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Minimal sensitivity optimisation of perturbative wavefunctions

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Abstract. Stevenson's principle of minimal sensitivity is applied directly to configuration space wavefunctions calculated in first-order perturbation theory. The redundant parameters, which comprise the essential elements of minimal sensitivity calculations, actually become functions of configuration space, giving the method considerable flexibility and potential accuracy. It is shown that the method is exact in an illustrative class of simple cases, and, for the more realistic case of the ground state wavefunction of the quartic oscillator, it is considerably more accurate than the closely related perturbative variational approach, particularly in the asymptotic region.

1. Introduction

Stevenson's principle of minimal sensitivity (PMS) (Stevenson 1981) provides a powerful instrument for optimising and extending the useful domain of approximation methods, particularly perturbation theory. It asserts that *if an approximation depends on parameters of which the true result is known to be independent, then, in the absence of further information, that approximation is optimised by choosing those parameters so as to minimise the approximation's sensitivity to small variations in their values.* The optimised approximation is thus the one which most closely mimics the true result's independence of redundant parameters.

The insertion of such redundant parameters into a given problem can often be accomplished in a natural and straightforward fashion. For example, if a quantum system is described by a Hamiltonian H, one constructs an approximating Hamiltonian $H_0(\{\lambda_i\})$, which is exactly diagonalisable for all values of the parameters in the set $\{\lambda_i\}$. One can then write

$$H = H_0(\{\lambda_i\}) + V(\{\lambda_i\}), \tag{1.1a}$$

where, of course,

$$V(\{\lambda_i\}) \equiv (H - H_0(\{\lambda_i\})), \tag{1.1b}$$

and then proceed to calculate an approximation to any physical quantity of interest by applying orthodox perturbation methods to the form (1.1a). Such a perturbative approximation will normally be dependent on the parameters in the set $\{\lambda_i\}$, though it is clear from (1.1) that the true result is independent of them. Thus we may invoke PMS to choose the *optimum* values of the parameters in the set $\{\lambda_i\}$ *for that particular approximation.* In general, PMS can be expected to select *different* values of these redundant parameters for perturbative approximations to *different* physical quantities—

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indeed we can expect it to choose different values of the redundant parameters for different *orders* of perturbative approximation to the *same* physical quantity. It is precisely this element of adaptability which gives PMS its often surprising power and accuracy. Given an *indication* of the correct answer by the basic approximation method (e.g., perturbation theory), PMS locates the *optimum* redundant parameter values for the *approximation at hand.* Of course, the firmer is the indication of the correct answer—e.g., the more closely $H_0(\{\lambda_i\})$ is capable of approximating H—the better one can expect the PMS optimised result to be. Thus PMS allows much scope for future development of the art of good approximations. The technically redundant parameters of the set $\{\lambda_i\}$ are, paradoxically, at their most useful when they are most nearly 'meaningful', i.e., when they can be chosen so that $H_0(\{\lambda_i\})$ is a *good* approximation to H—at least for the problem at hand.

Stevenson (1981) has not given a proof of PMS, indeed he considers it to be not really susceptible to proof, although it embraces well known special cases, such as the first-order perturbative version of the Rayleigh–Ritz variational principle for quantum ground states, which *are* susceptible to proof. PMS rests on its clear-cut intuitive appeal, bolstered by a growing array of successful applications and theorems for special cases (Stevenson 1981, Caswell 1979). Although not sanctified by a general theorem, the status of PMS is, as Stevenson points out, no more nebulous than that of unoptimised perturbation theory itself (Stevenson 1981).

Stevenson actually formulated PMS for application to the orthodox perturbative expansions of renormalisable quantum field theories, where the redundant parameters arise from the true results' independence of the renormalisation scheme utilised (Stevenson 1981). As the first to explicitly present a formal, general statement of PMS, Stevenson was, however, acutely aware of its wider implications, and gave as one example of these a PMS treatment of the energy level spectrum of the anharmonic oscillator along the general lines of equation (1.1) (Stevenson 1981). Caswell (1979) had earlier made a similar application of PMS to this same problem (although he did not explicitly state PMS in its general form), and both Caswell and Stevenson obtained the energy levels of the quartic oscillator to 1–2% accuracy already from PMS optimised *first*-order perturbation theory (Stevenson 1981, Caswell 1979) (ironically, the ground state energy, for which this first-order PMS calculation is just an orthodox application of the Rayleigh–Ritz variational principle, is the *least* accurately determined of these levels).

These successes of PMS in determining energy levels prompted the present investigation of its efficacy for determining the corresponding configuration space eigenfunctions. One possible approach to these wavefunctions, suggested by that conventionally used with the Rayleigh–Ritz variational principle optimisation of the approximate ground state energy, is to simply substitute the PMS *energy optimised* values of the redundant parameters into the corresponding approximated wavefunctions. Such 'variational wavefunctions' are, however, well known to normally have accuracies inferior to those of their corresponding approximated energy eigenvalue (Dicke and Wittke 1960). Moreover, this approach is not in keeping with strict PMS, which requires that the redundant parameters be determined from the approximation to that quantity which one *actually desires to calculate*, i.e., from approximated wavefunction *itself* in this instance.

Direct application of PMS to approximated configuration space eigenfunctions can be expected to lead, in general, to *different* values of the redundant parameters at *different* points of configuration space. Thus, strict adherence to PMS in this instance

leads to the somewhat unfamiliar circumstance of the redundant parameters becoming *functions* of configuration space. It is clear this has the potential to be a source of heightened calculational power, for the PMS wavefunctions are free to differ in *functional form* from the approximate wavefunctions which underlie them—a considerable enhancement in adaptability relative to the traditional 'variational wavefunctions'. These PMS wavefunctions are normalised to unity *a posteriori*.

In § 2 we apply PMS to calculating both the energy eigenvalues and the energy eigenfunctions of a test harmonic oscillator problem, treated in perturbation theory, where the redundant parameter is the square of an unknown oscillator frequency, i.e. in the language of equation (1.1),

$$H = \tfrac{1}{2}(p^2 + x^2) \tag{1.2a}$$

and

$$H_0(\lambda) = \tfrac{1}{2}(p^2 + \lambda x^2). \tag{1.2b}$$

We find that PMS applied to *first-order* perturbative approximations, whether of the energy eigenvalues or eigenfunctions, for this problem, always leads to $\lambda = 1$, i.e., the *exact answer*. A little thought reveals that this is not a fortuitous occurrence for the harmonic oscillator, but one example of a theorem covering a broad class of similar problems. We are able to show that if, for a Hamiltonian of the form

$$H = H' + \sum_{i=1}^{N} V_i, \tag{1.3a}$$

we write the approximating Hamiltonian

$$H_0(\{\lambda_i\}) = H' + \sum_{i=1}^{N} \lambda_i V_i, \tag{1.3b}$$

then PMS applied to first- (or higher-) order perturbation theory must yield $\lambda_i = 1$, $i = 1, 2, \ldots, N$, i.e., the exact result. This illustrates quite dramatically the 'benevolent paradox' (Stevenson 1981) of the ability of PMS to make perturbation theory into a non-perturbative technique. It also throws some heuristic light on the not infrequent occurrence that PMS yields excellent results already from first-order perturbation theory, with the accuracy improving only slowly as one goes to higher orders (Stevenson 1981).

In § 3 we apply PMS directly to the first-order perturbative calculation of the ground state wavefunction of the quartic oscillator, whose exact Hamiltonian is

$$H = \tfrac{1}{2}(p^2 + x^4), \tag{1.4a}$$

and for which we use an harmonic oscillator approximating Hamiltonian which is essentially the same as that of equation (1.2*b*),

$$H_0(\lambda) = \tfrac{1}{2}(p^2 + \lambda^2 x^2). \tag{1.4b}$$

Technical ambiguities in the PMS determination of λ as a function of x are resolved by the physical requirement that the resulting wavefunction be continuous and normalisable. This is in accord with Stevenson's admonition to make the maximum sensible use of available information when determining an approximation—a broad principle which simultaneously embraces and transcends PMS (Stevenson 1981).

The resulting PMS ground state wavefunction is compared with the exact (numerically computed) result as well as the corresponding variational ground state wavefunction and its first-order perturbative correction. The PMS wavefunction is superior to

these other closely related approximate wavefunctions, especially in the asymptotic region, where the latter have very large fractional errors. This improvement is important, for example, in determining the expectation values of high-order moments of x. Using the PMS wavefunction to compute the expectation value of the Hamiltonian yields a ground state energy approximation which is more than an order of magnitude more accurate than the already good values determined by the variational principle itself or its first perturbative correction.

2. Exact results from perturbative PMS in an illustrative class of cases

For the harmonic oscillator problem of equation (1.2) we readily calculate the energy eigenvalues in first-order perturbation theory (i.e., including both the zeroth- and first-order contributions),

$$E_n^{(0,1)}(\lambda) = (n+\tfrac{1}{2})\lambda^{1/2}[1+\tfrac{1}{2}(1-\lambda)\lambda^{-1}] = (n+\tfrac{1}{2})(\tfrac{1}{2})(\lambda^{1/2}+\lambda^{-1/2}), \qquad n=0,1,2,\ldots, \tag{2.1a}$$

as well as the ground state energy eigenfunction to first order,

$$\psi_{n=0}^{(0,1)}(x;\lambda) = (\lambda^{1/2}/\pi)^{1/4}\exp(-\tfrac{1}{2}\lambda^{1/2}x^2)[1+\tfrac{1}{8}(1-\lambda)\lambda^{-1}(1-2\lambda^{1/2}x^2)]. \tag{2.1b}$$

We now apply PMS by setting the derivative of these approximations with respect to λ (the redundant parameter) to zero (Stevenson 1981, Caswell 1979)

$$\partial E_n^{(0,1)}(\lambda)/\partial\lambda = -(n+\tfrac{1}{2})(\tfrac{1}{4})(1-\lambda)\lambda^{-3/2} = 0 \tag{2.2a}$$

and

$$\partial\psi_0^{(0,1)}(x;\lambda)/\partial\lambda = -(\lambda^{1/2}/\pi)^{1/4}\exp(-\tfrac{1}{2}\lambda^{1/2}x^2)(\tfrac{1}{8})(1-\lambda)\lambda^{-2}[1-(\tfrac{1}{8})(1+2\lambda^{1/2}x^2)^2] = 0. \tag{2.2b}$$

We see that equations (2.2) are all solved by $\lambda = 1$, which yields the *exact* results, when substituted into equations (2.1). Equation (2.2*b*) also has an extraneous x-dependent solution for λ, which is discarded, as it would render the approximate solution (2.1*b*) non-normalisable. We shall return to this matter of resolving ambiguities in PMS in the more realistic problem treated in § 3.

The above treatment can be readily extended to the complete set of energy eigenfunctions by calculating and utilising the generating function of these first-order perturbed eigenfunctions,

$$\begin{aligned} G^{(0,1)}(x;s;\lambda) &\equiv \sum_{n=0}^{\infty} s^n \psi_n^{(0,1)}(x;\lambda)(n!)^{-1/2} \\ &= (\lambda^{1/2}/\pi)^{1/4}\exp\{-\tfrac{1}{2}[\lambda^{1/2}x^2 + 2(2\lambda^{1/2})^{1/2}xs + s^2]\} \\ &\quad \times\{1+\tfrac{1}{8}(1-\lambda)\lambda^{-1}[1-2(2\lambda^{1/2})^{1/2}xs - 2\lambda^{1/2}x^2]\}. \end{aligned} \tag{2.3}$$

We readily find that the equation

$$\partial G^{(0,1)}(x;s;\lambda)/\partial\lambda = 0 \tag{2.4}$$

is again solved by $\lambda = 1$ (for all x and s).

Our laborious verification that PMS always yields exact results already from first-order perturbation theory for this test problem suggests the theorem that this is true as well for the whole class of similar problems defined by equation (1.3). Indeed, the kth-order contribution to the perturbative expansion of any physical quantity governed by the system (1.3) must consist of a sum of terms, each of which has a coefficient of the form

$$\prod_{i=i}^{N} (1-\lambda_i)^{n_i}, \tag{2.5a}$$

where each $n_i \geqslant 0$ and

$$\sum_{i=1}^{N} n_i = k. \tag{2.5b}$$

For $k \geqslant 2$, such coefficients are all *stationary* in the N-dimensional variable $(\lambda_1, \lambda_2, \ldots, \lambda_N)$ at the point $\lambda_1 = \lambda_2 = \ldots = \lambda_N = 1$. Thus, the second- and higher-order contributions to the perturbative expansion of any physical quantity governed by equation (1.3) must be stationary at the exact solution point $\lambda_1 = \lambda_2 = \ldots = \lambda_N = 1$. Since the exact solution is independent of $(\lambda_1, \lambda_2, \ldots, \lambda_N)$, and thus obviously stationary everywhere, it follows that the zeroth- plus first-order perturbative contribution (i.e., the perturbative approximation to first order), which is the exact result minus all the perturbative contributions of order greater than or equal to two, must also be stationary at the exact solution point $\lambda_1 = \lambda_2 = \ldots = \lambda_N = 1$. Thus we have that any perturbative approximation to first- or higher-order arising from the system (1.3) is stationary at the exact solution point $\lambda_1 = \lambda_2 = \ldots = \lambda_N = 1$.

We turn now to a more realistic application of PMS.

3. Application of perturbative PMS to the ground state of the quartic oscillator

For the perturbative quartic oscillator system of equation (1.4), the zeroth-order (harmonic oscillator) ground state energy eigenvalue and eigenfunction are

$$E_0^{(0)}(\lambda) = \tfrac{1}{2}\lambda \tag{3.1a}$$

and

$$\psi_0^{(0)}(x;\lambda) = (\lambda/\pi)^{1/4} \exp(-\tfrac{1}{2}\lambda x^2), \tag{3.1b}$$

and the corresponding first-order results are

$$E_0^{(0,1)}(\lambda) = \tfrac{1}{2}\lambda[1 + (\tfrac{3}{4}\lambda^{-3} - \tfrac{1}{2})] \tag{3.2a}$$

and

$$\psi_0^{(0,1)}(x;\lambda) = (\lambda/\pi)^{1/4} \exp(-\tfrac{1}{2}\lambda x^2)\{1 + \tfrac{1}{8}[2\lambda x^2 - 1 - \lambda^{-1}x^4 - 3\lambda^{-2}x^2 + 3(\tfrac{3}{4}\lambda^{-3})]\}. \tag{3.2b}$$

To apply PMS, we differentiate equations (3.2) with respect to λ to obtain

$$\partial E_0^{(0,1)}(\lambda)/\partial\lambda = -\tfrac{1}{4}\lambda^{-3}(3 - \lambda^3) \tag{3.3a}$$

and

$$\begin{aligned}\partial\psi_0^{(0,1)}(x;\lambda)/\partial\lambda &= -(128\lambda^4)^{-1}(\lambda/\pi)^{1/4} \exp(-\tfrac{1}{2}\lambda x^2)\{[2(2\lambda x^2)^2 + 4(2\lambda x^2) - 14](2\lambda^3) \\ &\quad - [(2\lambda x^2)^3 + 9(2\lambda x^2)^2 + 33(2\lambda x^2) - 99]\}.\end{aligned} \tag{3.3b}$$

From equation (3.3*a*), the vanishing of $\partial E_0^{(0,1)}(\lambda)/\partial\lambda$ implies that $\lambda = 3^{1/3}$, which, when substituted into equation (3.2*a*), yields the 'variational' ground state energy estimate of $\frac{3}{8}(3)^{1/3} = 0.540\,844\ldots$. This may be compared with the exact result, $0.530\,181\ldots$, which is about 2% smaller (Stevenson 1981). When $\lambda = 3^{1/3}$ is substituted into equation (3.1*b*), the result is the 'variational' ground state eigenfunction, and when it is substituted into equation (3.2*b*), the result is the first-order perturbatively corrected version of this wavefunction, which we subsequently normalise numerically. Plots, on both linear and log scales, of these approximate wavefunctions are given together with the exact (numerically computed) ground state wavefunction in figures 1–4. Both of these approximate wavefunctions are seen to suffer from very severe fractional errors for $|x| \gg 1$, and the perturbatively corrected version has, in addition, an unphysical change of sign in this region, although it is more accurate than the simple variational wavefunction for $|x| \leqslant 1$. These features are also reflected by the numbers given in table 1.

The procedure to obtain the PMS optimised ground state wavefunction $\psi_0^{(0,1)}(x,\lambda)$ is to set $\partial\psi_0^{(0,1)}/\partial\lambda = 0$ in (3.3*b*) and substitute the resulting value of $\lambda(x)$ into (3.2*b*). We select among the multiple roots λ by taking into account the conditions of continuity and normalisability of $\psi_0^{(0,1)}$. It turns out that the required $\lambda(x)$ is positive everywhere.

At $x = 0$, equation (3.3*b*) has only one real root, $\lambda = (99/28)^{1/3}$, which, not coincidentally, differs from the 'variational' $\lambda = (3)^{1/3}$ by less than 6%. The continuity criterion then allows the tracing of this root to $|x| \approx 0.72$, where it crosses with another 'unphysical' one which $\to\infty$ as $|x| \to 0$ and $\to 0$ as $|x| \to \infty$. We discuss the region

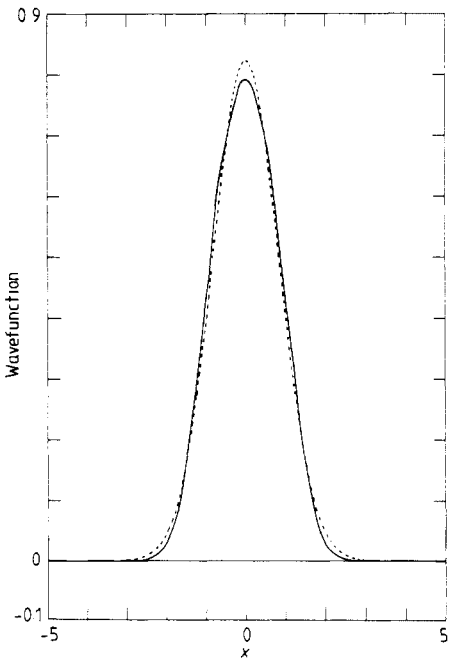

Figure 1. Variational ground state wavefunction approximation (broken curve) for the quartic oscillator against the exact solution (full curve) on a linear scale.

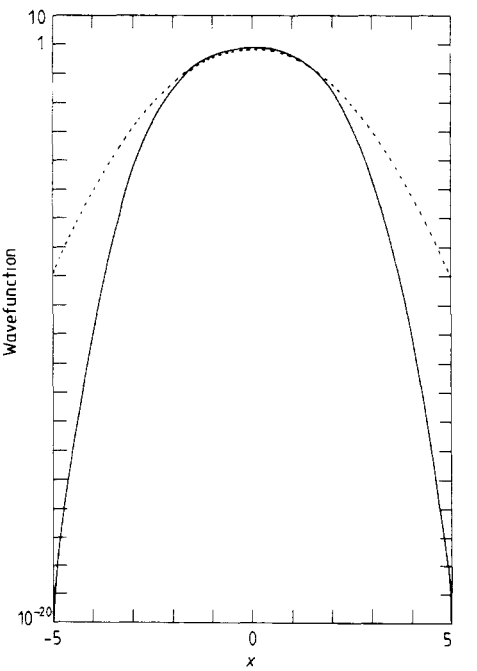

Figure 2. Variational approximation (broken curve) against exact ground state wavefunction (full curve) for the quartic oscillator on a log scale.

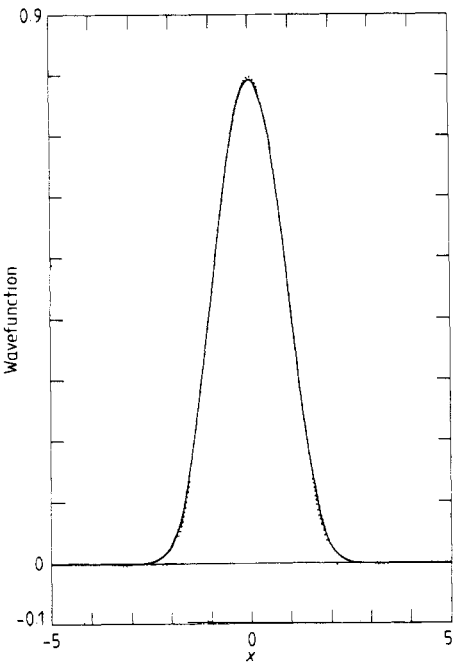

Figure 3. Perturbatively corrected variational approximation (broken curve) against exact ground state wavefunction (full curve) for the quartic oscillator on a linear scale.

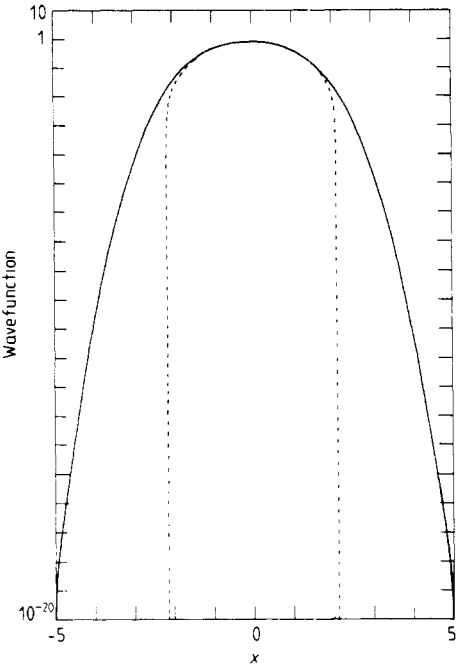

Figure 4. Perturbatively corrected variational approximation (broken curve) against exact ground state wavefunction (full curve) for the quartic oscillator on a log scale.

Table 1. Quartic oscillator ground state wavefunction.

$\lvert x\rvert$	Exact solution	Variational approximation	Perturbatively corrected variational approximation	$\lambda(x)$	$((\lvert x\rvert/\sqrt{2})^3+3)^{1/3}$	PMS approximation
0	0.793	0.823	0.796	1.52	1.44	0.795
0.5	0.691	0.687	0.692	1.52	1.45	0.692
1.0	0.427	0.400	0.425	1.50	1.50	0.425
1.5	0.159	0.162	0.152	1.60	1.61	0.156
2.0	2.84×10^{-2}	4.60×10^{-2}	1.39×10^{-2}	1.78	1.80	2.73×10^{-2}
2.5	1.90×10^{-3}	9.08×10^{-3}	-1.17×10^{-2}	2.02	2.04	1.74×10^{-3}
3.0	3.72×10^{-5}	1.25×10^{-3}	-5.53×10^{-3}	2.31	2.32	3.05×10^{-5}
3.5	1.65×10^{-7}	1.20×10^{-4}	-1.18×10^{-3}	2.61	2.63	1.11×10^{-7}
4.0	1.29×10^{-10}	8.03×10^{-6}	-1.47×10^{-4}	2.94	2.95	6.40×10^{-11}
4.5	1.38×10^{-14}	3.75×10^{-7}	-1.16×10^{-5}	3.27	3.28	4.44×10^{-15}
5.0	1.57×10^{-19}	1.22×10^{-8}	-5.93×10^{-7}	3.60	3.61	2.83×10^{-20}

$0.72\leqslant|x|\leqslant0.85$ in more detail below. From (3.2*b*) and the normalisability criterion, we must have $\lambda x^2\to+\infty$ as $|x|\to\infty$, so that (3.3*b*) fixes the asymptotic behaviour of the required root to be $\lambda\sim|x|/\sqrt{2}$. The continuity criterion then allows the tracing of this root back to $|x|\approx0.85$ where it again crosses with the 'unphysical' root. This procedure thus determines the required root for $0\leqslant|x|\leqslant0.72$ and $|x|\geqslant0.85$.

In the region $0.72 \leqslant |x| \leqslant 0.85$ there is no real root which satisfies the continuity requirements at the limits of the interval. Here we achieve continuity and satisfy PMS by requiring that $|\partial\psi/\partial\lambda|$ *be locally minimised.*

One can very crudely summarise the behaviour of the resulting $\lambda(x)$, for all x, by the approximate formula,

$$\lambda(x) \approx ((|x|/\sqrt{2})^3 + 3)^{1/3}. \tag{3.4}$$

Indeed, equation (3.4) differs from the actual $\lambda(x)$ by no more than 10%, and much less than this for most x, as is indicated in figure 5 and table 1. Inserting the actual $\lambda(x)$ into equation (3.2*b*) and normalising, we arrive at the PMS ground state wavefunction approximation, which we plot together with the exact wavefunction on both linear and log scales in figures 6 and 7, with some representative corresponding numbers also given in table 1. In figure 6 the PMS and exact ground state wavefunctions are almost indistinguishable, while the log scale in figure 7 shows the PMS wavefunction to be decreasing marginally too rapidly for $|x| \gg 1$, the asymptotic region of extremely small amplitude, where the PMS result is nevertheless vastly more accurate than the closely related variational and perturbatively corrected variational results shown in figures 2 and 4 and in table 1. We note, in passing, that the rapid, if small, variations in $\lambda(x)$ in the region $0.6 \leqslant |x| \leqslant 0.9$, as shown in figure 5, have no counterpart in the resulting PMS wavefunction, shown in figure 6. Indeed, in this region the PMS wavefunction is monotonic and virtually linear, and differs from the exact wavefunction by less than one half percent.

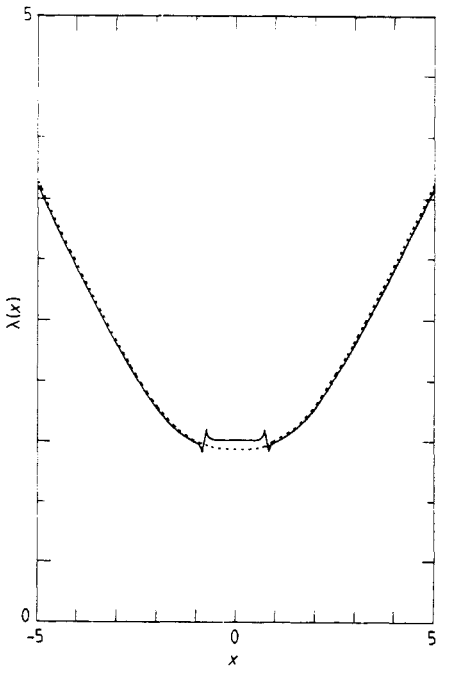

Figure 5. PMS $\lambda(x)$ (full curve) and its approximation $[(|x|/\sqrt{2})^3 + 3]^{1/3}$ (broken curve) for the quartic oscillator.

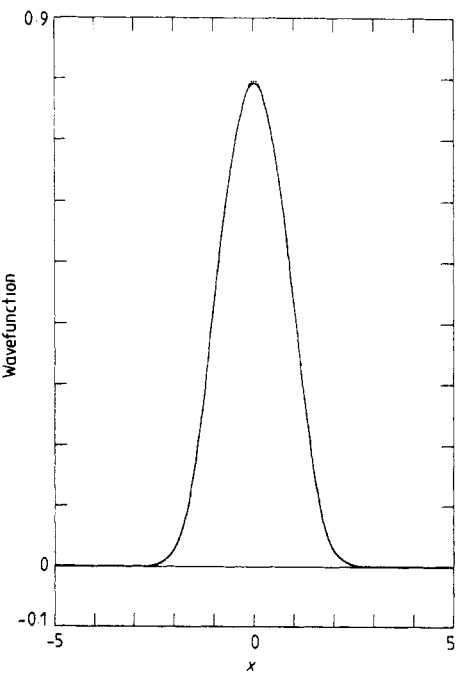

Figure 6. PMS approximation (broken curve) against exact ground state wavefunction (full curve) for the quartic oscillator on a linear scale.

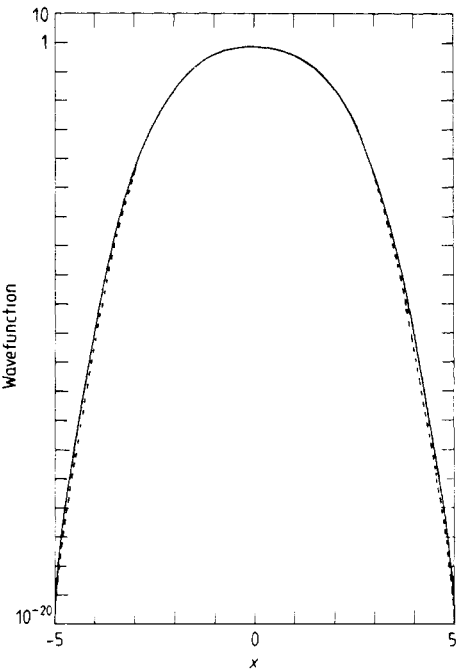

Figure 7. PMS approximation (broken curve) against exact ground state wavefunction (full curve) for the quartic oscillator on a log scale.

Finally, we note that the energy expectation value computed using the variational wavefunction is 0.5408 . . . , as noted previously, about 2% too high, and that computed using the perturbatively corrected variational wavefunction is 0.5371 . . . , about 1.3% too high, while that computed using the PMS wavefunction is 0.5307 . . . , only 0.1% too high. In this instance, PMS applied to the wavefunction gives a much more accurate energy result than does its direct application to the energy itself.

4. Conclusion

We believe that perturbative PMS applied directly to wavefunctions will prove to be an important technique. Also, the general approach of having the redundant PMS parameters become *functions* of some of the continuum variables describing a system may prove valuable in a variety of problems as a means of greatly enhancing the accuracy of traditional approximation methods. For example, statistical mechanics calculations might be tackled using PMS perturbation theory, with the redundant parameters becoming functions of macroscopic variables such as temperature.

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