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The Quadrature Discretization Method (QDM) in the solution of the Schrödinger equation

Heli Chen [a,*] and Bernie D. Shizgal [b,*]

[a] *Department of Mathematics, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z4*
[b] *Department of Chemistry, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1*

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The Quadrature Discretization Method (QDM) is employed in the solution of several one-dimensional Schrödinger equations that have received considerable attention in the literature. The QDM is based on the discretization of the wave function on a grid of points that coincide with the points of a quadrature. The quadrature is based on a set of non-classical polynomials orthogonal with respect to a weight function. For a certain class of problems with potentials of the form that occur in supersymmetric quantum mechanics, the ground state wavefunction is known. In the present paper, the weight functions that are used are related to the ground state wavefunctions if known, or some approximate form. The eigenvalues and eigenfunctions of four different potential functions discussed extensively in the literature are calculated and the results are compared with published values.

1. Introduction

The Quadrature Discretization Method (QDM) was originally developed for the solution of kinetic theory problems [7,47,49], the Fokker–Planck equation [38,51], and has been recently applied to the Schrödinger equation [48,50]. The details of the methodology were previously presented by Shizgal [47], Shizgal and Blackmore [49], Blackmore and Shizgal [7] and Shizgal and Chen [50]. The latter reference also discussed the relationship of the Fokker–Planck equation and the Schrödinger equation. It has also been recently applied to fluid dynamics problems [39,62,63]. The method involves the creation of polynomial basis sets [10,13,28,43] for each problem considered. The usual methods for basis set construction can lead to algorithms that are numerically unstable [11]. However, Gautschi [29] has developed a stable accurate method for the generation of orthonormal basis sets for arbitrary weight function referred to as the Stieltjes procedure.

[*] Also with the Institute of Applied Mathematics.

There have been numerous papers on the solution of the elementary one-dimensional Schrödinger equation,

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + V(y)\right]\psi(y) = E\psi(y), \tag{1}$$

with different methods and several choices for the potential function $V(y)$ [2–6,8,9, 12,14–27,30–37,40–42,44–46,52,53,55–61,64]. Some of the potentials studied include the Non-Polynomial Oscillator (NPO) potential of the form

$$V(y) = y^2 + \frac{\lambda y^2}{1 + gy^2}. \tag{2}$$

Mitra [41] employed Hermite polynomials as basis functions and reduced the Schrödinger equation to matrix form. Mitra obtained the eigenvalues and eigenfunctions by numerical diagonalization and reported numerical results for the first three eigenvalues. Kaushal [36] described a perturbative approach and compared with the previous numerical results. Bessis and Bessis [6] demonstrated that the matrix elements of the potential with Hermite basis functions can be done analytically and the numerical integrations by Mitra are unnecessary. Flessas [27] showed that for particular relationships between λ and g there are some exact results for the eigenvalues of this potential. For example, if $\lambda = -4g - 2g^2$, then $E_1 = 1 - 2g$ and, if $\lambda = -7g^2 - 6g \pm g\sqrt{25g^2 - 12g + 4}$, then $E_2 = (9g + \lambda)/g$. These results are useful for benchmarking different numerical methods. Hautot [33] reconsidered the calculation of the matrix elements of the Hamiltonian for this potential in the Hermite basis set. Lai and Lin [37] reported additional exact solutions not discovered by Flessas, and also introduced a Pade approximant analysis. Fack and Van den Berghe [18] employed several different finite difference schemes to solve for the eigenvalues and eigenfunctions for this problem. They employed a fine grid of points and diagonalized matrices of dimensions 200×200. They compared their results with available numerical results of previous workers, as well as for models with known exact results. Varshni [55] and Witwit [57,59] extended the earlier work to a three-dimensional version of this potential. Scherrer et al. [46] employed the continued fraction developed by Risken for the solution of the Fokker–Planck equation.

We have also considered the potential given by

$$V(y) = y^6 - 3y^2, \tag{3}$$

considered by Sinha et al. [53]. This potential belongs to the class of potentials that arise in supersymmetric quantum mechanics [12,14] and are the same class that results in the transformation of the Fokker–Planck equation to the Schrödinger equation [16, 17,42,44,45,50]. These authors consider a comparison of the SWKB results [12,14] and an exact calculation of the eigenvalues from a direct integration of the Schrödinger equation.

Kaluza [35] considered the anharmonic sextic oscillator defined by the potential

$$V(y) = \frac{1}{2}y^2 + 2y^4 + \frac{1}{2}y^6. \tag{4}$$

Kaluza employed an analytical Lanczos procedure to generate the tridiagonal matrix representative of the Hamiltonian for this potential. Since the algorithm is analogous to a Schmidt orthogonalization procedure, it suffers from considerable roundoff error. This problem was aleviated by using multiple precision arithmetic. Braun et al. [8] employed a finite difference approach to study the same potential and was able to reproduce the numerical results of Kaluza and extend the precision of many of the higher eigenvalues.

A fourth potential that we consider in this paper is of the form

$$V(y) = y^2 + \varepsilon y^4, \tag{5}$$

which has been studied by several workers. Banerjee et al. [5] and Banerjee [4] employed a non-perturbative method with the product of scaled Gaussian and a polynomial as weight function to calculate the eigenvalues for this potential for various values of ε. Fernandez et al. [22] and Arteca et al. [2] applied a variational method to obtain the eigenvalues and compared with Banerjee's results. Fernandez and Castro [23] obtained the eigenvalues of this potential by solving the corresponding Riccati equation with Pade approximants. Recently, Fernandez and Tipping [26] improved the solution of the Riccati equation for this potential with a separation of the eigenfunctions into odd and even parity. Fack and Van den Berghe employed a finite-difference method to solve this problem. Witwit [60,61] extended the work to two and three-dimensional problems. The QDM was recently applied with considerable success to the two-dimensional Schrödinger equation with the Henon–Heles potential function [50].

A great many papers have appeared on the calculation of the spectra of generalized anharmonic oscillators and their discussion here is beyond the scope of the present paper. Ari and Demiralp [1] and Taseli and Demiralp [54] employed characteristic function and Wronskian approaches to determine the spectra of such generalized anharmonic oscillators. These authors propose alternate methods that do not involve the direct calculation of the matrix elements of the Hamiltonian in the Schrödinger equation. The QDM also does not require the direct integration of matrix elements. The discrete representation of the Hamiltonian involves only function evaluations of the potential. A brief summary of the QDM is presented in section 2. Further details were presented by Shizgal and Chen [50,51]. The applications to the four potential functions given by equations (2)–(5) are presented and discussed in section 3. A summary of the results is provided in section 4.

2. The solution of the Schrödinger equation with the QDM

The basic methodology of the QDM has been discussed by Shizgal and Chen in a previous paper [50] and it is also presented in the preceeding paper [38]. The matrix

representative of the Hamiltonian in the Schrödinger equation in the basis set $\{S_n(y)\}$ is given by

$$H_{nm} = -\int S_n(y) S_m''(y)\,\mathrm{d}y + \int S_n(y) V(y) S_m(y)\,\mathrm{d}y. \tag{6}$$

With an integration by parts in the first integral, we have that

$$H_{nm} = \int S_n'(y) S_m'(y)\,\mathrm{d}y + V_{nm}, \tag{7}$$

where $V_{nm} = \int S_n(y) V(y) S_m(y)\,\mathrm{d}y$. The eigenvalues and the eigenfunctions can be calculated with the numerical diagonalization of equation (7). The disadvantage of this representation is that the matrix elements are generally evaluated numerically except for certain special models. The appropriateness of the choice of basis set can be acertained to some extent from the structure of H_{nm}. If, for example, H_{nm} is tridiagonal as in the work of Kaluza [35], the convergence of the eigenvalues is expected to be rapid.

We now consider the transformation to the polynomial basis set $\{R_n(y)\}$ given by

$$S_n(y) = \sqrt{w(y)} R_n(y), \tag{8}$$

where we choose the weight function as expressible in the form $w(y) = \exp(-\int W(y')\,\mathrm{d}y')$. This form of weight function is related to the steady state distribution function given by a Fokker–Planck equation [38]. Equation (10) can be rewritten in terms of $R_n(y)$ as given by

$$H_{nm} = \int w \left[R_m' + \frac{w'}{2w} R_m \right] \left[R_n' + \frac{w'}{2w} R_n \right] \mathrm{d}y + V_{nm}. \tag{9}$$

If one of the cross terms in the integrand above is integrated by parts, one gets that

$$H_{nm} = \int w R_n' R_m'\,\mathrm{d}y + \left[V_{nm} - \widetilde{V}_{nm} \right], \tag{10}$$

where

$$\widetilde{V}(y) = \frac{1}{4} W^2(y) - \frac{1}{2} W'(y). \tag{11}$$

If the matrix representative H_{nm} is transformed back to the discrete representation [38, 50] with the transformation **T** (equation (30) of [38]), that is,

$$H_{ij} = \sum_{n=0}^{N} \sum_{m=0}^{N} T_{in} H_{nm} T_{mj}, \tag{12}$$

one finds that

$$H_{ij} = \sum_{k=0}^{N} D_{ki} D_{kj} + \left[V(y_i) - \widetilde{V}(y_i) \right] \delta_{ij}, \tag{13}$$

where further details concerning the derivation of equation (13) are described in [50]. If the potential of interest can be factorized in accordance with equation (11), then a possible choice of weight function would be given by the "equilibrium distribution function" [50] or the ground state wave function. For this choice, the term in $(V(y_i) - \widetilde{V}(y_i))\delta_{ij}$ is zero, since $\widetilde{V}(y) = V(y)$. The extension to two and three-dimensional problems is straightforward [50] and involves the direct product of the one-dimensional spaces.

For the class of potentials that can be written as given by equation (11), the ground state wavefunction is known and given by

$$\psi_0(y) = C \exp\left[-\frac{1}{2}\int W(y)\,\mathrm{d}y\right], \tag{14}$$

and the corresponding eigenvalue is zero. The function $W(y)$ is referred to as the superpotential [12,14]. These are the class of potentials that result in the transformation of the Fokker–Planck equation into the Schrödinger equation [16,17,42,44,45]. In this case, it is easy to choose the weight function such that $\widetilde{V}(y) = V(y)$.

3. Calculations and results

The main purpose of this paper is to consider the solution of the Schrödinger equation with the QDM and to study the rate of the convergence of the eigenvalues versus the number of grid points (equivalently, basis functions) for different weight

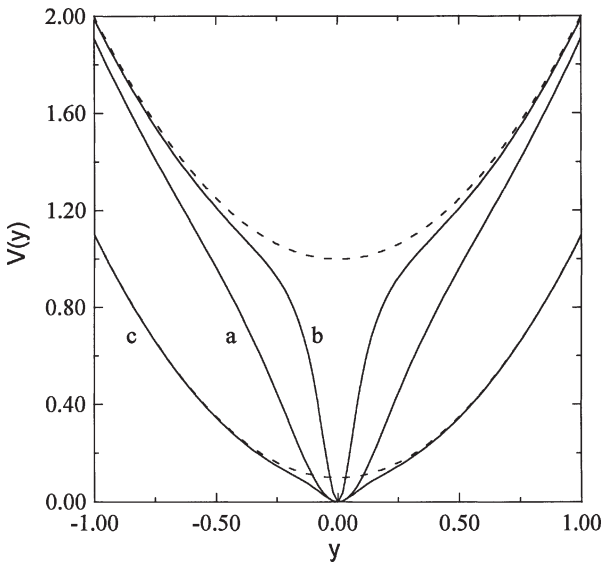

Figure 1. The Non-Polynomial Oscillator (NPO) potential, $V(y) = y^2 + \lambda y^2/(1 + gy^2)$. λ and g equal to (a) 10, 10, (b) 100, 100, and (c) 10, 100. The dash lines are the corresponding harmonic potential $V(y) = y^2 + \lambda/g$.

Table 1
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 0,\ g = 0$		
5	1.00000000	3.00000000	5.00000000	7.00000000	9.00000000
			$\lambda = 1,\ g = 1$		
10	1.23249101	3.51099389	5.62484751	7.83801690	10.32756366
15	1.23235091	3.50743657	5.59055567	7.65537404	9.72679150
20	1.23235080	3.50738872	5.58979112	7.64836479	9.68550819
25	1.23235072	3.50738837	5.58977905	7.64820406	9.68407574
30	1.23235072	3.50738835	5.58977894	7.64820127	9.68404264
35		3.50738835	5.58977893	7.64820124	9.68404202
40			5.58977893	7.64820124	9.68404202
			$\lambda = 10,\ g = 1$		
6	2.78731371	7.45133700	11.12235424	15.06719730	20.93409663
8	2.78330674	7.42328164	10.82111289	14.02801379	17.85478222
10	2.78256744	7.41859167	10.73364911	13.61840145	16.71237123
12	2.78239417	7.41766006	10.70974937	13.46807104	16.19788329
15	2.78231986	7.41756091	10.70207942	13.40273170	15.91402388
20	2.78233128	7.41750446	10.70106074	13.38898345	15.82571826
25	2.78233044	7.41750609	10.70102615	13.38834923	15.81924074
30	2.78233052	7.41750588	10.70102563	13.38832431	15.81888806
35	2.78233052	7.41750590	10.70102557	13.38832353	15.81887214
40		7.41750590	10.70102558	13.38832349	15.81887152
45			10.70102558	13.38832349	15.81887149
50					15.81887149
			$\lambda = 100,\ g = 1$		
10	9.35966852	26.70397902	41.44872496	53.83672948	64.45752724
15	9.35941391	26.70599835	41.44097043	53.83975078	64.19541577
20	9.35941813	26.70596477	41.44110330	53.83909110	64.18782502
25	9.35941803	26.70596566	41.44109963	53.83909383	64.18745791
30	9.35941803	26.70596563	41.44109976	53.83909326	64.18744198
35		26.70596563	41.44109975	53.83909327	64.18744105
40			41.44109975	53.83909326	64.18744100
45				53.83909326	64.18744100

[a] $w(y) = \exp(-\alpha y^2)$, where α is chosen for the fatest convergence.

functions. The basis functions, $R_n(x)$, are orthonormal with respect to the weight function, $w(x)$. Our interest is to try to suggest the weight function that provides optimal convergence of the eigenvalues. We consider four different one-dimensional potentials in the Schrödinger equation that have received considerable attention in the literature over the past decade. If the convergence for one-dimensional problems can be optimized, there would be a considerable savings in computer time when applied to two- and three-dimensional problems. This has been demonstrated by Shizgal and Chen [50] in the application of the QDM to the two-dimensional Henon–Heles potential.

Table 2
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 1,\ g = 10$		
10	1.11770702	3.54168906	6.69900727	11.03978681	16.69475171
30	1.05932983	3.08883073	5.09038673	7.13612019	9.26980877
50	1.05929698	3.08809133	5.08285715	7.09048160	9.08892124
60	1.05929690	3.08809085	5.08284796	7.09037430	9.08805809
70	1.05929689	3.08809085	5.08284769	7.09037053	9.08801960
80	1.05929688		5.08284768	7.09037041	9.08801815
90	1.05929688		5.08284768	7.09037041	9.08801810
100					9.08801810
			$\lambda = 10,\ g = 10$		
10	1.65877686	4.53929108	8.04585051	13.12551490	19.66357857
30	1.58013523	3.88195452	5.85711306	8.03082593	10.30455803
50	1.58002278	3.87904292	5.83286153	7.90413992	9.88876928
70	1.58002235	3.87903684	5.83276776	7.90315755	9.88233330
80	1.58002233	3.87903683	5.83276755	7.90315433	9.88230079
90	1.58002233	3.87903683	5.83276753	7.90315417	9.88229884
100			5.83276753	7.90315416	9.88229873
110				7.90315416	9.88229873
			$\lambda = 100,\ g = 10$		
10	5.82541635	12.16555870	15.97213490	22.13479362	29.83816388
30	5.79404439	11.57646135	13.66813086	16.22502482	18.70150089
50	5.79394465	11.57221790	13.62913696	15.99309324	17.99876164
70	5.79394241	11.57219684	13.62877371	15.98848089	17.97250413
90	5.79394231	11.57219677	13.62877143	15.98843454	17.97208972
100	5.79394230	11.57219678	13.62877142	15.98843423	17.97208598
110	5.79394230	11.57219678	13.62877142	15.98843421	17.97208565
120				15.98843421	17.97208562
130					17.97208562

[a] $w(y) = \exp(-\alpha y^2)$, where α is chosen for the fatest convergence.

The first potential that we have chosen and which has been studied extensively [3,6,9,18,25,27,32–34,36,37,40,41,46,52,55,57,59] is the NPO model (equation (2)) shown in figure 1 as the solid curves. The dashed curves are the harmonic potentials, $V(y) = y^2 + \lambda/g$, for $\lambda = g = 100$ and $\lambda = g = 10$ (upper curve) and for $\lambda = 10$ and $g = 100$ (lower curve); the potential departs from harmonic in the vicinity of the origin. The deep narrow anharmonic well near the origin gets deeper and narrower with increasing g. Many of the previous calculations have emphasized the calculation of the ground state eigenvalue for large g. For situations where the potential is close to harmonic, it would appear useful to use the scaled Hermite polynomials as basis functions based on the weight function, $w_1(y) = \exp(-\alpha y^2)$, where α is a scaling parameter.

Table 3
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 1$, $g = 100$		
10	1.74034331	6.61289499	14.45434406	25.73416848	40.57425497
50	1.01083691	3.04192292	5.19309999	7.64468189	10.57282857
100	1.00841233	3.00987806	5.00989049	7.01481472	9.03654508
150	1.00841061	3.00983181	5.00927636	7.00985617	9.00959190
160	1.00841061	3.00983178	5.00927573	7.00984803	9.00951745
170	1.00841060	3.00983177	5.00927557	7.00984578	9.00949511
180	1.00841060	3.00983177	5.00927553	7.00984517	9.00948856
			$\lambda = 10$, $g = 100$		
10	2.12557689	8.03895659	17.66231586	31.55531547	49.82378424
50	1.09321568	3.19606870	5.54663516	8.42645412	11.98070336
100	1.08408954	3.09891916	5.09892856	7.13621223	9.24759634
150	1.08406343	3.09831922	5.09279892	7.09883559	9.09763231
160	1.08406338	3.09831770	5.09277453	7.09859179	9.09597926
170	1.08406335	3.09831722	5.09276616	7.09850083	9.09530236
180	1.08406335	3.09831706	5.09276332	7.09846755	9.09503285
			$\lambda = 100$, $g = 100$		
10	2.92175390	9.34160581	19.45189904	34.28680807	53.64778578
50	1.84742726	4.11049745	6.47955464	9.57139193	13.28590654
100	1.83638157	3.98422018	5.93857806	8.04492347	10.17201242
150	1.83633621	3.98310435	5.92841712	7.98535022	9.95499695
170	1.83633594	3.98309903	5.92834037	7.98458485	9.95023642
180	1.83633590	3.98309857	5.92833282	7.98449794	9.94960676

[a] $w(y) = \exp(-\alpha y^2)$, where α is chosen for the fatest convergence.

For this NPO potential, we have carried out an extensive analysis of the behavior versus the two parameters g and λ and for different weight functions. The results are summarized in tables 1–10. In tables 1–3 with g = 1, 10 and 100, we use the weight function for scaled Hermite polynomials and vary the scaling parameter α for each of the first 5 eigenvalues so as to get the value of α that yields the most rapid convergence. The QDM is implemented, as discussed in the previous papers [38,50], by constructing the orthogonal polynomials for the chosen weight function with the algorithm described by Gautschi [29]. The quadrature points are then determined [10,13,28,43] and the eigenvalues calculated from the numerical diagonalization of the QDM representative of the Hamiltonian (equation (13)). The results are shown for $\lambda = 1$, 10 and 100 in each table. In table 1, we reproduce exactly (to 9 significant figures) the harmonic oscillator eigenvalues for $\lambda = 0$. With increasing g, it is seen that the eigenvalues are getting increasingly equally spaced consistent with an harmonic potential. The underlined portion of each eigenvalue indicates the convergence to that number of significant figures. For $g = 1$, 10 and 100 in tables 1–3, we get convergence of the eigenvalues with 25–45, 60–120, 170–180 quadrature points, respectively. The

Table 4
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 1,\ g = 1$		
10	1.23272180	3.50666367	5.59128149	7.64562064	9.69097632
20	1.23235720	3.50737573	5.58980527	7.64815336	9.68412556
30	1.23235100	3.50738781	5.58978006	7.64819920	9.68404558
40	1.23235074	3.50738831	5.58977901	7.64820110	9.68404226
50	1.23235073	3.50738835	5.58977894	7.64820123	9.68404204
60	1.23235072	3.50738835	5.58977893	7.64820124	9.68404202
70	1.23235072		5.58977893	7.64820124	9.68404202
			$\lambda = 10,\ g = 1$		
10	2.78258502	7.41837822	10.73118613	13.60393371	16.67001724
15	2.78231869	7.41755973	10.70193987	13.40125193	15.90594518
20	2.78233137	7.41750412	10.70105591	13.38888589	15.82484591
25	2.78233043	7.41750611	10.70102592	13.38834461	15.81917812
30	2.78233053	7.41750587	10.70102563	13.38832411	15.81888465
35	2.78233051	7.41750590	10.70102557	13.38832352	15.81887198
40	2.78233052	7.41750590	10.70102558	13.38832349	15.81887151
45	2.78233052		10.70102558	13.38832349	15.81887149
50					15.81887149
			$\lambda = 100,\ g = 1$		
10	9.35945915	26.70572641	41.44628014	53.91385775	64.86511926
15	9.35941761	26.70596964	41.44114465	53.84147035	64.23043100
20	9.35941803	26.70596558	41.44110119	53.83917850	64.19022920
25	9.35941803	26.70596563	41.44109978	53.83909702	64.18763807
30		26.70596563	41.44109975	53.83909346	64.18745616
35			41.44109975	53.83909328	64.18744228
40				53.83909327	64.18744111
45				53.83909326	64.18744101
50				53.83909326	64.18744100
55					64.18744100

[a] $w(y) = \exp(-y^2\sqrt{1 + \lambda/(1 + 0.5g)})$.

convergence is clearly much slower for the large values of g. The results in table 3 for the largest eigenvalues are converged to no less that 3 significant figures. The slow convergence for large g is due to the narrow anharmonic form of the potential near the origin; see figure 1.

For the results in table 1, the values of α were chosen arbitrarily. The interest in this paper is to develop techniques to optimize the convergence by selecting a weight function related in some way to the potential. Mitra [41] chose $\alpha = \sqrt{1 + \lambda}$, and Bessis and Bessis [6] suggested $\alpha = \sqrt{1 + \lambda/(1 + 0.5g)}$. In tables 4–6, we show the results analogous to those in tables 1–3 using the value of α suggested by Bessis and Bessis. It is clear that the convergence in tables 1–3 is faster than the convergence in tables 4–6.

Table 5
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 1,\ g = 10$		
10	1.06515662	3.08692234	5.08700592	7.08838586	9.09234744
30	1.06003407	3.08794408	5.08337022	7.09012096	9.08856179
50	1.05946708	3.08805698	5.08296831	7.09031284	9.08814362
100	1.05930820	3.08808859	5.08285570	7.09036658	9.08802645
150	1.05929829	3.08809057	5.08284868	7.09036993	9.08801914
170	1.05929756	3.08809071	5.08284816	7.09037018	9.08801860
180	1.05929736	3.08809075	5.08284802	7.09037025	9.08801845
			$\lambda = 10,\ g = 10$		
10	1.61407526	3.87252286	5.85545056	7.90700483	9.98909626
30	1.58268033	3.87852707	5.83441119	7.90231956	9.88401555
50	1.58046212	3.87895272	5.83303946	7.90301643	9.88258285
100	1.58003812	3.87903382	5.83277730	7.90314922	9.88230893
150	1.58002355	3.87903660	5.83276829	7.90315378	9.88229952
170	1.58002282	3.87903674	5.83276784	7.90315400	9.88229905
180	1.58002265	3.87903677	5.83276773	7.90315406	9.88229894
			$\lambda = 100,\ g = 10$		
10	5.89164179	11.65464995	14.22630311	17.92322840	22.47689280
30	5.79569188	11.57183960	13.62953798	15.99205694	17.99649871
50	5.79404301	11.57217532	13.62879829	15.98841237	17.97213192
100	5.79394280	11.57219667	13.62877155	15.98843409	17.97208577
130	5.79394234	11.57219677	13.62877143	15.98843420	17.97208563
140	5.79394232	11.57219677	13.62877142	15.98843420	17.97208562
150	5.79394231	11.57219677	13.62877142	15.98843421	17.97208562
160	5.79394230	11.57219678		15.98843421	
170	5.79394230	11.57219678			

[a] $w(y) = \exp(-y^2\sqrt{1 + \lambda/(1 + 0.5g)})$.

We have extended the previous efforts by employing a weight function chosen empirically but taking into account the form of the potential. Our previous experience [50,51] has suggested that a useful choice of weight function would be derived from the "superpotential" associated with the potential. This would require the solution of the Riccati equation [23] which is as difficult if not more so than the solution of the Schrödinger equation. However, we have also shown that this choice of weight function is not always the best choice [51]. Nevertheless, we have used an empirical weight function of the form

$$w_1(y) = \exp\left(-\alpha_1 y^2\right) / \left(1 + gy^2\right)^{\alpha_2}. \tag{15}$$

The results obtained with this weight function are shown in tables 7–9. In table 10, we list the values of α_1 and α_2 in the weight function. For all pairs of λ and g, we obtain convergence of the eigenvalues to 9–10 significant figures with no more than 60 quadrature points. It is useful to compare the convergence of λ_5 for $\lambda = 100$ and

Table 6
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 1,\ g = 100$		
10	1.00943021	3.00981139	5.00980562	7.00981397	9.00989938
30	1.00902768	3.00981943	5.00959630	7.00982620	9.00973614
50	1.00883028	3.00982338	5.00949367	7.00983220	9.00965609
100	1.00860665	3.00982785	5.00937742	7.00983900	9.00956543
150	1.00851699	3.00982964	5.00933081	7.00984172	9.00952908
170	1.00849611	3.00983006	5.00931996	7.00984236	9.00952062
180	1.00848760	3.00983023	5.00931554	7.00984261	9.00951717
			$\lambda = 10,\ g = 100$		
10	1.09402833	3.09811836	5.09791649	7.09814755	9.09889054
30	1.08994543	3.09819977	5.09580087	7.09827100	9.09723424
50	1.08798805	3.09823881	5.09478843	7.09833030	9.09644473
100	1.08583151	3.09828179	5.09367433	7.09839559	9.09557603
150	1.08499665	3.09829842	5.09324340	7.09842085	9.09524005
170	1.08480631	3.09830221	5.09314518	7.09842660	9.09516348
180	1.08472929	3.09830374	5.09310544	7.09842893	9.09513250
			$\lambda = 100,\ g = 100$		
10	1.92323022	3.98167955	5.97436235	8.01099094	10.12548823
30	1.87989757	3.98225971	5.94937345	7.98317686	9.96554325
50	1.86200758	3.98260632	5.94066820	7.98370029	9.95876339
100	1.84549528	3.98292370	5.93271091	7.98417970	9.95257021
150	1.84038615	3.98302127	5.93026369	7.98432709	9.95066627
170	1.83936741	3.98304068	5.92977655	7.98435641	9.95028732
180	1.83897462	3.98304816	5.92958881	7.98436771	9.95014127

[a] $w(y) = \exp(-y^2\sqrt{1 + \lambda/(1 + 0.5g)})$.

$g = 100$ in tables 9 and 3. In table 3, λ_5 is converged to 9.950 with 180 quadrature points, whereas it is converged to 9.94916096 with 50 points in table 9. This demonstrates the usefulness of the QDM and the use of specific weight functions to accelerate the convergence. This could mean a great decrease in computational times for two- and three-dimensional problems.

In table 11, we compare the present results for λ_1 with the results reported in the literature by other workers. The methods used by others have been summarized in the introduction to the paper. The weight function used is of the form given by equation (15) with values of α_1 and α_2 which are chosen empirically for different values of λ and g. The QDM results shown in this table are converged to the significant figures shown – either 12 or 14. The most difficult parameter region is for $g = 500$ and, as can be seen from the results in the table, we have achieved remarkable convergence with $g = 500$. The only other work to compare with are the results by Bessis and Bessis [6] and by Chaudhuri and Mukherjee [9]. The QDM results are far superior to the previous results.

Table 7
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 1,\ g = 1$		
5	1.39754248	6.00256900	11.66691170	27.12138709	52.46889173
10	1.23347542	3.50334632	5.91911961	7.73245910	13.42453838
12	1.23235218	3.50738518	5.60432140	7.63808491	10.50025290
15	1.23235072	3.50738845	5.58977876	7.64821025	9.68403519
20	1.23235072	3.50738835	5.58977894	7.64820124	9.68404205
25		3.50738835	5.58977893	7.64820124	9.68404202
30			5.58977893		9.68404202
(b)	1.23235072	3.50738835	5.58977892	7.64820121	9.68404195
(c)	1.23235353	3.50739706	5.58983355	7.64906899	
			$\lambda = 10,\ g = 1$		
5	2.78138892	8.72184392	14.67163572	29.92249451	55.15913549
10	2.78233156	7.41816173	10.81174060	13.48916964	18.62437460
12	2.78233088	7.41751699	10.70458231	13.40672751	16.36170232
15	2.78233052	7.41750593	10.70102881	13.38872711	15.82253275
20	2.78233052	7.41750590	10.70102558	13.38832349	15.81887215
25		7.41750590	10.70102558	13.38832349	15.81887149
30					15.81887149
(c)	2.78233054	7.41767206	10.70448059	13.39000325	
			$\lambda = 100,\ g = 1$		
5	9.35957820	26.76092127	41.56662303	60.49260798	91.26562732
10	9.35941835	26.70595968	41.44117242	53.84491548	64.45670875
12	9.35941804	26.70596556	41.44110930	53.83926961	64.20476806
15	9.35941803	26.70596563	41.44109980	53.83909597	64.18766807
20	9.35941803	26.70596563	41.44109975	53.83909326	64.18744157
25			41.44109975	53.83909326	64.18744100
30					64.18744100
(c)	9.35941803	26.70596563	41.44109975	53.83909296	

[a] $w(y) = \exp(-\alpha_1 y^2)/(1 + gy^2)^{\alpha_2}$, where α_1 and α_2 are given in table 10. Results from (b) Fack and Van den Berghe [18], (c) Lai and Lin [37].

Figure 2 shows the variation of the error in λ_1 for the NPO model ($g = \lambda = 10$) versus the number of quadrature points, N, for four different weight functions. λ_1^{exact} is defined as the eigenvalue converged to 14 significant figures calculated with the QDM. The fourth weight function (d) gives the most rapid convergence. The significant improvement with weight function (d) over the scaled Gaussian weight function can be explained with the variation of the eigenfunction shown in figures 3 and 4. The convergence of the eigenvalue depends on the accurate determination of the eigenfunction near the origin. Figures 3 and 4 show the details of the ground state eigenfunction near the origin. The solid curves are determined with the new weight function (equation (15)) and $N = 140$. This is considered to be very close to the exact result. The other results are obtained with $N = 25$. Figure 3 is for $g = \lambda = 100$

Table 8
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 1,\ g = 10$		
8	1.09475078	3.28354065	6.07364598	10.01493041	33.92974057
10	1.06078000	3.10750137	5.34002953	7.84826441	12.39506550
12	1.05934121	3.08925905	5.10521689	7.20306392	9.76442476
15	1.05929700	3.08810693	5.08309896	7.09455928	9.11338782
20	1.05929690	3.08809085	5.08284789	7.09037308	9.08806709
25	1.05929688	3.08809085	5.08284767	7.09037041	9.08801812
30	1.05929688		5.08284768	7.09037041	9.08801810
35			5.08284768		9.08801810
			$\lambda = 10,\ g = 10$		
10	1.67530513	4.31996615	9.75230993	10.43741586	29.54884661
20	1.58002638	3.87916818	5.83491979	7.91869454	9.97591517
25	1.58002232	3.87903807	5.83278723	7.90346720	9.88457979
30	1.58002233	3.87903684	5.83276775	7.90315728	9.88233966
35	1.58002233	3.87903683	5.83276753	7.90315420	9.88229915
40		3.87903683	5.83276753	7.90315416	9.88229873
45				7.90315416	9.88229873
(b)	1.58002233	3.87903683	5.83276752	7.90315413	9.88229866
			$\lambda = 100,\ g = 10$		
10	7.48981433	8.03655640	44.09323078	49.71269815	149.70360371
20	5.79394731	11.57682425	13.70481854	16.27467472	19.37491150
25	5.79394193	11.57225713	13.62958358	16.00289112	18.03283044
30	5.79394232	11.57219704	13.62878139	15.98861076	17.97411182
35	5.79394230	11.57219678	13.62877147	15.98843650	17.97211015
40	5.79394230	11.57219678	13.62877142	15.98843422	17.97208593
45			13.62877142	15.98843421	17.97208562
50				15.98843421	17.97208562

[a] $w(y) = \exp(-\alpha_1 y^2)/(1+gy^2)^{\alpha_2}$, where α_1 and α_2 are given in table 10. (b) Results from Fack and Van den Berghe [18].

for three different weight functions: Hermite polynomials ($*$), scaled Hermite polynomials ($+$) and the new weight function ($\circ$). Figure 3(B) shows the eigenfunction on a small scale near the origin. From the figure we see that the points generated from the scaled Gaussian weight function can not describe the rapid variation of the eigenfunction near the origin. However, the new weight function, with a denser grid of quadrature points near the origin where the potential (figure 1) and the eigenfunction vary rapidly, is better. It is clear that the results with the new weight function (equation (15)) gives the best convergence. Figure 4 shows the behavior near the origin for three different pairs of values of g and λ. Figure 4(B) shows the small scale behavior near the origin, whereas figure 4(C) shows the small scale behavior at large positions from the origin. The dashed curve is the result with the Gaussian weight function.

Table 9
The convergence of eigenvalues[a] with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

N	λ_1	λ_2	λ_3	λ_4	λ_5
			$\lambda = 1,\ g = 100$		
10	1.04129101	3.29082677	6.43712676	10.95519923	55.86316463
15	1.00859774	3.01435281	5.04709144	7.22004103	9.67669200
20	1.00841165	3.00986701	5.00988241	7.01509885	9.04372955
25	1.00841060	3.00983203	5.00928092	7.00992522	9.01020204
30	1.00841060	3.00983177	5.00927556	7.00984573	9.00949652
35		3.00983177	5.00927551	7.00984496	9.00948602
40			5.00927551	7.00984495	9.00948596
45				7.00984495	9.00948596
			$\lambda = 10,\ g = 100$		
10	1.45426410	5.01654653	29.97472996	72.98922478	243.24844347
15	1.08980088	3.18022872	5.48420299	8.49756777	12.20388108
20	1.08416996	3.10035001	5.11504606	5.81559287	7.21912972
25	1.08406448	3.09836640	5.09342462	7.10472597	9.12859105
30	1.08406336	3.09831782	5.09277943	7.09864757	9.09661478
35	1.08406331	3.09831701	5.09276222	7.09845465	9.09492189
40	1.08406334	3.09831700	5.09276191	7.09844919	9.09486638
45	1.08406334	3.09831700	5.09276189	7.09844907	9.09486470
50			5.09276190	7.09844907	9.09486466
55			5.09276190		9.09486466
			$\lambda = 100,\ g = 100$		
10	0.25273328	58.55206092	526.35484897	565.24148666	1785.60704400
20	1.89936536	4.43121455	8.05177942	12.63918879	27.70284628
30	1.83635795	3.98374475	5.93607533	8.03086862	10.15714058
40	1.83633587	3.98309869	5.92833557	7.98453363	9.95000108
50	1.83633584	3.98309834	5.92832858	7.98444358	9.94916197
60	1.83633583	3.98309834	5.92832857	7.98444352	9.94916096
65	1.83633583		5.92832857	7.98444352	9.94916096
(b)	1.83633444	3.98309836	5.92832790	7.90315413	9.88229866

[a] $w(y) = \exp(-\alpha_1 y^2)/(1 + gy^2)^{\alpha_2}$, where α_1 and α_2 are given in table 10. (b) Results from Fack and Van den Berghe [18].

Table 10
$(\alpha_1,\ \alpha_2)$ used for tables 7–9.

g/λ	1	10	100
1	(1, 10)	(1.2, 10)	(3, 12)
10	(1.4, 6)	(2, 8)	(2, 14)
10	(1.4, 6)	(2, 8)	(2, 14)
100	(2, 6)	(2.4, 8)	(2.5, 16)

Table 11
Comparison of results of λ_1 with $V(y) = y^2 + \lambda y^2/(1 + gy^2)$.

λ	1	10	100	500
		$g = 1$		
QDM	1.232350723406	2.782330515932	9.359418026324	21.65874769959
(a)	1.23235072	2.78233052	9.35941803	
(b)	1.23235072			
(c)	1.24213			
(d)	1.23235353	2.78233054	9.35941803	
(e)	1.23237205	2.782330	9.35941803	21.6587477
(f)	1.23235	2.78233	9.3594	
		$g = 10$		
QDM	1.059296880862	1.580022327392	5.793942300193	16.73274738223
(a)	1.05929688	1.58002233	5.79394230	
(b)		1.58002233		
(e)	1.05929700	1.5800249	5.793947	16.73919
(f)	1.05929	1.58002	5.794	
		$g = 100$		
QDM	1.008410597947	1.084063335494	1.836335833449	5.083683913501
(a)	1.00841060	1.08406334	1.83633583	
(b)			1.83633444	
(c)		1.08411	1.8411	
(e)	1.0084106	1.0840543	1.8363850	5.0840857
(f)	1.00841	1.08406	1.8364	
		$g = 500$		
QDM	1.001849154630	1.084063335494	1.18486023962	1.92317625551
(a)				
(c)			1.18451	1.92255
(e)	1.0018491	1.0184910	1.1848632	1.9232260

(a) Scherrer et al. [46], (b) Fack and Van den Berghe [18], (c) Chaudhuri and Mukherjee [9], (d) Lai and Lin [37], (e) Bessis and Bessis [6], (f) Mitra [41].

If the potential belongs to the class of potentials in supersymmetric quantum mechanics [12,14], then the ground state eigenfunction is known with the eigenvalue equal to zero. This is the case for the potential given by equation (3), considered by Sinha et al. [53]. The weight function that corresponds to the superpotential is of the form

$$w_2(y) = \exp\left(-y^4/4\right). \tag{16}$$

The basis set was determined following the prescription by Gautschi [29] and the quadrature points as described in the earlier papers. For this choice of weight function, $V(y) \equiv \widetilde{V}(y)$, and the representative of the Hamiltonian in the QDM representation is from equation (13) given by $H_{ij} = \sum_k D_{ki} D_{kj}$. We have studied the convergence of the eigenvalues for this potential with three different weight functions, one of which

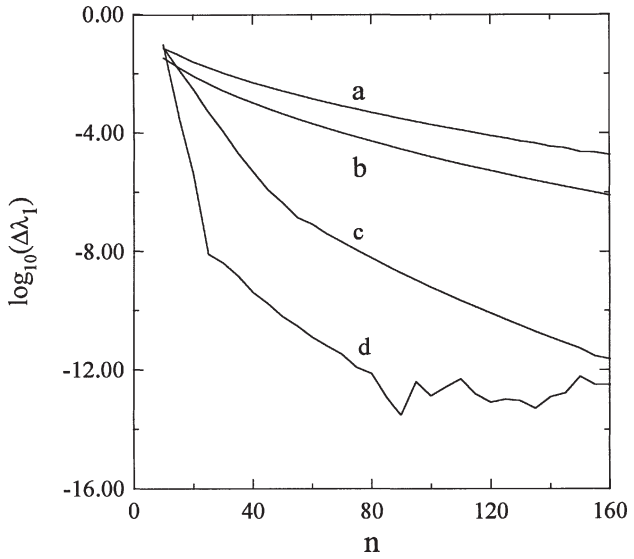

Figure 2. Variation of the error in λ_1, $\Delta\lambda_1 = |\lambda_1 - \lambda_1^{\text{exact}}|$, for the NPO potential versus the number of grid points, N, for different weight functions. (a) $w(y) = \exp(-y^2)$, (b) $w(y) = \exp(-y^2 \times \sqrt{1+\lambda/(1+0.5g)})$, (c) $w(y) = \exp(-5.8y^2)$, (d) $w(y) = \exp(-2y^2)/(1+gy^2)^8$; $\lambda = g = 10$.

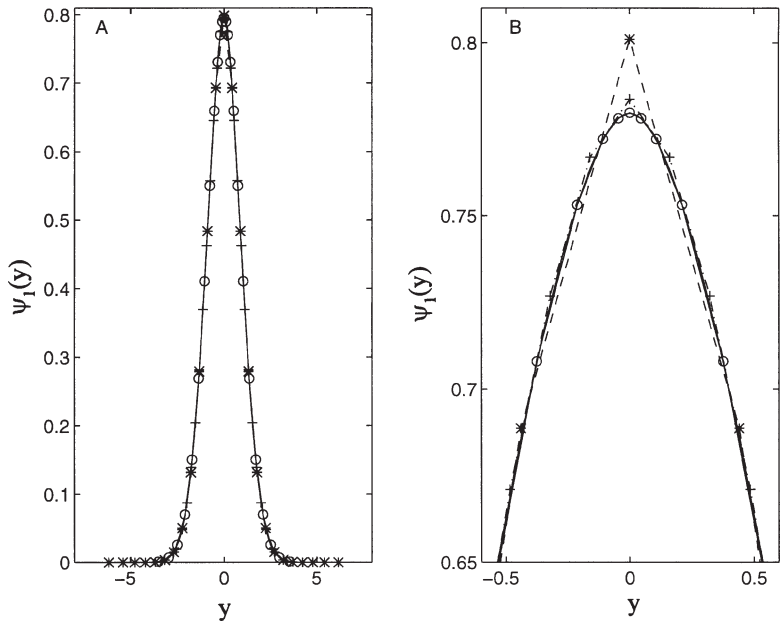

Figure 3. Ground state eigenfunction for the NPO potential with $g = \lambda = 100$, $N = 25$, with different weight functions. $(*)$ $w(y) = \exp(-y^2)$, $(+)$ $w(y) = \exp(-17y^2)$ and $(\circ)$ $w(y) = \exp(-3y^2)/(1+gy^2)^8$. The solid curve is for the last weight function with $N = 140$. (A) Full scale, (B) small scale near the origin.

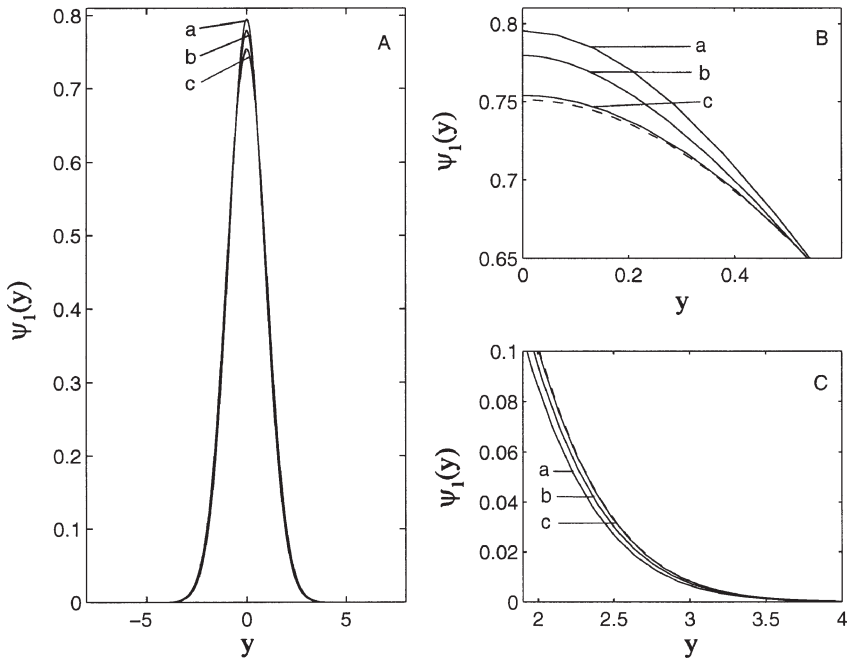

Figure 4. Ground state of eigenfunction for the NPO potential. λ and g are equal to (a) 10, 10, (b) 100, 100, (c) 10, 100, and (- - -) 0, 0. (A) Full scale, (B) small scale near the origin, (C) small scale at large positions from the origin.

corresponds to the Hermite polynomials, $w_1(y)$, defined earlier with α = 5, and another given by

$$w_3(y) = \exp\left(-y^4/4 - 5y^2\right). \tag{17}$$

The results with the three weight functions are shown in table 12. The overall convergence is very similar with all three weight functions, although $w_2(y)$ appears to give marginally faster convergence, in particular for the first eigenvalue. Our results are consistent with the results of Sinha et al. [53] to the precision that they report in their paper.

The third potential chosen was studied by Braun et al. [8] and Kaluza [35] and also belongs to the class of potentials in supersymmetric quantum mechanics. Kaluza chose basis functions such that the matrix representative of the Hamiltonian is tridiagonal. The generation of the basis set is essentially a Gram–Schmidt orthogonalization which is subject to considerable round-off errors [11,47]. Kaluza avoids these numerical difficulties by using symbolic algebraic techniques in *Mathematica*. For arbitrary weight functions, this analytic approach is not feasible, whereas the Gautschi algorithm is generally convergent. Braun et al. employ a spectral method of solution based on Chebyshev polynomials on a finite interval where the cutoff at $y = 8$ is an additional parameter. They use up to 512 grid points and report eigenvalues up to 18 significant

Table 12
The convergence of eigenvalues for SE with $V(y) = y^6 - 3y^2$.

N	λ_1	λ_3	λ_5	λ_{10}
		$w_1(y) = \exp(-5y^2)$		
5	3.20578381	19.34421619		
10	1.92166391	11.48428663	24.44773756	
15	1.93541230	11.67877474	25.22960745	72.68872477
20	1.93548442	11.68098869	25.25435384	71.64137641
25	1.93548209	11.68097117	25.25461676	71.57368183
30	1.93548210	11.68097087	25.25460450	71.57923539
35		11.68097089	25.25460490	71.57902800
40			25.25460488	71.57903698
45				71.57903668
50				71.57903669
		$w_2(y) = \exp(-y^4/4)$		
5	1.95003306	13.51720225		
10	1.93549705	11.68815652	25.58769695	
15	1.93548226	11.68108903	25.26571988	75.81549114
20	1.93548210	11.68097109	25.25463882	72.04071624
25		11.68097089	25.25460546	71.58445530
30			25.25460488	71.57920993
35				71.57903737
40				71.57903670
45				71.57903669
		$w_3(y) = \exp(-y^4/4 - 5y^2)$		
5	4.54466778	23.73100470		
10	2.23089971	13.39054786	31.59035642	
15	1.94701006	11.78606709	25.89623300	83.65936104
20	1.93570651	11.68371077	25.28051990	73.07062002
25	1.93548392	11.68099725	25.25493023	71.64923337
30	1.93548212	11.68097108	25.25460771	71.57992969
35	1.93548210	11.68097089	25.25460489	71.57904422
40		11.68097089	25.25460488	71.57903671
45				71.57903669

figures. We have chosen the weight function

$$w_4(y) = \exp\left(-2y^2 - y^4/2\right) \tag{18}$$

and determined the matrix representative of the Hamiltonian in the "polynomial basis" representation (equation (10)) with $V_{nm} - \widetilde{V}_{nm} = 2$. The matrix elements of the Hamiltonian are determined with the quadrature define by the weight function (equation (18)). Because of the symmetry of the potential, the eigenfunctions are of either even or odd parity. The matrix H_{nm} of dimension $N \times N$ can be decomposed into two matrices for the odd and even eigenfunctions each of dimension $(N/2) \times (N/2)$. Since the matrix H_{nm} is pentadiagonal, the submatrices of even and odd parity are

Table 13
The convergence of eigenvalues[a] of even parity with $V(y) = (1/2)y^2 + 2y^4 + (1/2)y^6$.

N	λ_1	λ_3	λ_5	λ_7
1	1.00000000000000000			
3	1.00000000000000000	15.832389169799		
5		15.124216267224	40.6232236023546	
8		15.118931530866	36.367167641896	66.261603950851
10		15.118929992544	36.343021051640	62.648395926012
15		15.118929986242	36.342716214160	62.356049424923
20		15.118929986242	36.342716212413	62.356028944861
25			36.342716212413	62.356028944603
30				62.356028944604
35				62.356028944604

N	λ_{20}	λ_{30}	λ_{40}	λ_{48}
20	438.4415064273			
30	310.4920471524	848.8060217068		
40	309.4993497820	588.5806628599	1346.579274312	
50	309.4993484837	566.4282265701	947.4614543288	1597.421054106
55	309.4993484837	566.4026817440	893.9968790569	1364.247596709
60		566.4026355012	872.0907745529	1248.445773964
65		566.4026354734	868.2562193165	1183.544197185
70		566.4026354734	868.1457422322	1149.943901457
75			868.1452015357	1138.668487703
80			868.1452006773	1137.541785229
85			868.1452006767	1137.522672203
90			868.1452006767	1137.522588690
95				1137.522588541
100				1137.522588541

[a] $W(y) = \exp(-2y^2 - y^4/2)$.

tridiagonal. The convergence of the eigenvalues from the numerical diagonalization of these tridiagonal matrices is rapid.

The final potential studied is given by equation (5). This potential is not in the class of potentials in supersymmetric quantum mechanics. We have in the first instance used scaled Hermite polynomials and the associated quadrature points to determine the eigenvalues with equation (13). The convergence of the lower order eigenvalues is shown in table 14 for three values of ε. The scaling is very important in order that the grid points are distributed over the region of y where the eigenfunctions are concentrated. With the notion that the optimal weight function should be the square of the ground state eigenfunction, we have fitted, to polynomials, the ground state eigenfunction determined previously with Hermite quadrature points. This is an alternative to solving the Riccati equation for the superpotential [22]. The fit is reasonably accurate, but $V(y)$ is not exactly equal to $\widetilde{V}(y)$. In table 15, we show the convergence of the eigenvalues with this alternate weight function. The results with this weight function show a moderate improvement in the rate of convergence. We

Table 14
The convergence of eigenvalues with $V(y) = y^2 + \varepsilon y^4$.

N	λ_1	λ_3	λ_5	λ_{10}
		$\varepsilon = 10$[a]		
12	2.44917485	16.63595545	35.88068953	94.30085478
15	2.44917408	16.63591955	35.88506209	95.81165911
20	2.44917407	16.63592150	35.88517148	96.15949348
25	2.44917407	16.63592149	35.88517122	96.15623411
30		16.63592149	35.88517122	96.15626312
35				96.15626298
40				96.15626298
		$\varepsilon = 100$[b]		
10	4.99945382	34.87447875	75.72914876	253.32604009
12	4.99941563	34.87402295	75.88739267	201.40793502
15	4.99941758	34.87398862	75.87689375	205.27637088
20	4.99941755	34.87398427	75.87700463	204.79428957
25	4.99941755	34.87398426	75.87700403	204.79476335
30		34.87398426	75.87700403	204.79477459
35				204.79477451
40				204.79477451
		$\varepsilon = 10000$[c]		
10	22.86146298	160.68335404	350.84170426	1022.19210882
12	22.86161867	160.68601691	350.38352262	924.84691394
15	22.86160889	160.68588347	350.43503532	944.02953926
20	22.86160887	160.68591272	350.43589703	947.71986787
25	22.86160887	160.68591261	350.43589621	947.68562278
30		160.68591261	350.43589622	947.68596392
35			350.43589622	947.68596166
40				947.68596167
45				947.68596167

[a] $w(y) = \exp(-6y^2)$.
[b] $w(y) = \exp(-10y^2)$.
[c] $w(y) = \exp(-60y^2)$.

find, for example, that with the new weight function for $\varepsilon = 100$, λ_1 is converged to 9 significant figures with 15 points, whereas 20 points are required with scaled Hermite polynomials. Similarly, λ_3 is converged to 8 significant figures with 20 points, whereas 25 are required with scaled Hermite polynomials. The choice of weight function is clearly important for the rapid convergence of the eigenvalues.

4. Summary

In the present paper, we have provided an extensive study of the use of the Quadrature Discretization Method (QDM) in the solution of the Schrödinger equation for several one-dimensional potential functions considered recently by several other

Table 15
The convergence of eigenvalues with $V(y) = y^2 + \varepsilon y^4$ calculated by fitting weight function to ground state eigenfunction.

N	λ_1	λ_3	λ_5	λ_{10}
		$\varepsilon = 10$[a]		
10	2.44917318	16.63603391	35.86694240	107.31938413
12	2.44917406	16.63593038	35.88380588	98.84824260
15	2.44917407	16.63592170	35.88516632	96.71828902
20		16.63592149	35.88517122	96.16096863
25		16.63592149	35.88517122	96.15625913
30				96.15626298
35				96.15626298
		$\varepsilon = 100$[b]		
12	4.99941762	34.87397375	75.87733275	210.04422203
15	4.99941755	34.87398436	75.87701004	205.20313119
20	4.99941755	34.87398426	75.87700401	204.79819433
25		34.87398426	75.87700403	204.79477654
30			75.87700403	204.79477452
35				204.79477451
40				204.79477451
		$\varepsilon = 10000$[c]		
10	22.86160088	160.68728162	350.26068143	1055.94778633
12	22.86160897	160.68596913	350.42650209	973.50076873
15	22.86160887	160.68591446	350.43583997	952.12677503
20	22.86160887	160.68591261	350.43589612	947.72238259
25		160.68591261	350.43589622	947.68593841
30			350.43589622	947.68596166
35				947.68596167
40				947.68596167

[a] $w(y) = \exp(-(y^4 + 5y^2)/2)$.
[b] $w(y) = \exp(-(2y^4 + 6y^2))$.
[c] $w(y) = \exp(-(50y^4 + 25y^2))$.

researchers. The main theme of this paper is to determine the optimum set of basis functions, equivalently the weight function, that provides rapid convergence of the eigenvalues versus the number of basis functions or grid points. Although this work is restricted to one-dimensional problems, the extension to two- and three-dimensions is straightforward [50]. The eigenvalues can be determined by the numerical diagonalization of the representative of the Hamiltonian in either the polynomial or the discrete basis. The work in this paper generally employed the discretized version of the Hamiltonian at a set of points that correspond to the quadrature points associated with the chosen weight function. The distribution of grid points is determined by the weight function, which controls the convergence of the eigenvalues and eigenfunctions. We have demonstrated in this paper the flexibility of the QDM in that arbitrary weight functions can be employed to improve the rate of convergence. In

some cases, the improvement is remarkable such as for the nonpolynomial oscillator.

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