \tag{3.13}$$

We require that both $T+B=w$ and $q+B-T=0$. We then take $N(T)/D(B)$ as an estimate of the continuum limit for the cube of the original series. Because the $S(w)$ may be small, it is best to numerically normalize the original series by working with $S(w^*)a^q\sum_w^W a^{-3w}\times[S(w)/S(w^*)]$, where w^* is of the order of $W/2$. This is the basic technique used in estimating all of the various series expressions appearing in (3.10) and (3.11).

It is important to note that although the use of Padé analysis can be very effective, there are some potential pitfalls. In particular, the series expression in (3.11) corresponding to $a^\rho\sum_{w=\text{even}}a^{-3w}R(\rho;w)$ can be ignored, despite the fact that according to (3.9a) each of the coefficients is nonzero. The simple reason for this is that this series really corresponds to the ratio of two series of the form

$$a^\rho\frac{((a^{-3})^0)\hat{C}_r(\rho;0;0)}{\hat{C}_r(0;0;0)+a^{-3}\hat{C}_r(0;1;0)+\cdots}\,, \tag{3.14}$$

in accordance with the remarks made in the context of (3.5). If we assume that the denominator expression in (3.14) represents some finite value [being the expansion for the 0th-order moment of (3.3)] then the constant nature of the numerator requires that the subsequent multiplication by $a^{\rho=2,4}$ yield zero in the continuum limit. Thus the proper way to Padé approximate the cited series in (3.11) is to require that the relation for the Padé degrees in (3.13) satisfy $q+B-T=q(\neq 0)$. Clearly, the above may also be true for some of the other series expressions in (3.10) and (3.11). From our numerical experiments this seems particularly true for the $w=$even series in (3.10); we should also ignore it because its Padé approximant (according to $q+B-T=0$), although numerically stable, leads to inconsistencies with certain relative moment relations to be derived.

In the tables we give the various Padé-generated sequences corresponding to the various $R^{(1)}$ and $R^{(2)}$ series in (3.10) and (3.11). The results correspond to taking $W\leq 45$, and $L_0=10^4$ [i.e., $E=\frac{1}{4}(a_fL_0)^2$]. That is, we numerically estimated $R^{(1)}$, for instance, by taking $R(\rho;w;a_f)/a_f$, for the appropriate ρ and w values, and a_f sufficiently small. Note, numerical error propagation may be of concern in our scheme, so a_f cannot be too small.

In general one proceeds to determine the total moments from the relative moments in accordance with the appropriate counterpart to (3.1). This relation deserves further explanation. Note that we have emphasized its validity for p = even only. The reason for this is that because of the double support structure for $\psi^{(w)}(L;a_f)$, as explained in the context of (2.8), the more complete lattice expression for all the moments, even and odd, becomes

$$\mu(p)=a^{1+p}\sum_L L^p \sum_w a^{-3w}\psi^{(w)}(L;a_f) \tag{3.15}$$

$$=a^{1+p}\left[\sum_\rho B\binom{p}{\rho}(-a_fL_0)^{p-\rho}\sum_{\tilde{L}}\tilde{L}^\rho\psi^{(w)}(-L_0+\tilde{L};a_f)+\sum_\rho B\binom{p}{\rho}(a_fL_0)^{p-\rho}\sum_{\tilde{L}}\tilde{L}^\rho\psi^{(w)}(L_0+\tilde{L};a_f)\right]. \tag{3.16}$$

Because of the implicit assumption that $\psi^{(w)}(-L;a_f)=\psi^{(w)}(L;a_f)$, we have that $\psi^{(w)}(-L_0-\tilde{L};a_f)=\psi^{(w)}(L_0+\tilde{L};a_f)$. Because of this (3.16) becomes $\mu(p=\text{odd})=0$ and $\mu(p=\text{even})=$Eq. (3.1). We have noted in the context of the discussion pertaining to (3.1) that for every $[1+(p=\text{even})/2]$ even-order moments, $p+1$ relative moments must be determined. Clearly this specific situation implies a nonuniqueness between specifying the total moments and determining a set of relative moments that satisfy (3.1). The specific lattice model chosen, and the subsequent Padé analysis, serve to choose a specific set of relative moments satisfying (3.1). Nonetheless, we can find a continuum model whose moments correspond to the relative moments (modulo a factor of 2) satisfying (3.1) also. This latter set of relative moments *do not* correspond to the relative-moment solutions provided by the specific lattice model (2.2) and its subsequent Padé analysis.

For purposes of comparison, we discuss the simple continuum model mentioned above. Simply translate the harmonic oscillator by x_τ. Denote the new solution (translated) by $\Upsilon(x)=\psi(x_\tau+x)$. Clearly, for both even and odd p

$$\mu(p)=\int dx(x_\tau+x)^p\Upsilon(x) \tag{3.17}$$

$$=\sum_\rho B\binom{p}{\rho}(x_\tau)^{p-\rho}\int dx\, x^\rho\Upsilon(x)\ . \tag{3.18}$$

For p = even, the expressions $\tilde{\mu}(p)=\frac{1}{2}\int dx\, x^p\Upsilon(x)$ are a solution to (3.1). Note that while $\mu(p=\text{odd})=0$, as determined by (3.16), and also the relative-moment solutions to (3.1) are not required to have any additional special properties, we find that the $\tilde{\mu}(\rho)$ do have the additional property of satisfying

$$\mu(p=\text{odd})=0=\sum_\rho B\binom{p}{\rho}(x_\tau)^{p-\rho}\tilde{\mu}(\rho)\ . \tag{3.19}$$

We can say even more about $\tilde{\mu}$'s. Because $\Upsilon(x)$ satisfies

$$\Upsilon''+(E-\tfrac{1}{4}(x+x_\tau)^2)\Upsilon=0\ , \tag{3.20}$$

the moments $\tilde{\mu}(\rho)$ obey a recursive relation of the form

$$\tfrac{1}{4}\tilde{\mu}(p+2)=p(p-1)\tilde{\mu}(p-2)-\sqrt{E}\,\tilde{\mu}(p+1)\ . \tag{3.21}$$

We also know from (3.19) that for $p=1$

$$\tilde{\mu}(1)=-x_\tau\tilde{\mu}(0)\ . \tag{3.22}$$

In addition, from (3.18) $\mu(0)=\tilde{\mu}(0)\neq 0$. Because of this and (3.22), clearly $\tilde{\mu}(1)/\tilde{\mu}(0)=-2\sqrt{E}$. This is very different from the relative-moment solutions provided by the lattice model (2.2) and the subsequent Padé analysis; although these do yield a reasonable set of relative-moment solutions to (3.1), as we shall now see.

The lattice model (2.2) and subsequent Padé analysis yield the results quoted in the tables. Notice that neither of the entries in Table I, corresponding to the results for $\mu_r(1)/\mu_r(0)$, are of a negative nature; nor of the magnitude of the solution $\tilde{\mu}(1)/\tilde{\mu}(0)$, quoted above. In order to assess the extent of agreement between (2.2) and the known moments, (1.2), we explicitly rewrite things in normalized form:

$$\mu(0)=2\mu_r(0)\ , \tag{3.23}$$

TABLE I. Padé results for even and odd series expansion for $\mu_r(\rho=1)/\mu_r(0)$ of Eq. (3.10), $E=4.5$, $L_0=9999$.

(w = even)	(w = odd)
8.672×10^{-2}	1.275×10^{-2}
8.235×10^{-2}	1.602×10^{-2}
8.147×10^{-2}	1.578×10^{-2}
7.893×10^{-2}	1.600×10^{-2}
7.961×10^{-2}	1.534×10^{-2}
7.583×10^{-2}	1.521×10^{-2}
7.901×10^{-2}	1.522×10^{-2}
6.346×10^{-2}	1.521×10^{-2}
7.877×10^{-2}	1.574×10^{-2}
7.648×10^{-2}	1.520×10^{-2}

TABLE II. Padé results for even and odd series expansion for $\mu_r(\rho=2)/\mu_r(0)$ of Eq. (3.11), $E=4.5$, $L_0=9999$.

(w = even)	(w = odd)
5.234×10^{-3}	-1.082×10^{-1}
-6.548×10^{-3}	-1.359×10^{-1}
7.342×10^{-3}	-1.339×10^{-1}
-7.495×10^{-3}	-1.358×10^{-1}
6.385×10^{-3}	-1.302×10^{-1}
-5.807×10^{-3}	-1.307×10^{-1}
3.404×10^{-3}	-1.305×10^{-1}
-3.268×10^{-3}	-1.306×10^{-1}
-3.005×10^{-3}	-1.307×10^{-1}
-6.634×10^{-3}	-1.304×10^{-1}

TABLE III. Padé results for even and odd series expansion for $\mu_r(\rho=3)/\mu_r(0)$ of Eq. (3.10), $E=4.5$, $L_0=9999$.

(w =even)	(w =odd)
3.033×10^{-2}	-9.547×10^{-2}
1.714×10^{-2}	-8.640×10^{-2}
1.361×10^{-2}	-8.691×10^{-2}
1.739×10^{-2}	-8.332×10^{-2}
8.339×10^{-2}	-7.690×10^{-2}
8.266×10^{-2}	-8.745×10^{-2}
8.346×10^{-2}	-8.223×10^{-2}
8.457×10^{-2}	1.497×10^{-1}
8.450×10^{-2}	-8.650×10^{-1}
8.564×10^{-2}	

TABLE IV. Padé results for even and odd series expansion for $\mu_r(\rho=4)/\mu_r(0)$ of Eq. (3.11), $E=4.5$, $L_0=9999$.

(w =even)	(w =odd)
2.409×10^{-1}	7.958×10^{-1}
2.588×10^{-1}	7.254×10^{-1}
2.597×10^{-1}	7.299×10^{-1}
2.484×10^{-1}	7.146×10^{-1}
2.598×10^{-1}	6.914×10^{-1}
2.724×10^{-1}	6.998×10^{-1}
2.599×10^{-1}	6.965×10^{-1}
1.410×10^{-1}	6.970×10^{-1}
3.032×10^{-1}	6.967×10^{-1}

$$\frac{\mu(2)}{2\mu_r(0)}=x_\tau^2+2x_\tau\hat{\mu}_r(1)+\hat{\mu}_r(2)\ , \qquad (3.24)$$

$$\frac{\mu(4)}{2\mu_r(0)}=x_\tau^4+4x_\tau^3\hat{\mu}_r(1)+6x_\tau^2\hat{\mu}_r(2)+4x_\tau\hat{\mu}_r(3)+\hat{\mu}_r(4)\ , \qquad (3.25)$$

$\hat{\mu}_r\equiv\mu_r()/\mu_r(0)$. From (1.2), the normalized moments corresponding to the left-hand side of (3.24) and (3.25) are, respectively, $x_\tau^2=4E$ and x_τ^4+8. From this it is clear that we require

$$2x_\tau\hat{\mu}_r(1)+\hat{\mu}_r(2)=0 \qquad (3.26)$$

and

$$4x_\tau^3\hat{\mu}_r(1)+6x_\tau^2\hat{\mu}_r(2)+4x_\tau\hat{\mu}_r(3)+\hat{\mu}_r(4)=8\ , \qquad (3.27a)$$

or

$$16E\hat{\mu}_r(2)+4x_\tau\hat{\mu}_r(3)+\hat{\mu}_r(4)=8\ . \qquad (3.27b)$$

We proceed to show the extent to which the data in the tables is consistent with the various relations (3.26) and (3.27). Looking at (3.26) we note that for some inexplicable reason the even-column entries in Tables I and V are inconsistent with (3.26) if we take into account the data in Tables II and VI, respectively. As an example, if we take the typical limit of Table I to be $\mu_r(1)=0.0152$ (odd-column Table I); and $\mu_r(2)=-0.130$ (ignoring the erratic nature of the even column in Table II, due to possible error propagation) we have $4\sqrt{4.5}(0.0152)+(-0.130)=0.1289-0.130$. This is in reasonable agreement with (3.26). The corresponding analysis for $E=10.5$ is $4\sqrt{10.5}(0.0041)+(-0.056)=0.053-0.056$. This is also in reasonable agreement with (3.26); furthermore, the last entry in Table VI's odd column is indicative of even better agreement.

Using the odd column of Table II (VI), and the even and odd columns of Tables III and IV (VII and VIII) the result of verifying (3.27b) for $E=4.5(10.5)$ is

$$16\times4.5(-0.130)+8\sqrt{4.5}(0.9428-0.082+0.0085)+(0.7+0.26)=6.35\ , \qquad (3.28)$$

$$16\times10.5(-0.056)+8\sqrt{10.5}(0.6172-0.0183+0.0031)+(0.225+0.048)=6.47\ . \qquad (3.29)$$

Although the above fall short of the theoretical answer 8, this may be due to the fact that the expansions in question [(3.10) and (3.11)] are only analyzed to lowest order. Of course numerical accuracy may be a significant factor. Despite the above, bearing in mind the known values for the moments on the left-hand side of (3.24) and (3.25), the above results yield reasonably accurate values for the moments in question. This is particularly true for (3.24), in light of the very good agreement with relation (3.26).

TABLE V. Padé results for even and odd series expansion for $\mu_r(\rho=1)/\mu_r(0)$ of Eq. (3.10), $E=10.5$, $L_0=9999$.

(w =even)	(w =odd)
4.280×10^{-2}	3.579×10^{-3}
4.064×10^{-2}	4.493×10^{-3}
4.021×10^{-2}	4.428×10^{-3}
3.896×10^{-2}	4.491×10^{-3}
3.929×10^{-2}	4.318×10^{-3}
3.868×10^{-2}	4.320×10^{-3}
3.903×10^{-2}	4.177×10^{-3}
3.897×10^{-2}	4.286×10^{-3}
3.903×10^{-2}	4.104×10^{-3}
3.878×10^{-2}	4.097×10^{-3}

TABLE VI. Padé results for even and odd series expansion for $\mu_r(\rho=2)/\mu_r(0)$ of Eq. (3.11), $E=10.5$, $L_0=9999$.

(w =even)	(w =odd)
1.281×10^{-3}	-4.638×10^{-2}
-1.601×10^{-3}	-5.824×10^{-2}
1.791×10^{-3}	-5.740×10^{-2}
-1.822×10^{-3}	-5.820×10^{-2}
1.557×10^{-3}	-5.580×10^{-2}
-1.454×10^{-3}	-5.600×10^{-2}
-1.012×10^{-3}	-5.594×10^{-2}
-2.036×10^{-3}	-5.599×10^{-2}
-1.911×10^{-3}	-5.594×10^{-2}
-2.075×10^{-3}	-5.347×10^{-2}

TABLE VII. Padé results for even and odd series expansion for $\mu_r(\rho=3)/\mu_r(0)$ of Eq. (3.10), $E=10.5$, $L_0=9999$.

(w = even)	(w = odd)
1.129×10^{-2}	-2.064×10^{-2}
6.380×10^{-3}	-1.851×10^{-2}
5.065×10^{-3}	-1.862×10^{-2}
6.462×10^{-3}	-1.836×10^{-2}
3.151×10^{-3}	-1.834×10^{-2}
2.928×10^{-3}	-1.837×10^{-2}
3.490×10^{-3}	-1.526×10^{-2}
3.054×10^{-3}	-1.858×10^{-2}
3.253×10^{-3}	-1.820×10^{-2}
3.382×10^{-3}	

TABLE VIII. Padé results for even and odd series expansion for $\mu_r(\rho=4)/\mu_r(0)$ of Eq. (3.11), $E=10.5$, $L_0=9999$.

(w = even)	(w = odd)
4.424×10^{-2}	2.571×10^{-1}
4.756×10^{-2}	2.344×10^{-1}
4.777×10^{-2}	2.358×10^{-1}
4.750×10^{-2}	2.309×10^{-1}
4.814×10^{-2}	2.234×10^{-1}
4.809×10^{-2}	2.260×10^{-1}
4.790×10^{-2}	2.249×10^{-1}
4.792×10^{-2}	2.255×10^{-1}
4.702×10^{-2}	2.252×10^{-1}

IV. POLYA-PADÉ RECONSTRUCTION

The general problem of reconstructing a function from its moments is a difficult one in which attention to possible questions of nonuniqueness should be paid.[5] Although much is known for the reconstruction of functions which define nondecreasing Stieltjes measures,[10] such may not be the general situation, as in the harmonic-oscillator problem. In a recent work[6] we have formulated an intuitively appealing reconstruction program which appears adequate for an approximate reconstruction of multiple-turning-point problems, particularly within domains centered about the various turning points. We present a succinct description of the basic formalism, and refer the reader to the cited reference for more details.

Assuming the quantized energy E is known[8,9] and a sufficient number of moments are also known, the Fourier transform of the wave function becomes

$$\tilde{\psi}(k)=\frac{1}{\sqrt{2\pi}}\int dx\, e^{-ikx}\psi(x) \tag{4.1}$$

$$=\frac{1}{\sqrt{2\pi}}\sum_{p=0}^{P}\frac{(-ik)^p}{p!}\mu(p)+O(k^{P+1})\,. \tag{4.2}$$

For definiteness, we will outline the Polya-Padé program for the two-turning-point-problem harmonic oscillator. We want to define a "Polya-Padé" representation as given below:

$$\tilde{\psi}(k)=\frac{1}{\sqrt{2\pi}}\sum_{p=0}^{P}\frac{(-ik)^p}{p!}\mu(p) \tag{4.3}$$

$$=\frac{1}{\sqrt{2\pi}}\left[\exp(-ikx_\tau^{(+)})\sum_d\left[\frac{R_d^{(+)}}{-ik-P_d^{(+)}}\right]+\exp(-ikx_\tau^{(-)})\left[\sum_d\frac{R_d^{(-)}}{-ik-P_d^{(-)}}\right]\right]\quad(x_\tau^{(\pm)}\equiv\pm x_\tau)\,. \tag{4.4}$$

It should be noted that the summations in (4.4) correspond to the partial-fraction decomposition of a corresponding Padé approximant of numerator and denominator degrees T and B, respectively. We symbolize this by

$$\sum_d\frac{R_d^{\pm}}{-ik-P_d^{\pm}}=\{T;B;-ik\}\,. \tag{4.5}$$

The importance of this fact will be stressed shortly.

The motivation for attempting to define such a representation as (4.4) stems from the simple nature of its inverse Fourier-transform expression, which takes on the form of a discrete generalized Laplace representation about each of the respective turning points:

$$\psi_{\text{approx}}(x)=\left\{\begin{matrix}-\Sigma_d^{(+)}R_d^{(+)}\exp(-\Delta^{(+)}P_d^{(+)})\\ \text{if }\Delta^{(+)}>0\\ \Sigma_d^{(-)}R_d^{(+)}\exp(-\Delta^{(+)}P_d^{(+)})\\ \text{if }\Delta^{(+)}<0\end{matrix}\right\}+\left\{\begin{matrix}-\Sigma_d^{(+)}R_d^{(-)}\exp(-\Delta^{(-)}P_d^{(-)})\\ \text{if }\Delta^{(-)}>0\\ \Sigma_d^{(-)}R_d^{(-)}\exp(-\Delta^{(-)}P_d^{(-)})\\ \text{if }\Delta^{(-)}<0\end{matrix}\right\}, \tag{4.6}$$

$\Sigma^{(\pm)}\equiv$summation over those terms for which $\mathrm{Re}(P_d)\gtrless 0$, $\Delta^{(\pm)}\equiv x-x_\tau^{(\pm)}$.

It is proven in the cited work on Polya-Padé approximants[6] that the choice of degrees B and T in (4.5) determine the maximum order of continuous derivatives for (4.6), including at the turning points. Specifically, if $B-T=2+N$, then

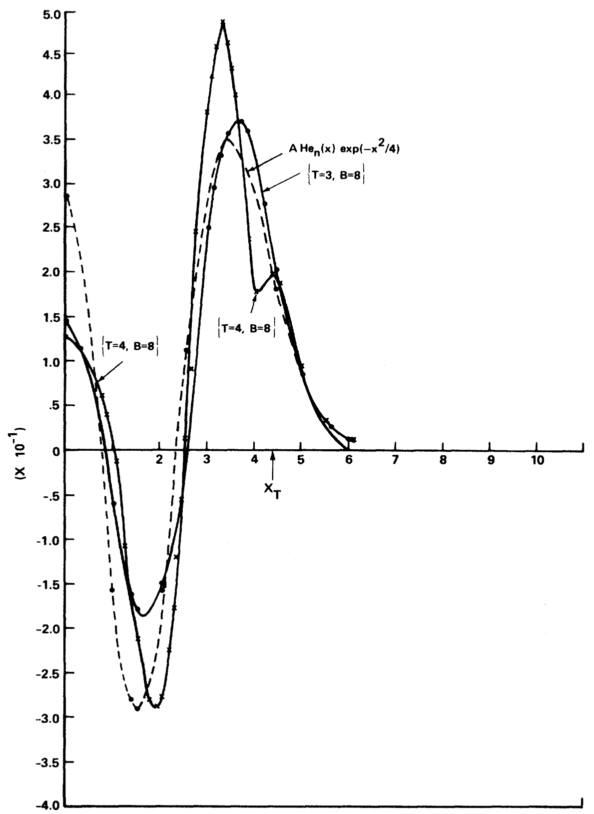

FIG. 1. Comparison of actual solution $A_n \mathrm{He}_n(x) \times \exp(-x^2/4)$, $n=4$, and Polya-Padé approximants $\{T=3, B=8\}$ and $\{T=4, B=8\}$. $A_4=(6\sqrt{\pi})^{-1}$.

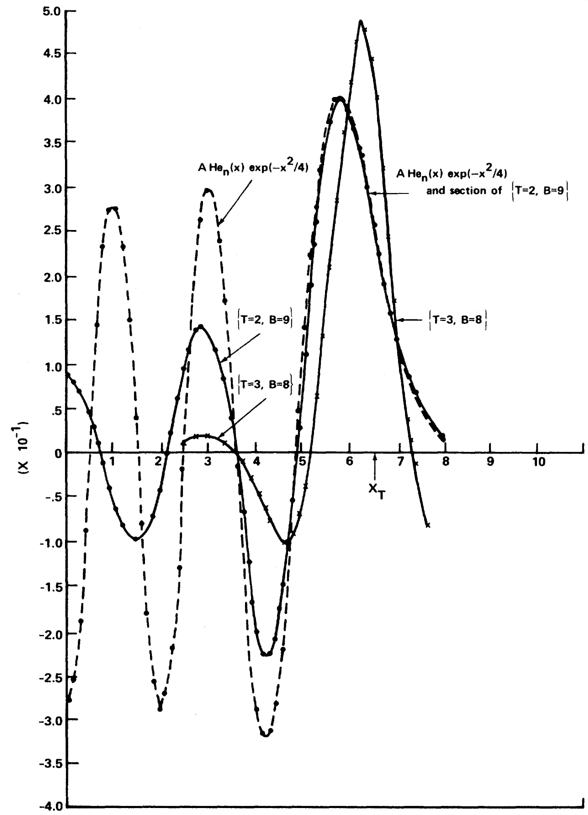

FIG. 2. Comparison of actual solution $A_n \mathrm{He}_n(x) \times \exp(-x^2/4)$, $n=10$, and Polya-Padé approximants $\{T=3, B=8\}$ and $\{T=2, B=9\}$. $A_{10}=(1890\sqrt{\pi})^{-1}$.

(4.6) has continuous derivatives up to order N. Accordingly, as N increases, one expects the Polya-Padé approximants to better determine the wave-function solution, $\psi(x)$, since the exact solution is known to be infinitely differentiable. This is corroborated by the appended plots. (See Figs. 1 and 2.)

The basic procedure for determining (4.5) is as follows. We use Borel transform theory[11] to express the Fourier transform according to the integral expression

$$\sqrt{2\pi}\,\tilde{\psi}(k)=\sum_p \frac{\mu(p)}{p!}(-ik)^p \rightarrow \frac{1}{2\pi i}\oint \frac{\exp(-iks)}{s}\left[\sum_{p=0} \frac{\mu(p)}{s^p}\right] . \tag{4.7}$$

The integrand expression is rewritten in terms of the Padé approximant

$$\sum_{p=0} \frac{\mu(p)}{s^p}=\{M;M+1;s^{-1}\} \tag{4.8a}$$

$$=s\sum_d \frac{A_d}{s-B_d} . \tag{4.8b}$$

Taking the loop integral (4.7) around all poles of (4.8b), one obtains the formal representation

$$\tilde{\psi}(k)=(2\pi)^{-1/2}\sum_d A_d \exp(-ikB_d) . \tag{4.9}$$

One is then able to decompose the B_d poles into two sets, each of which corresponds to a group of poles clustered around the respective turning point. Denoting each of these groups by $B_d^{(\pm)}$ we further decompose (4.9) according to

$$\tilde{\psi}(k)=(2\pi)^{-1/2}\{\exp(-ikx_\tau^{(+)})[\Sigma_d^{+} A_d^{(+)}\exp(-ik(B_d-x_\tau^{(+)}))]+\exp(-ikx_\tau^{(-)})[\Sigma_d^{-} A_d^{(-)}\exp(-ik(B_d^{(-)}-x_\tau^{(-)}))]\} . \tag{4.10}$$

Comparing (4.10) with (4.4) and (4.5) it is clear that the series expressions in (4.10) are expanded in k and subsequently Padé analyzed.

We have commented on the significance of the appended data and the above formalism, already. In closing, we state the observation that the extent of the variation of the poles, $B_d^{(\pm)}$, about the respective turning points seems to correspond to the extent of the domain, centered about $x_\tau^{\pm}$, for which satisfactory agreement between the actual solution and (4.6) is noted.[6] The curves correspond to the implementation of a Polya-Padé ansatz based on the actual moments for the harmonic oscillator. The wave functions are normalized by $\mu(0)=1$, so

$$A_n=\frac{2^{(n/2-1)}(n/2)!}{n!\sqrt{\pi}} ,$$

$n=$even.

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