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Choosing Step Sizes for Perturbative Methods of Solving the Schrödinger Equation

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General rules are here developed for choosing step sizes consistent with preset accuracy for the solution of the one-dimensional Schrödinger equation. These rules are then particularized for the case of perturbative methods lying upon piecewise constant reference potential and verified experimentally for two cases. To help the reader, the algorithms of the basic versions of these methods are summarized in the Appendix.

1. INTRODUCTION

The problem of choosing step sizes for perturbative methods in solving the radial Schrödinger equation has been investigated in several papers, e.g., [1, 2]. However, the basic arguments of these procedures are rather empirical and do not lead always to fully reliable rules; see also [3]. Therefore a more systematic treatment appears to be necessary and this is done in the present paper.

2. CONSTRUCTION OF ERROR BOUNDS

Our problem is to find a partition of $[a, b]$ so that the *local* truncation error of the numerical solution for the Schrödinger equation

$$y'' + (E - V(x))\, y = 0, \qquad x \in [a, b], \qquad y(a) = y_a\,, \qquad y'(a) = y'_a\,, \quad (2.1)$$

to be maintained under some preset level ϵ for any energy E within the range of interest $[E_{\min}\,, E_{\max}]$. The rules which will be obtained can also be applied to find partitions consistent with some preset level for the accumulated error, as seen at the end of this section.

We restrict ourselves here only to perturbative methods. It is well known that they yield, at coarse partitions, results which are fully satisfactory in describing numerous physical phenomena. This is equivalent to saying that, for many physical problems, these methods do not need small steps. In this case an accurate estimation of the local truncation error requires *several* terms in its expansion to be taken, in contradistinction to the case of small step sizes, when the leading term only is usually sufficient.

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A second area of concern is the energy dependence of the error. Indeed, if we write Eq. (2.1) in some current interval $[x_i, x_{i+1} = x_i + h]$, $\delta \equiv x - x_i$, $0 \leqslant \delta \leqslant h$, as

$$y'' + (E - \bar{V} - \Delta V)y = 0, \qquad \Delta V = \mathscr{V} - \bar{V}, \tag{2.2}$$

where $\bar{V}$ is the reference potential of the employed perturbative method, one sees that the accuracy of the results actually depends on the size of the relative perturbation

$$\sigma(E) = |\Delta V|/|\mathscr{V} - E|. \tag{2.3}$$

Consequently, the largest error should arise when the current value of the energy E approaches the potential curve, i.e.,

$$E \simeq E_t \equiv \int_0^h d\delta\, \mathscr{V}(x_i + \delta)/h. \tag{2.4}$$

This is the basic assumption of the so-called artificial turning point procedure examined in [4].

This argument is, however, not sufficient. In fact, it guarantees that the largest error arises at $E \simeq E_t$ but this is true only for some averaged quantities such as the function

$$P(E) = \left(\int_0^h d\delta\, D^2(E, \delta)\right) \Big/ \int_0^h d\delta\, y^2(x_i + \delta), \tag{2.5}$$

where $D(E, \delta)$ is the deviation of the numerical solution from the exact one,

$$D(E, \delta) = y(x_i + \delta) - y^{\text{comput}}(x_i + \delta).$$

It might not be true for individual quantities such as the relative error at certain $\delta = \delta_c$,

$$R(E) = |D(E, \delta_c)|/|y(x_i + \delta_c)|. \tag{2.6}$$

The following two-stage strategy then emerges to find formulas for the local error associated with a perturbative method:

(i) use the turning point energy E_t and take *several* terms to describe the actual error at $\delta = h$;

(ii) examine the energy dependence of the error at $\delta = h$.

These individual pieces of information are finally merged into a single descriptor which is then used to evaluate the appropriate step size.

In the following we apply this strategy to the three versions, CPM(k), $k = 0, 1, 2$, of the perturbative methods with constant reference potential. Their algorithms are summarized in the Appendix.

First, we need to construct accurate representation for the exact solution of Eq. (2.2). To this aim we take as many terms as necessary in the perturbation expansion for the

transfer matrix elements at $E = E_t$. With the notations used in the Appendix, $E = E_t$ means $F = 0$.

The terms given below are sufficient for this purpose. These are:

A. Terms from the parabolic perturbation (A6). The first three of these are already written in the Appendix and can be specified at once for $F = 0$ simply by taking the leading terms in the series expansion for the auxiliary functions ξ, η, ζ, ρ, φ, τ. One finds, for instance,

$$u^0 = 1, \quad u^1 = -\frac{h^3}{12}(V_1 + hV_2), \quad u^2 = -\frac{h^6}{6!}\left(\frac{1}{2}V_1^2 + \frac{5}{7}V_1V_2h + \frac{11}{42}V_2^2h^2\right),$$

etc. We also add the third-order corrections. Their calculation is rather simple and the results read:

$$u^3 = \frac{h^9}{9!}\left(V_1^3 + \frac{17}{5}V_1^2V_2h + \frac{607}{165}V_1V_2^2h^2 + \frac{71}{55}V_2^3h^3\right), \tag{2.7a}$$

$$v^3 = \frac{h^{11}}{10!}\left(\frac{2}{3}V_1^2V_2 + \frac{4}{33}V_1V_2^2h + \frac{874}{1289}V_2^3h^2\right), \tag{2.7b}$$

$$u^{3'} = \frac{h^9}{9!}\left(8V_1^2V_2 + 16V_1V_2^2h + \frac{64}{1289}V_2^3h^2\right), \tag{2.7c}$$

$$v^{3'} = -\frac{h^9}{9!}\left(V_1^3 + \frac{13}{5}V_1^2V_2h + \frac{343}{165}V_1V_2^2h^2 + \frac{7}{15}V_2^2h^3\right). \tag{2.7d}$$

B. Terms from the residual perturbation (A5). Here we only retain the first-order corrections. One finds that, for $F = 0$, all of them are zero.

C. Mixed terms from the perturbations (A5) and (A6). From these we retain only the lowest-order terms resulting from the first member in the r.h.s. of Eq. (A5) and the whole perturbation (A6). They read:

$$u^C = \frac{h^8}{7!}\gamma_3\left(\frac{1}{20}V_1 + \frac{1}{18}V_2h - \frac{1}{5\cdot 6!}\gamma_3h^2\right), \tag{2.8a}$$

$$v^C = \frac{h^9}{90\cdot 7!}\gamma_3\left(V_1 + V_2h + \frac{1}{11\cdot 5!}\gamma_3h^2\right), \tag{2.8b}$$

$$u^C = \frac{h^7}{7!}\gamma_3\left(\frac{1}{10}V_1 + \frac{1}{10}V_2h - \frac{1}{15\cdot 5!}\gamma_3h^2\right), \tag{2.8c}$$

$$v^{C'} = \frac{h^8}{7!}\gamma_3\left(\frac{1}{20}V_1 + \frac{2}{45}V_2h - \frac{1}{5\cdot 6!}\gamma_3h^2\right). \tag{2.8d}$$

The expressions

$$T_{ij} = t_{ij}^0 + t_{ij}^1 + t_{ij}^2 + t_{ij}^3 + t_{ij}^C, \qquad i,j = 1,2, \tag{2.9}$$

contain sufficient terms so that T_{ij} can be thought of as a fairly accurate representation of the elements of the exact transfer matrix, Eq. (A7). To compress the writing, the following notations have been used: $t_{11} = u$, $t_{12} = v$, $t_{21} = u'$, $t_{22} = v'$.

When a CPM(k), $k = 0, 1, 2$, is applied it produces results whose relative local error reads:

$$\epsilon_{ij} = \left| t_{ij} - \sum_{m=0}^{k} t_{ij}^{m} \right| / | t_{ij} |$$

$$\simeq \left| t_{ij}^{C} + \sum_{m=k+1}^{3} t_{ij}^{m} \right| / | T_{ij} |, \qquad \text{for} \quad i = 1, j = 1, 2, \text{ and } i = j = 2. \tag{2.10a}$$

The case $i = 2, j = 1$ plays a special role because $t_{21}^{0} = t_{21}^{1} = 0$. As such, for this case, the only appropriate error will be the absolute one,

$$\epsilon_{21} = \left| t_{21}^{C} + \sum_{m=k+1}^{3} t_{21}^{m} \right|. \tag{2.10b}$$

We now come to the second stage. Clearly, only the terms which vanish at $F = 0$ might be suspected of exhibiting the disturbing factor F in their expressions. These are t_{21}^{0}, t_{21}^{1}, the coefficients of V_1^3 in t_{12}^{3} and t_{21}^{3}, and the terms under B. The first two are

$$t_{21}^{0} = F\eta, \qquad t_{21}^{1} = -\tfrac{1}{4} V_2 F\rho,$$

the next two are exactly zero for $F \neq 0$, while the terms under B read

$$t_{11}^{B} = \frac{1}{80}\left(\mathscr{V}_3 + \frac{h}{2}\mathscr{V}_4\right) F\varphi, \quad t_{12}^{B} = -\frac{1}{112}\mathscr{V}_4 F\tau, \quad t_{21}^{B} = -F t_{12}^{B}, \quad t_{22}^{B} = -t_{11}^{B}. \tag{2.11}$$

The ratios $| t_{ij}^{B} | / | t_{ij} | \simeq | t_{ij}^{B} | / | t_{ij}^{0} | \equiv \mathscr{E}_{ij}$ provide us with the energy dependent components of the error (EDCE):

$$\mathscr{E}_{11} = \mathscr{E}_{22} = \frac{1}{80}\left|\mathscr{V}_3 + \frac{h}{2}\mathscr{V}_4\right| \cdot | F | \cdot | \varphi | / | \xi | \simeq \frac{1}{5 \times 7!}\left|\mathscr{V}_3 + \frac{h}{2}\mathscr{V}_4\right| \cdot | F | h^7, \tag{2.12a}$$

$$\mathscr{E}_{12} = \mathscr{E}_{21} = \frac{1}{112} | \mathscr{V}_4 | \cdot | F | \cdot | \tau | / | \eta | \simeq \frac{4}{35 \cdot 9!} | \mathscr{V}_4 | \cdot | F | h^8. \tag{2.12b}$$

The estimates given in the RHS of Eqs. (2.12a), (2.12b) are obtained from the series expansions of the functions ξ, η, φ, and τ in which only the leading term has been retained. Thus, they are valid only in the limit of small $| Z | = | F | h^2$. In the case when $| F |$ is very large asymptotic expansions for φ and τ should be used. As these are

$$\varphi(F, h) \simeq -h^3\xi(F, h)/(3F^2), \qquad \tau(F, h) \simeq h^4\eta(F, h)/(30F^2),$$

the result is that

$$\mathscr{E}_{11} = \mathscr{E}_{22} = \frac{h^3}{240 \mid F \mid} \left| \mathscr{V}_3 + \frac{h}{2} \mathscr{V}_4 \right|, \tag{2.12c}$$

$$\mathscr{E}_{12} = \mathscr{E}_{21} = \frac{h^4}{3360 \mid F \mid} \mid \mathscr{V}_4 \mid. \tag{2.12d}$$

The formulas (2.12a)–(2.12d) show that the EDCEs are *bounded* functions of $\mid F \mid$. They actually indicate that for small $\mid F \mid$ each $\mathscr{E}_{ij}$ increases linearly with $\mid F \mid$, reaches some maximum, and finally, for large $\mid F \mid$, damps out as $\mid F \mid^{-1}$. This allows one to understand several experimental features reported in the literature. For instance, in papers [5–9] it was noted that the results given by the CPM(0) and CPM(1) are practically independent of energy. We can now explain this as coming from the fact that both the energy range $[E_{\min}, E_{\max}]$ and the step sizes used in these investigations correspond to small $\mid Z \mid$. Consequently, the EDCEs are given by Eqs. (2.12a), (2.12b). Thus, they decrease with h as h^p, $p \geqslant 7$, i.e., much faster than the leading term of the local error for these methods. In fact, the latter decreases as h^3 for the CPM(0) and as h^5 for the CPM(1). In contrast, for the CPM(2), as seen in the results reported in [4, 10], the EDCEs might play some role. One can now say even more, namely, that they are significant only in the intervals where $\mathscr{V}_3$ and $\mathscr{V}_4$ are large.

Another experimental feature which we can now understand quantitatively is that the perturbative methods are by far more appropriate in solving the Schrödinger equation at higher energies. This comes from the fact that, as explained, the EDCEs are bounded functions for the perturbative methods while they are strict increasing functions of $\mid F \mid$ for classical methods. In the case of the Numerov method, for instance, the local error is proportional to $\mid F \mid^3 h^6/240$ (see formula (3.2) in Ref. [11]), i.e., it is *cubic* in $\mid F \mid$.

As shown, there are six individual relevant errors, ϵ_{11}, ϵ_{12}, ϵ_{21}, ϵ_{22}, $\mathscr{E}_{11}$, and $\mathscr{E}_{12}$. An appropriate unique descriptor of these is their maximum value,

$$\lambda(h) = \sup\{\epsilon_{11}, \epsilon_{12}, \epsilon_{21}, \epsilon_{22}, \mathscr{E}_{11}, \mathscr{E}_{12}\}. \tag{2.13}$$

Thus, to find the step size consistent with a preset level ϵ for the local error, one has to solve the equation $\lambda(h) = \epsilon$. Once the root h is found the procedure is repeated in the next interval, i.e., that which originates in $x_{i+1} = x_i + h$, and so on.

If n is the total number of steps of the resultant partition it is reasonable to assume that the product $n\epsilon$ gives a realistic bound for the accumulated error. However, in so doing, the accumulated error plays the role of an output quantity rather than of an input parameter, as required in most applications.

To solve the inverse problem, i.e., how to get ϵ when the upper bound for the accumulated error, TOLV, is imposed, we use a preliminary computation. To be specific, once the method and the integration limits are chosen, we carry out a preliminary computation which generates the partition consistent with some input ϵ_0 for the local error. (We have always taken $\epsilon_0 = 1$.) Let n_0 be the resultant number of

intervals. As the local error for CPM(k) reads $(C_k)_i^{2k+3}\, h_i^{2k+3}$, then, with the assumption that it just equals ϵ_0,

$$\epsilon_0 = (C_k)_i^{2k+3}\, h_i^{2k+3}, \tag{2.14}$$

one can determine an average $\tilde{C}_k$,

$$\tilde{C}_k = n_0 \epsilon_0^{1/(2k+3)} \sum_{i=1}^{n_0} \frac{1}{h_i}. \tag{2.15}$$

$\tilde{C}_k$ is practically independent of ϵ. Therefore, once $\tilde{C}_k$ is found from the preliminary computation, it is used in the current calculation (i.e., with TOLV as input parameter). The link between TOLV and ϵ is

$$\text{TOLV} = (b - a)\, \tilde{C}_k \epsilon^{2(k+1)/(2k+3)}. \tag{2.16}$$

3. Numerical Results

We take the two examples which were also investigated in [9]:

(a) Saxon–Woods potential

$$\mathscr{V}(x) = u_0/(1 + t) + u_1 t/(1 + t)^2, \qquad t = \exp[(x - x_0)/a_0], \tag{3.1}$$

with $u_0 = -50$, $x_0 = 7$, $a_0 = 0.6$, $u_1 = -u_0/a_0$. The integration domain is [$a = 0$, $b = 15$] and the energy domain is [$E_{\min} = -50$, $E_{\max} = 0$];

(b) Morse potential

$$\mathscr{V}(x) = Dt(t - 2), \qquad t = \exp[a_0(x_0 - x)], \tag{3.2}$$

with $D = 188.3455$, $a_0 = 0.711248$, $x_0 = 1.9975$. The two domains are [$a = 0$, $b = 20$] and [$E_{\min} = -180$, $E_{\max} = 0$].

The factors $\tilde{C}_k$ are determined in a preliminary computation. They are $\tilde{C}_0 = 0.75$, $\tilde{C}_1 = 0.8$, $\tilde{C}_2 = 0.45$ for potential (a) and $\tilde{C}_0 = 2.5$, $\tilde{C}_1 = 3.7$, and $\tilde{C}_2 = 1.4$ for potential (b).

In a first set of tests we compare, for several test energies within the energy domain, the relative deviations at $x = b$ of the computed solutions from the exact ones, at various values of the input TOLV, for the same initial conditions $y_a = 0$, $y_a' = 1$. The test energies were $E_i = E_{\min} + 5i$, where $i = 0, 1, 2, \ldots, 20$ for (a) and $i = 0, 1, 2, \ldots, 36$ for (b). The solutions computed with the CPM(2) at TOLV $= 10^{-6}$ (potential (a)) and TOLV $= 10^{-4}$ (potential (b)) are taken as reference.

In Table I, results are given in upper entries for the quantities

$$\Delta = \sup_i \{|\, y^{\text{comput}}(E_i\,;b) - y^{\text{ref}}(E_i\,;b)|/|\, y^{\text{ref}}(E_i\,;b)|, \\ |\, y^{\text{comput}'}(E_i\,;b) - y^{\text{ref}'}(E_i\,;b)|/|\, y^{\text{ref}'}(E_i\,;b)|\}/\text{TOLV}, \tag{3.3}$$

TABLE I

Values of Accumulated Error/Preset Accumulated Error, Eq. (3.3), for the Two Potentials

	Preset TOLV					
	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
Saxon–Woods						
CPM(0)	0.05	0.06	0.05			
	(21)[a]	(64)	(203)			
CPM(1)	0.03	0.05	0.08	0.13	0.14	
	(14)	(24)	(39)	(67)	(115)	
CPM(2)	0.05	0.09	0.11	0.09	0.06	0.03
	(8)	(11)	(15)	(22)	(32)	(46)
Morse						
CPM(0)	0.25	0.25				
	(105)	(333)				
CPM(1)	0.10	0.11	0.12			
	(57)	(101)	(178)			
CPM(2)	0.08	0.11	0.07	0.07		
	(21)	(28)	(39)	(55)		

[a] The number of steps of the corresponding partitions is indicated in parentheses.

i.e., the ratio between the maximum value of the experimental accumulated error and the preset level TOLV; the lower entries indicate the total number of steps of the resultant partition. The computations were stopped when the partition became so narrow that it would be no longer relevant for our purpose.

One sees that, while unity would be the ideal value for each Δ, the experimental values are smaller by an order of magnitude. This can easily be understood because the local error reaches its maximum at different energies in different intervals. Thus, when the equation is solved over the entire integration domain for one and the same energy, there are only a few intervals in which the local error approaches its upper bound while it is much smaller in all the others; in turn, this leads to smaller values for the accumulated error. With this point in mind one can conclude that our procedure is safe.

The same partitions can also be used to solve the eigenvalue problem. In this case the appropriate descriptor for the accumulated error in the wavefunctions is the upper value, in the whole spectrum, of the absolute error in eigenvalues,

$$\Delta E = \sup_i | E_i^{\text{ref}} - E_i^{\text{comput}} | \tag{3.4}$$

(i now stands for the eigenvalue label). This was our second set of tests and the results are presented in Table II. These data are useful in drawing some conclusions concerning the efficiency of these methods. For instance, only 22 steps are necessary for

TABLE II

The Upper Values of the Absolute Errors of the Eigenvalues Computed for the Two Potentials by the Three CPM Versions

	Preset TOLV					
	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
Saxon–Woods (units TOLV $\times 10^{-2}$)						
CPM(0)	3.4	2.4	2.0			
CPM(1)	2.0	3.1	4.3	5.0	5.4	
CPM(2)	3.1	3.3	6.9	8.9	4.8	4.0
Morse (units TOLV $\times 10^{-1}$)						
CPM(0)	1.4	1.4				
CPM(1)	0.3	0.3	0.4			
CPM(2)	0.2	0.4	0.4	0.2		

CPM(2) in the case of the Saxon–Woods potential to obtain all eigenvalues with absolute error of at most 8.9×10^{-5}. For the same accuracy the method of Numerov requires $h < 1/32$, i.e., more than 480 steps (see Table VI in Ref. [9]).

APPENDIX

ALGORITHMS OF THE PERTURBATIVE METHODS BASED ON CONSTANT REFERENCE POTENTIAL

These algorithms were reported previously in several papers [4–10] and with different notations. Here we summarize them in a consistent notation.

To solve the one-dimensional Schrödinger equation

$$y'' + (E - \mathscr{V}(x_i + \delta))\, y = 0, \qquad y(0) = y_0\,, \qquad y'(0) = y_0'\,, \tag{A1}$$

on a single interval $0 \leqslant \delta \leqslant h$, $\delta = x - x_i$, we first approximate $\mathscr{V}$ by a parabola,

$$\tilde{\mathscr{V}}(x_i + \delta) = \bar{V} + V_1\left(\delta - \frac{h}{2}\right) + V_2\left(\delta^2 - \frac{h^2}{3}\right), \tag{A2}$$

so that we are left with the approximate equation

$$\tilde{y}'' + (E - \tilde{\mathscr{V}}(x_i + \delta))\, \tilde{y} = 0, \qquad \tilde{y}(0) = y_0\,, \qquad \tilde{y}'(0) = y_0'\,. \tag{A3}$$

The optimal values of $\bar{V}$, V_1, and V_2, i.e., the ones which generate the smallest deviation of the solution of Eq. (A3) from the one of the original equation, (A1), are given by

$$\bar{V} = \frac{1}{288}[19(V^1 + V^6) + 75(V^2 + V^5) + 50(V^3 + V^4)], \tag{A4a}$$

$$V_1 = \frac{1}{336h}[950V^4 + 1250V^3 - (611V^1 + 1025V^2 + 175V^5 + 389V^6)], \tag{A4b}$$

$$V_2 = \frac{25}{84h^2}[5(V^1 + V^6) + 6(V^2 + V^5) - 11(V^3 + V^4)], \tag{A4c}$$

where $V^m = (x_i + (m-1)h/5)$, $m = 1, 2, \ldots, 6$. The deviation of the parabolic potential from the original one reads

$$\Delta\tilde{V} = \frac{\mathscr{V}_3}{120}h^3[20(\delta/h)^3 - 30(\delta/h)^2 + 12\delta/h - 1] + \frac{\mathscr{V}_4}{840}h^4[35(\delta/h)^4 - 60(\delta/h)^2 + 32\delta/h - 3] + \mathcal{O}(h^5), \tag{A5}$$

where $\mathscr{V}_m \equiv d^m\mathscr{V}(x_i + \delta)/d\delta^m|_{\delta=0}$. The exact solutions at $\delta = h$ of Eqs. (A1) and (A3) coincide within $\mathcal{O}(h^7)$.

To summarize, the original $\mathscr{V}$ is written as a sum of three terms,

$$\mathscr{V}(x_i + \delta) = \bar{V} + \Delta V + \Delta\tilde{V}.$$

The most important of them is, of course, the constant $\bar{V}$. It is taken as the reference potential. The next important term is ΔV,

$$\Delta V = V_1\left(\delta - \frac{h}{2}\right) + V_2\left(\delta^2 - \frac{h^2}{3}\right) \tag{A6}$$

and it is considered as the main perturbation. The last term, $\Delta\tilde{V}$, plays the role of a residual perturbation. The solution of Eq. (A1) then reads

$$\begin{pmatrix} y(h) \\ y'(h) \end{pmatrix} = \begin{pmatrix} u(h) & v(h) \\ u'(h) & v'(h) \end{pmatrix}\begin{pmatrix} y(0) \\ y'(0) \end{pmatrix}, \tag{A7}$$

where each element of the transfer matrix is written as perturbation series from $\Delta V + \Delta\tilde{V}$. For instance,

$$u(h) = u^0(h) + u^1(h) + u^2(h) + \cdots, \tag{A8}$$

The algorithms described in [4–10] consider only the parabolic perturbation ΔV. The algorithms of the constant reference potential perturbative methods (CPM) are labeled through the last order retained from the parabolic perturbation. Only CPM(k)

with $k = 0, 1$, and 2 have been reported so far. Their truncation errors are $\mathcal{O}(h^3)$, $\mathcal{O}(h^5)$, and $\mathcal{O}(h^{7\sim9})$, respectively. The expressions of the first three individual contributions are

$$u^0(h) = \xi, \qquad u^1(h) = -\frac{1}{4}(V_1 + V_2 h)\zeta,$$
$$u^2(h) = \frac{1}{32} V_1^2 h\rho - \frac{1}{16} V_1 V_2(2\varphi - h^2\rho) - \frac{1}{480} V_2^2 h(57\varphi - 16h^2\rho), \tag{A9a}$$

$$v^0(h) = \eta, \qquad v^1(h) = \frac{1}{4} V_2\rho,$$
$$v^2(h) = \frac{1}{32} V_1^2\varphi + \frac{1}{16} V_1 V_2 h\varphi + \frac{1}{32} V_2^2\left(6\tau + \frac{16}{15} h^2\varphi\right), \tag{A9b}$$

$$u^{0'}(h) = F\eta, \qquad u^{1'}(h) = -\frac{1}{4} V_2 F\rho,$$
$$u^{2'}(h) = \frac{1}{32} V_1^2\left(7\rho - \frac{1}{3} h^2\zeta\right) + \frac{1}{16} V_1 V_2 h\left(7\rho - \frac{1}{3} h^2\zeta\right)$$
$$+ V_2^2\left[-\frac{1}{12}(3\varphi - 5h^2\rho) + \frac{1}{32} F\left(6\tau + \frac{16}{15} h^2\varphi\right)\right], \tag{A9c}$$

$$v^{0'}(h) = \xi, \qquad v^{1'}(h) = \frac{1}{4}(V_1 + V_2 h)\zeta,$$
$$v^{2'}(h) = \frac{1}{32} V_1^2 h\rho + \frac{1}{16} V_1 V_2(2\varphi + h^2\rho) + \frac{1}{480} V_2^2 h(63\varphi + 16h^2\rho). \tag{A9d}$$

Here $F \equiv \overline{V} - E$ and ξ, η, ζ, ρ, φ, and τ are the values at $\delta = h$ of the following functions:

$$\xi(F, \delta) = (\exp(F^{1/2}\delta) + \exp(-F^{1/2}\delta))/2 = \cos(|F|^{1/2}\delta) \quad \text{for} \quad F \leqslant 0,$$
$$= \cosh(F^{1/2}\delta) \quad \text{for} \quad F > 0; \tag{A10a}$$

$$\eta(F, \delta) = (\exp(F^{1/2}\delta) - \exp(-F^{1/2}\delta))/(2F^{1/2}) = \sin(|F|^{1/2}\delta)/|F|^{1/2} \quad \text{for} \quad F < 0,$$
$$= \delta \quad \text{for} \quad F = 0,$$
$$= \sinh(F^{1/2}\delta)/F^{1/2} \quad \text{for} \quad F > 0; \tag{A10b}$$

$$\zeta(F, \delta) = (\delta\xi(F, \delta) - \eta(F, \delta))/F; \tag{A10c}$$

$$\rho(F, \delta) = (-\delta^2\eta(F, \delta)/3 + \zeta(F, \delta))/F; \tag{A10d}$$

$$\varphi(F, \delta) = -(5\rho(F, \delta) + \delta^2\zeta(F, \delta)/3)/F; \tag{A10e}$$

$$\tau(F, \delta) = (7\varphi(F, \delta) - \delta^2\rho(F, \delta))/(10F). \tag{A10f}$$

Their series expansions in powers of $Z = F\delta^2$ read

$$\xi(F, \delta) = \sum_{q=0}^{\infty} \frac{1}{(2q)!} Z^q, \tag{A11a}$$

$$\eta(F, \delta) = \delta \sum_{q=0}^{\infty} \frac{1}{(2q+1)!} Z^q, \tag{A11b}$$

$$\zeta(F, \delta) = 2\delta^3 \sum_{q=0}^{\infty} \frac{(q+1)}{(2q+3)!} Z^q, \tag{A11c}$$

$$\rho(F, \delta) = -\frac{4}{3} \delta^5 \sum_{q=0}^{\infty} \frac{(q+1)(q+2)}{(2q+5)!} Z^q, \tag{A11d}$$

$$\varphi(F, \delta) = -\frac{8}{3} \delta^7 \sum_{q=0}^{\infty} \frac{(q+1)(q+2)(q+3)}{(2q+7)!} Z^q, \tag{A11e}$$

$$\tau(F, \delta) = \frac{8}{15} \delta^9 \sum_{q=0}^{\infty} \frac{(q+1)(q+2)(q+3)(q+4)}{(2q+9)!} Z^q. \tag{A11f}$$

In practical computations for $|Z| > Z_{\text{threshold}}$ definitions (A10) should be used, while for $|Z| \leqslant Z_{\text{threshold}}$ series expansions (A11) should be used. For IBM 360 or 370 computers $Z_{\text{threshold}}$ is taken as unity for single-precision calculations and as 0.06 for double-precision calculations. In both cases the number of terms retained in the series is seven for ξ; six for η; five for ζ, ρ, and φ; and four for τ. The computational effort/step for the three versions (CPU time on an IBM 370/135) is around 1.7, 2.3, and 4.2 msec, respectively, for single-precision calculations and 2.3, 3.1, and 5.2 msec, respectively, for double precision calculations. Clearly, this is several times larger than for the method of Numerov (around 0.5 msec for single precision). However, as a rule, this is compensated by the number of steps required for the same accuracy which is significantly smaller for perturbative methods; see Tables I and II as well as the discussion at the end of Section 3.

Note also some relationships between the auxiliary functions. These are useful for various operations with the computed solutions.

Differentiation with respect to δ:

$$\frac{\partial \xi}{\partial \delta} = F\eta, \quad \frac{\partial \eta}{\partial \delta} = \xi, \quad \frac{\partial \zeta}{\partial \delta} = \delta\eta, \quad \frac{\partial \rho}{\partial \delta} = -\frac{1}{3}\delta\zeta, \quad \frac{\partial \varphi}{\partial \delta} = \delta\rho, \quad \frac{\partial \tau}{\partial \delta} = -\frac{1}{10}\delta\varphi. \tag{A12}$$

Differentiation with respect to F:

$$\frac{\partial^{k+1}\xi}{\partial F^{k+1}} = \frac{\delta}{2} \frac{\partial^k \eta}{\partial F^k} \tag{A13a}$$

and

$$\frac{\partial \eta}{\partial F} = \frac{1}{2}\zeta, \quad \frac{\partial^2 \eta}{\partial F^2} = -\frac{3}{4}\rho, \quad \frac{\partial^3 \eta}{\partial F^3} = -\frac{3}{8}\varphi, \quad \frac{\partial^4 \eta}{\partial F^4} = \frac{15}{8}\tau. \tag{A13b}$$

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