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Improvement of numerical integration algorithms by means of coordinate transformations

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Abstract. We study the effect of coordinate transformations on numerical integration algorithms and the Richardson extrapolation. Present method is based on Hermitian transformed eigenvalue equations and symmetrical tridiagonal matrices.

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1 Introduction

Simple numerical methods based on finite difference commonly provide accurate solutions to the Schrödinger equation. In the case of slowly converging sequences of single calculations, Richardson extrapolation of several such runs, each with an appropriate constant steplength, greatly improves the results. It is well-known that smaller steplengths are necessary where the potential changes abruptly, whereas larger steps may appropriately describe those regions where the potential is smooth. Consequently, a variable steplength appears to be necessary when the potential exhibits both behaviours. Such methods are more difficult to program because it is necessary to choose the steplength according to the behaviour of the potential. In addition to it, a variable steplength may result in a less accurate Richardson extrapolation.

An interesting alternative approach is to perform a change of variable $x(r)$ with inverse $r(x)$, from the original variable r to the new variable x, that converts a constant steplength $\Delta x = h$ into a variable one $\Delta r \approx (\mathrm{d}r/\mathrm{d}x)h$. In this way, one can apply Richardson extrapolation to the equation in the variable x, while at the same time incorporating the advantages of a variable steplength in the variable r. For example, the logarithmic transformation $r(x) = \exp(Kx)$ has proved suitable for long-range potentials such as Coulomb interactions [1]. In this case, we clearly appreciate that the variable steplength $\Delta r \approx K\exp(Kx)h = Krh$, goes to zero at origin ($r \to 0$), where the potential changes abruptly, and increases as we move far from it ($r \to \infty$), where the potential is smoother. However, it is held to be a disadvantage of this transformation that it maps the original coordinate interval $(0, \infty)$ onto $(-\infty, \infty)$. In order to remedy this inconvenience, it is customary to divide the interval of the variable r into two parts $(0, 1)$ and $(1, \infty)$ and to apply the logarithmic transformation only to the latter, so that the new variable x ranges from 0 to ∞ [1]. This split requires a more careful programming of the finite difference method if one does not want to spoil the great velocity of convergence provided by Richardson extrapolation.

The Euler transformation has proved suitable for the calculation of critical screening parameters which are particular values of the potential strength such that a bound state lies exactly at the rim of the potential well. In this case the wavefunction tends extremely slowly to a finite nonzero value at infinity, and the numerical integration should proceed to considerably large values of the coordinate in order to produce sufficiently accurate results. The parametrized Euler transformation

$$r = \frac{Kx}{1-x} \tag{1}$$

maps the original coordinate interval $(0, \infty)$ onto $(0, 1)$ and makes the integration of the Schrödinger equation more efficient if one chooses the adjustable parameter K judiciously [2].

Recently, Killingbeck, Jolicard and Grosjean (KJG) proposed the alternative change of variable [3]

$$1 + Kr = \exp(Kx) \tag{2}$$

to solve the Schrödinger equation for the spiked harmonic oscillator

$$-\frac{\mathrm{d}^2\Psi}{\mathrm{d}r^2} + \left(r^2 + \lambda r^{-M}\right)\Psi = E\Psi,\ M > 0, \tag{3}$$

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and other similar models by means of a shooting method. Equation (2) maps the interval $(0,\infty)$ onto itself, and becomes an identical transformation $r \approx x$ at sufficiently small values of x. Both the Euler and KJG transformations are free from the difficulty outlined above for the logarithmic transformation. Notice that the KJG transformation is suitable for the behaviour of the potential-energy function of the spiked oscillator because it provides a steplength that increases with the variable: $\Delta r \approx (1+Kr)h$. We see that Δr is small at the spiked tail of the potential close to the origin, and increases as the propagation of the wavefunction enters the more easily tractable harmonic-oscillator region. Combining a shooting algorithm and Richardson extrapolation Killingbeck *et al.* obtained considerably more accurate results than those given earlier by other methods based on smaller steplengths and more discretization intervals [3]. The authors concluded that sufficiently large values of K made the algorithm suitable for Richardson extrapolation, and pointed out that the number of steps N and the steplength h should be chosen so that Δr is sufficiently small close to origin, and not too large at the upper limit of integration.

Killingbeck *et al.* [3] transformed the variable leaving the wavefunction unchanged; consequently, their modified Schrödinger equation is non-Hermitian, and the resulting discretization matrix nonsymmetrical. In order to exploit the matrix form of their approach, which has proved suitable for shooting methods, one has to resort to special algorithms for nonsymmetrical matrices.

Motivated by the remarkable results produced by the KJG transformation, we have decided to rewrite the finite difference method in the form of a symmetrical matrix to take advantage of well-known and sufficiently-tested standard routines for diagonalization. In this way, potential users of the method may profit from available libraries of powerful routines for symmetric tridiagonal matrices.

In order to illustrate the effect of the coordinate transformations on the algorithms for numerical integration we choose several simple quantum-mechanical models with singular potentials. Such potentials are relevant, for example, to interatomic interactions in molecular physics between an ion and a neutral atom, or between two neutral atoms [4]. We also mention models for phenomena related to cold fusion [5] and the description of short-range and long-range interactions in molecular physics and high-energy scattering [6]. Long-range Coulomb-like effective potentials are relevant to Hartree-Fock approaches in atomic and molecular physics [1].

In Section 2 we derive two Hermitian Schrödinger equations in an arbitrary variable x. In Section 3 we show how to obtain symmetric matrices in both cases by appropriate substitution of finite differences for derivatives. In Section 4 we calculate the ground-state eigenvalue of the Schrödinger equation (3) for the most difficult M values of the spiked oscillator problem and discuss the results. In Section 5 we choose the exactly solvable Schrödinger equation with a Coulomb potential in order to test the performance of the Euler and KJG transformations on several states of such a long-range potential. In Section 6 we comment on other approaches that have been applied to the Schrödinger equation with singular potentials. The main findings of this work are summarized in Section 7.

2 Change of variables

It is sufficient for our purposes to consider the Schrödinger equation

$$-\frac{\mathrm{d}^2\Psi}{\mathrm{d}r^2} + V(r)\Psi = E\Psi, \tag{4}$$

where either $r \in (0,\infty)$ or $r \in (-\infty,\infty)$ with the bound-state boundary conditions $\Psi(0) = \Psi(\infty) = 0$ in the former case and $\Psi(-\infty) = \Psi(\infty) = 0$ in the latter. We choose a one-to-one change of variable $x(r)$ with inverse $r(x)$ such that $\mathrm{d}x/\mathrm{d}r > 0$, and modify the wave function as $\Phi(x) = \Psi(r(x))/F(x)$ so that the resulting differential equation for $\Phi(x)$ is Hermitian. If we require that the scalar product has the same form for both variables,

$$\int \Psi^2 \mathrm{d}r = \int \Psi^2 \frac{\mathrm{d}r}{\mathrm{d}x}\mathrm{d}x = \int \Phi^2 \mathrm{d}x, \tag{5}$$

then we should choose

$$F(x) = \frac{1}{\sqrt{\mathrm{d}r(x)/\mathrm{d}x}}\cdot \tag{6}$$

The new wave function satisfies the Sturm-Liouville eigenvalue equation

$$-\frac{\mathrm{d}}{\mathrm{d}x}F^4\frac{\mathrm{d}}{\mathrm{d}x}\Phi + \left[V(r(x)) - F^3F'' - 2F^2F'^2\right]\Phi = E\Phi, \tag{7}$$

where primes indicate derivatives with respect to x.

Alternatively, one may modify the wave function as $\chi(x) = \Psi(r(x))/G(x)$, and set $G(x)$ so that no first derivative appears in the resulting differential equation. It is not difficult to verify that the appropriate $G(x)$ is just the reciprocal of $F(x)$:

$$G(x) = \sqrt{\frac{\mathrm{d}r(x)}{\mathrm{d}x}}, \tag{8}$$

and that we end with the *generalized* eigenvalue equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\chi + \left[V(r(x))G^4 - \frac{G''}{G} + 2\frac{G'^2}{G^2}\right]\chi = EG^4\chi. \tag{9}$$

Given that $G^4(x)$ is positive definite, this equation may be rewritten in an explicit Hermitian form by means of the Löwdin transformation $\Phi = G^2\chi$ that leads to

$$-\frac{1}{G^2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{1}{G^2}\Phi + \left[V(r(x)) - \frac{G''}{G^5} + 2\frac{G'^2}{G^6}\right]\Phi = E\Phi. \tag{10}$$

There is no doubt that equations (7, 10) are equivalent each other and to the original Schrödinger equation, although they exhibit different effective potentials and modified kinetic-energy terms that have been written in explicit Hermitian form. However, the corresponding matrix equations derived from discretization of those kinetic terms are not exactly equivalent as we will see below.

3 Discretization of the transformed equations

The next step is to obtain symmetrical discretized forms for the kinetic terms, with properties similar to the lowest order discretization of the second derivative in the standard Schrödinger equation

$$\frac{1}{h^2}\delta^2 = D^2 + \frac{h^2}{12}D^4 + \frac{h^4}{360}D^6 + \frac{h^6}{20160}D^8 + \cdots , \quad (11)$$

where D is the derivative operator and δ represents the centered second difference given by $\delta^2 f(x) = f(x-h) - 2f(x) + f(x+h)$. A relevant feature of equation (11) is that if we approximate D^2 by $\delta^2/\hbar^2$, then the error is a formal expansion containing only *even powers* of h, suitable for an efficient Richardson extrapolation. This process is analogous to the extrapolation method in the computation of integrals by means of the trapezoidal rule, where the correction is given by the Euler-McLaurin sum rule.

The matrix representation of the operator δ^2 is tridiagonal

$$[\delta^2]_{ij} = -2\delta_{ij} + \delta_{i,j+1} + \delta_{i+1,j}. \quad (12)$$

Therefore, in order to obtain the matrix representation of the kinetic-energy term in equation (10) one should multiply the tridiagonal matrix $[\delta^2]$ by a diagonal one $1/G(x)^2$, $x = ih$, from left and right. We thus obtain the symmetric representation

$$\left[-\frac{1}{G^2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{1}{G^2}\right]_{ij} \approx \delta_{ij}\frac{2}{G(ih)^4h^2} - \delta_{i,j+1}\frac{1}{G(ih)^2G((i+1)h)^2h^2} - \delta_{i+1,j}\frac{1}{G(jh)^2G((j+1)h)^2h^2} \cdot \quad (13)$$

The treatment of equation (7) is somewhat more complicated. One way of deriving an expansion analogous to equation (11) is to choose an average of two alternative combinations of forward $\Delta = \exp(hD) - 1$ and backward $\nabla = 1 - \exp(-hD)$ difference operators:

$$\left[-\frac{\mathrm{d}}{\mathrm{d}x}F^4\frac{\mathrm{d}}{\mathrm{d}x}\right] \approx -\frac{1}{2h^2}\left[\nabla F^4\Delta + \Delta F^4\nabla\right]. \quad (14)$$

In this way, the error exhibits only even powers of h as it follows from the fact that equation (14) is an even function of h.

From the matrix representation of the difference operators

$$[\Delta]_{ij} = -\delta_{ij} + \delta_{i+1,j}$$
$$[\nabla]_{ij} = \delta_{ij} - \delta_{i,j+1}, \quad (15)$$

(note that $[\Delta]^T = -[\nabla]$), one obtains the following matrix representation of the modified kinetic-energy operator

$$\left[-\frac{\mathrm{d}}{\mathrm{d}x}F^4\frac{\mathrm{d}}{\mathrm{d}x}\right]_{ij} \approx -\delta_{ij}\frac{F^4((i-1)h)+2F^4(ih)+F^4(i+1)h)}{h^2} + \delta_{i,j+1}\frac{F^4((i+1)h)+F^4(ih))}{2h^2} + \delta_{i+1,j}\frac{F^4((j+1)h)+F^4(jh))}{2h^2}\cdot \quad (16)$$

To those tridiagonal kinetic-energy matrices one has to add the diagonal terms that come from the effective potentials of equations (10) or (7). We may then obtain the desired eigenvalues by means of standard well-established algorithms for diagonalization of symmetric tridiagonal matrices.

4 Application to the spiked oscillator potential

We have carried out a set of calculations on the ground states of a family of spiked oscillators equation (3) with $\lambda = 10^{-4}$ and $M = 1, 3/2, 2, 5/2, 3, 7/2, 4$, using the KJG transformation equation (2) for a wide range of K values. In all the cases we have chosen a maximum value for the coordinate r equal to $r_{\max} = 10$, which proves sufficiently large for the harmonic oscillator, and therefore also for the spiked oscillators if λ is small enough (the most interesting and difficult case). The corresponding maximum value of the new variable $x_{\max}$ decreases with K. For each value of K the series of calculations starts with 512 intervals for the x variable, and their number is increased by an arbitrary scaling factor of 3/2 for a total of eight runs, resulting in a maximum number of steps of 8748. At each stage, we construct the Richardson extrapolation with all available previously computed values. The Fortran program is set to `REAL*16` that ensures a precision of more that 30 digits. The values of K are uniformly increased by an arbitrary scaling factor of 8 from $8^0 = 1$ through 8^{20}.

Although equations (7, 10) are equivalent, their corresponding discretization matrices are not (except in the limit $h \to 0$), and consequently they give different results for the straightforward integration. The main cause of this difference appears to be the abovementioned error series of even powers of the steplength that is readily removed by the Richardson extrapolation which brings both results into almost complete agreement.

At first sight the behaviour of our results in terms of K can be grouped in three cases: (a) $M = 1$, (b) $M = 3/2$ and $M = 2$, and (c) $M \geq 5/2$.

A common feature of all the calculations for cases (a) and (b) is that the eigenvalues obtained from direct diagonalization of the tridiagonal matrices are quite poor, and their accuracy deteriorates as K increases. On the other hand, the accuracy of the results for case (c) seems to improve slightly with K. Apparently, our naive idea that it is the concentration of mesh points in the interesting small-r

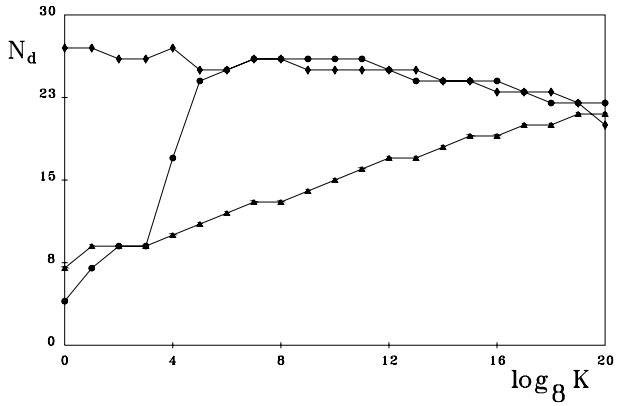

Fig. 1. Number of converged decimal digits N_d as a function of K, represented in the 8^K scale. Diamonds, triangles and circles correspond to $M = 1$, $M = 2$ and $M = 3$, respectively.

region by means of the transformation that improves the results is not altogether correct.

The effect of the value of K on the Richardson extrapolants is remarkable. Figure 1 shows the number of converged digits as a function of K for three representative cases of type (a), (b) and (c). We assume that a digit is converged if it does not change when comparing Richardson extrapolations with $n-1$ and n single evaluations. We have already tested this assumption on the exact ground-state eigenvalue $E = 2 + \sqrt{1+4\lambda}$ of the analytically solvable case $M = 2$.

Figure 1 shows that the best results for case (a) correspond to small values of K, that the accuracy slowly increases with K in case (b), and that in case (c) the precision increases sharply at small values of K, reaching a sort of optimal plateau ranging roughly from $K = 8^6$ up to $K = 8^{12}$, beyond which the accuracy decreases.

To understand those results it is convenient to pay attention to the relation between the exact eigenvalue E_{exact} and the result of a single numerical calculation with step h $E[h]$

$$E_{\text{exact}} = E[h] + \sum_{n=1}^{N} A_n h^{2n} + R_N(h). \qquad (17)$$

In this equation the unknown coefficients A_n depend on K but are independent of h, and the remainder R_N, which may be a complicated expression like the Euler-McLaurin formula, depends on of both K and h. If the remainder approaches zero sufficiently fast as h decreases, then one expects the Richardson extrapolation to do an efficient (often remarkable) job. But this favourable condition does not mean that the direct numerical integration is good; it may very well happen that $A_1, A_2, ...$ have large values, so that only after eliminating those power-series terms by the extrapolation one obtains accurate values for the energy E, even starting from poor values of $E[h]$. The fact that the value of K may not improve the straightforward integration, but that it does have a remarkably positive effect on the Richardson extrapolation suggests that the main role of the coordinate transformation is to somehow diminish the weight of the remainder of equation (17).

Some time ago Jamieson [7] derived an approximate expression for the remainder R_N for the spiked harmonic oscillator with $M = 6$. We have been unable to obtain a similar expression for the transformed equations which would be most useful to understand more clearly how the transformations work.

It is worth noticing that although the eigenvalues obtained by straightforward diagonalization of the matrices with the two discretization methods, based on the functions $F(x)$ and $G(x)$, are quite different, the set of extrapolations are in remarkable agreement. Apparently, the choice of the function that modifies the eigenfunction has more effect on the values of the coefficients A_n than on the remainder.

To give some examples of those features of the calculation, in Table 1 we show results of the straightforward diagonalization and the associated Richardson extrapolations. The impressive performance of the Richardson extrapolation is most noticeable in this table.

The Euler transformation also gives remarkable results for the eigenvalues of the spiked oscillators, although they do not appear to be as accurate as those coming from the KJG transformation.

5 Long-range potentials and excited states

In preceding sections we have seen that both the KJG and Euler transformations prove suitable for the treatment of potentials that change abruptly in a small neighborhood of the origin. Another numerical problem arises in the study of excited states of a potential well that approaches zero slowly. In such a case the integration should continue far from the origin in order to take into account the long tail of the wavefunction with sufficient accuracy. If one keeps constant the short steplength necessary to describe the region where the potential changes appreciably, then the number of points required to cover the entire region of meaningful values of the coordinate is enormous. On the other hand, a long steplength appropriate for the asymptotic region will not be fine enough to describe the region where the potential changes appreciably. Again, a properly chosen coordinate transformation may prove suitable for avoiding a variable steplength that would otherwise be advisable in such important and difficult problems.

The Euler and KJG transformations discussed above depend on an adjustable parameter K for fine tunning. It is clear that we should choose K so that $\mathrm{d}r/\mathrm{d}x$ does not increase too fast, because otherwise we will have an extremely large steplength at such great values of r as we have to include in our calculation. By simple inspection of the plots $\mathrm{d}r/\mathrm{d}x$ *vs.* r for the Euler and KJG transformations we conclude that the former requires large values of K whereas the latter requires small values of the adjustable parameter. The effect of such settings is particularly noticeable in the case of slightly bounded states whose wavefunctions have long tails that one has to take into account to obtain meaningful binding energies.

Table 1. Results from a single calculation of the eigenvalue and the best Richardson extrapolation as a function of the number of integration intervals, for the spiked oscillator with $M = 1$ and $K = 1$. The underlined digits are not converged.

Intervals	Single integration	Richardson extrapolation
512	3.00010 64405 96784	
768	3.00010 99942 88302	3.00011 28372 41516 40320 95501 39878
1152	3.00011 15736 60519	3.00011 28371 37807 45257 76433 46530
1728	3.00011 22755 94594	3.00011 28371 37807 78142 73473 45496
2592	3.00011 25875 63490	3.00011 28371 37807 78142 60123 07341
3888	3.00011 27262 15976	3.00011 28371 37807 78142 60123 11337
5832	3.00011 27878 39233	3.00011 28371 37807 78142 60123 11058
8748	3.00011 28152 27333	3.00011 28371 37807 78142 60123 11991

At first sight the Euler transformation appears to be most suitable for those long-range potentials because it shrinks the coordinate interval from $(0, \infty)$ onto $(0, 1)$ thus bypassing the problem of a too large integration region. However, as we will shortly see the KJG transformation also yields remarkably good results.

In order to test the performance of those transformations on a long-range potential, we choose the exactly solvable Schrödinger equation with a Coulomb interaction. It is sufficient for our present purposes to consider the radial Hamiltonian operator for s states

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{1}{r} \tag{18}$$

whose bound states $\Psi(r)$ satisfy $\Psi(0) = \Psi(r \to \infty) = 0$. Knowledge of the exact energies $E_n = -1/(4n^2)$, $n = 1, 2, ...$ enables us to test our results more easily.

We have carried out several calculations choosing $r_{\max} = 10\,000$ for the KJG transformation and $r_{\max} = \infty$ for the Euler transformation. For both transformations we started with a small number of initial intervals and successively increased them by a factor 3/2 seven times. In all the calculations we have resorted to a sequence of 7 Richardson extrapolations ranging from 2 to the maximum of the resulting 8 single evaluations. We have empirically estimated the degree of convergence by comparing two consecutive Richardson extrapolations (with $n-1$ and n single evaluations). As before, we can test this assumption because we know the exact energies.

Table 2 shows that both transformations give accurate results with a strikingly small number of mesh points. For comparison, notice that in order to obtain results of the same quality for the state $n = 8$ without a transformation we have to start with 700 intervals.

Table 2. Estimated errors in the calculation of the energies of the Coulomb potential by means of the Euler and KGJ transformations.

n	K	Transformation	Initial intervals	Estimated error
1	2	Euler	16	0
	1	KGJ	16	0
4	16	Euler	16	0
	1/2	KGJ	16	2×10^{-14}
8	128	Euler	16	0
	1/4	KGJ	16	1×10^{-11}
	1/2	KGJ	24	3×10^{-14}
16	256	Euler	16	2×10^{-11}
	256	Euler	24	8×10^{-14}
	256	Euler	36	0
	1/16	KGJ	24	7×10^{-12}
	1/32	KGJ	36	6×10^{-14}
32	1024	Euler	36	2×10^{-13}
	1/256	KGJ	36	2×10^{-14}

6 Other methods

Because of their mathematical and physical importance, singular potentials in general, and spiked harmonic oscillators in particular, have been treated by many methods. Those approaches that provide upper and lower bounds are useful to test the accuracy of more accurate numerical algorithms [8–10]. Perturbation theory with an appropriate renormalization of the perturbation series (variational perturbation theory) gives accurate eigenvalues [11,12]. The analytic continuation method is both simple and sufficiently accurate for most physical applications [13]. Expansion of the unknown eigenfunctions of H in a basis set of eigenfunctions of a properly chosen unperturbed Hamiltonian H_0 leads to a secular equation that one solves rapidly and accurately with today's personal computers [11,14–17]. In this case the addition of convenient nonlinear adjustable parameters greatly improves the velocity of convergence of the variational method [14–17]. The Lanczos algorithm has not produced the most accurate results for spiked harmonic oscillators [18], but one can in principle improve them as much as desired by enlargement of the basis set. The representation of the eigenfunctions by means of a B-spline basis set is another standard method that has yielded remarkably accurate results [19]. There are other numerical integration algorithms in addition to those discussed above that have also been applied to the potentials considered here [2,11,12,20].

The choice of one of the accurate approximate methods just mentioned is mainly a mater of taste because most of them give sufficiently accurate results for most physical applications. We believe that numerical integration is probably more flexible, than perturbation theory and the analytic continuation method. The expansion in a basis set requires the calculation of matrix elements that is far from being naive in the case of most singular potentials. The expansion in a B-spline basis set leads to a generalized eigenvalue equation that one expects to be less efficiently solved than the much simpler tridiagonal matrix equation produced by present numerical integration algorithm. For all these reasons we propose present method as a simple and accurate way of solving the Schrödinger equation with a singular potential energy-function.

7 Summary

The main contributions of this paper are:

- a development of discretized symmetric expressions of the transformed Schrödinger equation for the application of standard numerical routines for tridiagonal matrices;
- high-precision calculations that have enabled us to investigate the performance of different variable transformations in great detail. Under such conditions we have disclosed the amazing effect of the KJG transformation on the Richardson extrapolation, commonly used to improve the results of numerical integration algorithms;
- we have also shown that the Euler and KJG transformations are most suitable for long-range potentials as they yield accurate results with a remarkably small number of mesh points.

Present numerical results suggest that it may prove fruitful to carry out a rigorous mathematical investigation of the reasons for the remarkable improvement of Richardson extrapolation under appropriate coordinate transformations.

The changes of variable discussed throughout this paper are suitable when $r \in [0, \infty)$. We can think of similar transformations when $r \in (-\infty, \infty)$; for example,

$$r = \frac{Kx}{\sqrt{1-x^2}}, \; x = \frac{r}{\sqrt{K^2+r^2}} \tag{19}$$

that leads to a variable steplength determined by $\mathrm{d}r/\mathrm{d}x = (K^2+r^2)^{3/2}/K^2$.

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