

Improvements on a New Method for the Numerical Solution of the Schrödinger Equation*

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Two procedures are described for improving the accuracy and efficiency of a method recently proposed for the numerical solution of the bound state Schrödinger equation. Firstly, an analysis of the errors in the method dictates the most efficient way for obtaining accurate results and also allows for the use of extrapolation techniques. Secondly, an expansion around the solution for a harmonic oscillator potential yields a more rapidly convergent procedure. Illustrations for a simple one-dimensional potential are given.

1. INTRODUCTION

By considering an approximate closed form for the operator $\exp(-\beta H)$, where H is the Hamiltonian for the system and β is a real parameter, we have shown how it is possible to write down an approximate integral eigenvalue equation for the Schrödinger equation [1], which can then be solved by standard quadrature methods to obtain numerical approximations to the eigenvalues and eigenfunctions of the Schrödinger equation. For many potentials this method offers several advantages over the standard integration techniques, particularly with regard to obtaining information about a number of bound state eigenvalues from the one calculation. For a given required accuracy, our experience has been that the calculations can be performed with a comparable amount of computation to the more standard techniques, and in the case of nonlocal potentials [2, 3] with considerably less. The purpose of this paper is to point out two ways which have proved helpful in further reducing the amount of computation.

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2. EXTRAPOLATION TECHNIQUES

By considering the errors made in the solution by quadratures, it is possible to employ standard extrapolation methods to improve the eigenvalue estimates. To see this, we note that for sufficiently well-behaved potentials V (V bounded and differentiable to all orders), the operator expansion ([1, Eq. (2.10)]) enables us to write (for the ground state energy E_0 , for example)

$$e^{-\beta E_0} = e^{-\beta E_0(\beta)} + \sum_{j \geq 3} a_j \beta^j, \tag{2.1}$$

where $E_0(\beta)$ is the (exact) eigenvalue of the integral equation [1, Eq. (2.15)]

$$e^{-\beta E_0(\beta)} \psi_0(x; \beta) = \int_0^\infty e^{-\frac{1}{2}\beta V(x)} \langle x | e^{-\beta H_0} | x' \rangle e^{-\frac{1}{2}\beta V(x')} \psi_0(x'; \beta) dx' \tag{2.2}$$

and the coefficients a_j are well-behaved (in principle, the a_j 's could be obtained by perturbation theory, but that is not necessary for the purposes here). To simplify the notation, we have considered only the one-dimensional form of the Schrödinger equation in this paper, but the generalization to more than one dimension follows in a straightforward manner. For computational convenience, the integral is truncated at some (large) distance R under the assumption that $\psi_0(R) \rightarrow 0$ as $R \rightarrow \infty$.

In [1, 2] the approximation $E_0(\beta)$ was obtained by solving Eq. (2.2) by numerical quadratures; i.e., by replacing the integral equation by the matrix equation

$$e^{-\beta E_0(\beta)} \psi_i = \sum_{j=0}^N w_j A_{ij} \psi_j, \quad \psi_i = \psi_0(x_i; \beta), \tag{2.3}$$

$$A_{ij} = e^{-\frac{1}{2}\beta V(x_i)} \langle x_i | e^{-\beta H_0} | x_j' \rangle e^{-\frac{1}{2}\beta V(x_j')}$$

$x_i = i\Delta$, $0 \leq i \leq N$, $N\Delta = R$ (the range of the potential), and w_j is a weighting factor depending on the quadrature rule. Now it has been shown [4, 5] that each eigenvalue of an integral equation can be approximated by the eigenvalue of the corresponding matrix equation to an accuracy proportional to the error involved in the quadrature rule employed. Thus we may write

$$e^{-\beta E_0(\beta)} = e^{-\beta E_0(\beta, \Delta)} + \sum_{j \geq \sigma} b_j \Delta^j, \tag{2.4}$$

where $E_0(\beta, \Delta)$ is the (numerical value of) eigenvalue of Eq. (2.3), and σ is determined by the quadrature rule. Thus, from Eq. (2.1) we may write

$$e^{-\beta E_0} = e^{-\beta E_0(\beta, \Delta)} + \sum_{j \geq 3} a_j \beta^j + \sum_{j \geq \sigma} b_j \Delta^j, \tag{2.5}$$

or, taking logarithms and expanding, we obtain the following asymptotic expansion for E_0 ,

$$E_0 = E_0(\beta, \Delta) + \sum_{j \geq \nu} R_j \frac{\Delta^j}{\beta} + \sum_{j \geq 2} S_j \beta^j + \sum_{i \geq \nu} \sum_{j \geq 2} T_{ij} \Delta^i \beta^j, \quad (2.6)$$

where R_j , S_j , and T_{ij} are some constants, depending on the values of a_j , b_j .

For the trapezoidal rule ($\nu = 2$), for example,

$$\begin{aligned} E_0 = E_0(\beta, \Delta) + \frac{\Delta^2}{\beta} (R_2 + R_3 \Delta + R_4 \Delta^2 + \dots) \\ + S_2 \beta^2 + S_3 \beta^3 + \dots \\ + T_{22} \Delta^2 \beta^2 + \dots \end{aligned} \quad (2.7)$$

Thus we recover the conditions we noted before [1], namely, that $E_0(\beta, \Delta)$ is a good approximation to the actual eigenvalue provided $\Delta^2 \ll \beta$ and Δ and β are both small. Moreover, if Δ^2/β is kept constant as $\Delta, \beta \rightarrow 0$, we see that

$$E_0(\beta, \Delta) \rightarrow (E_0 - (\Delta^2/\beta) R_2).$$

Moreover, the convergence rate is quite slow; substituting $\Delta^2 \sim \beta$ into Eq. (2.7) we find

$$E_0 = E_0(\beta, \Delta) + R_2 \frac{\Delta^2}{\beta} + \sum_{j \geq 1} C_j \beta^{j/2}, \quad (\Delta^2/\beta \text{ constant}). \quad (2.8)$$

However, the final accuracy of the result depends not only on the ratio Δ^2/β , but on the value of R_2 ($= b_2$), which for the trapezoidal rule is quite small. This can be appreciated by noting that the integrand represented by Eq. (2.2) has the property that its values at the end points of the range of integration are equal. If the quadrature formulae were employed over the whole region, the Euler-Maclaurin formula [6], would imply that ν [in Eq. (2.4)] had a much larger value than 2. However, since the integrals were truncated at some large distance R , this is not entirely true, but certainly the value of R_2 can be seen to be small for large R .

Taking Simpson's Rule ($\nu = 3$) and a set of calculations performed such that Δ/β remains constant as $\Delta, \beta \rightarrow 0$, we find

$$E_0 = E_0(\beta) + \sum_{j \geq 2} C_j \beta^j, \quad (\Delta/\beta \text{ constant}), \quad (2.9)$$

so that the error term in the calculated value is $O(\beta^2)$ (at least asymptotically), and the results converge rapidly to the exact eigenvalue of H .

To illustrate this last result, we considered the one-dimensional Schrödinger equation with the potential $V(x) = 20 \tanh^2(x)$, which has the exact ground state

$\psi_0(x) = \text{sech}^3(x) \tanh(x)$, $E_0 = 11$. Using the power method of [1] we obtained a number of estimates of E_0 for different values of β (with $\beta = \Delta$). The results are illustrated in the first 3 columns of Table I (N here represents the number of grid points). The remaining columns of Table I demonstrate the increase in accuracy

TABLE I
Neville's Table for the Calculation of the Lowest Energy Value of the Potential,
 $V(x) = 20 \tanh^2(x)$

β	N	$E_0(\beta)$	$E_0(\beta_i\beta_j)$	$E_0(\beta_i\beta_j\beta_k)$	$E_0(\beta_i \cdots \beta_l)$	$E_0(\beta_i \cdots \beta_m)$
0.06667	150	10.934843				
			10.998761			
0.07143	140	10.925386		10.999899		
			10.998381		10.999920	
0.07692	130	10.913724		10.999888		10.999823
			10.997837		11.000003	
0.08333	120	10.899121		10.999816		
			10.997052			
0.09091	110	10.880506				

by extrapolation to the limit of small β using a Neville's table [6]. Successive columns to the right represent the values of the Neville's extrapolants, defined by (for example)

$$E_0(\beta_i\beta_j\beta_k) = [\beta_k^2 E_0(\beta_i\beta_j) - \beta_i^2 E_0(\beta_j\beta_k)] / (\beta_k^2 - \beta_i^2).$$

As is well known one must not continue extrapolating too far because of the loss of significant figures produced by this method [6]. On the other hand, one of the advantages of the Neville's Table lies just in the fact that it is easy to tell from the table itself when the extrapolation should be completed: for our particular calculation, we should not proceed beyond the cubic extrapolant. Of course, the overall accuracy (in this case to 6 significant figures) is determined by the accuracy of the individual estimates (3rd column), which, in turn, is controlled by deciding when the power method had converged (in this case when successive estimates differed by less than 0.001 % of the current value).

To determine the accuracy of the final result, we reconstructed the Neville's table several times, replacing, in turn, each estimate of E_0 by the value $E_0(\beta) - \epsilon$, where ϵ is the tolerance allowed in the power method, and we took the minus sign because the power method converges to the eigenvalue from above. One estimate of the error is then the largest difference suggested by each of these reruns. Applying this criterion suggests the result $E_0 = 10.9999 \pm 0.0001$. To obtain a similar accuracy without extrapolation requires a value of $N \approx 640$. Using the grid changing method described in [1], the calculation of E_0 then takes approximately 1 min on the CDC6400. Compared with this, each of the estimates needed for Table I take approximately 1 sec, so that the entire calculation can be performed in less than 5 sec.

3. THE HARMONIC OSCILLATOR APPROXIMATION

In using the iteration procedure (see [1, 7]) to project out the ground state of some system, it is clear that the convergence rate depends on the value of β ; in general, larger β implies a faster convergence rate [1, Eq. (4.3)]. However, at the same time using larger values of β increases the errors, so that although the method might converge more rapidly, the results will not be converging to the desired accuracy. This state of affairs can be improved by observing that since the errors in the expansion of the operator $\exp(-\beta H)$ depend upon the derivatives of $V(x)$, by absorbing as much of the variation of V into H_0 as possible, we may reduce the errors in the procedure.

One particularly convenient form occurs when H_0 is the Hamiltonian for a particle in a harmonic oscillator potential; i.e., $H_0 = (-\partial^2/\partial \mathbf{x}^2 + \omega^2 \mathbf{x}^2)$. A closed form for the Green's function $\langle \mathbf{x} | e^{-\beta H_0} | \mathbf{x}' \rangle$ needed for setting up the kernel in Eq. (2.2) has been given in [1], viz,

$$\langle \mathbf{x} | e^{-\beta H_0} | \mathbf{x}' \rangle = \left[\frac{\omega}{2\pi \sinh(2\beta\omega)} \right]^{3/2} \times \exp \left[-\frac{\omega}{2} \coth(2\omega\beta)(\mathbf{x}^2 + \mathbf{x}'^2) + \omega \operatorname{cosech}(2\omega\beta) \mathbf{x} \cdot \mathbf{x}' \right]. \quad (3.1)$$

Now, given an operator of the form $H = -\partial^2/\partial \mathbf{x}^2 + V(\mathbf{x})$, the division into $H = H_0 + U(\mathbf{x})$, $U(\mathbf{x}) = V(\mathbf{x}) - \omega^2 \mathbf{x}^2$, enables us to write

$$\langle \mathbf{x} | e^{-\beta H} | \mathbf{x}' \rangle \approx e^{-\frac{1}{2}\beta U(\mathbf{x})} \langle \mathbf{x} | e^{-\beta H_0} | \mathbf{x}' \rangle e^{-\frac{1}{2}\beta U(\mathbf{x}')}, \quad (3.2)$$

or, after rearranging,

$$\langle \mathbf{x} | e^{-\beta H} | \mathbf{x}' \rangle \approx e^{-\frac{1}{2}\beta \tilde{V}(\mathbf{x})} \frac{1}{(4\pi\gamma)^{3/2}} \exp[-(\mathbf{x} - \mathbf{x}')^2/4\gamma] e^{-\frac{1}{2}\beta \tilde{V}(\mathbf{x}')}, \quad (3.3)$$

where

$$\tilde{V}(\mathbf{x}) = V(\mathbf{x}) + \frac{\omega}{\beta} (\tanh(\beta\omega) - \beta\omega) \mathbf{x}^2,$$

and

$$\gamma = (\sinh/2\omega)(2\omega\beta).$$

Now, iteration, using the kernel Eq. (3.3) on to some initial function, will eventually produce the ground state energy value of H . Moreover, it is expected that this division of H (as against that based on the free particle case in [1]) will provide a faster rate of convergence by virtue of the choice of the additional parameter ω , which can be chosen to minimize the effect of the term $U(\mathbf{x})$ and hence reduce the errors.

Obviously, the ability to use this approach depends on being able to predict (in advance) a suitable value of ω . This can be done approximately if we note that Eq. (3.2) is exact for all β when $V(\mathbf{x}) = \omega^2\mathbf{x}^2$, i.e., when we are looking for the smallest eigenvalue for a harmonic oscillator. Now when $V(\mathbf{x}) \neq \omega^2\mathbf{x}^2$ we are suggesting that there exists a value of ω for which the lowest eigenfunction of the harmonic oscillator potential is a better approximation to the lowest eigenfunction for the potential $V(\mathbf{x})$ than the free particle wavefunction (as in [1]). If this is the case, a value of ω can be found by minimizing the variational quantity

$$\epsilon(\omega) = \int \Phi_0(\mathbf{x}) H\Phi_0(\mathbf{x}) d\mathbf{x}, \tag{3.4}$$

where $\Phi_0(\mathbf{x})$ is the ground-state harmonic oscillator wavefunction.

To illustrate these ideas, we have applied them to the simple problem of Section 2. Taking a range of values of ω , we calculated the corresponding estimates of E_0 using the power method of [1]. For the trapezoidal rule, we have the expansion Eq. (2.7), so that for constant (small) Δ ,

$$E_0 = E_0(\beta, \Delta) + \frac{C_0}{\beta} + \sum_{j \geq 2} C_j\beta^j,$$

where following the arguments of Section 2, the coefficient C_0 is very small. Unless β is so small that the second term on the right hand side dominates, the calculations performed in this manner should be linear in β^2 (at least over a range of values of small β). This is shown to be the case in Fig. 1, where we have plotted the results for a number of values of ω . The importance of these results can be seen from the curves for $\omega = 0$ and 2.9; using a value of $\omega = 2.9$ we are able to use a value of β approximately twice as large as that for $\omega = 0$ and will obtain as accurate results.

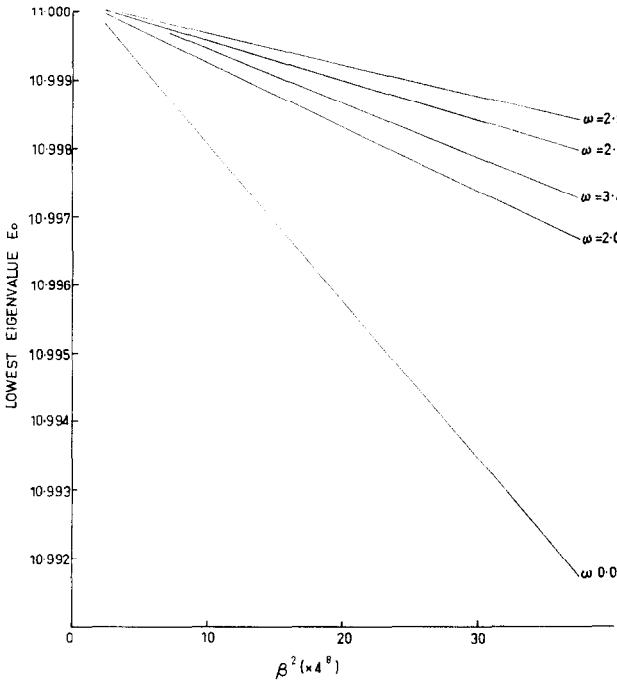


FIG. 1. Values of $E_0(\beta, \Delta)$ plotted against β^2 for different values of ω . For small β the errors are $O(\beta^2)$.

At the same time, the convergence rate will be greatly improved; (the number of iterations is essentially halved).

In Fig. 2 we have plotted the difference between the calculated and exact energy value against ω for a fixed value of β . It is seen that the best value of ω is approximately $\omega = 2.9$. In fact, this agrees very well with the value found from Eq. (3.4); for the one-dimensional harmonic oscillator we take

$$\Phi_0(x) = 2 \left(\frac{\omega^3}{\pi} \right)^{1/4} x e^{-\frac{1}{2}\omega x^2},$$

so that

$$\epsilon(\omega) = \frac{3\omega}{2} + 4 \sqrt{\frac{\omega^3}{\pi}} \int_0^\infty V(x) e^{-\omega^2 x^2} x^2 dx.$$

Putting $V(x) = 20 \tanh^2(x)$ into this expression, and calculating the value of ω which minimizes $\epsilon(\omega)$ numerically, we find $\omega = 2.94$.

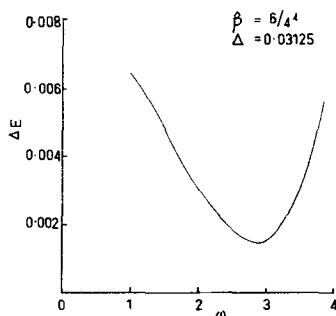


FIG. 2. Showing the error (ΔE) in the ground-state energy value as a function of the harmonic oscillator parameter ω . The calculations were performed with $\beta = 6/4^4$ and $\Delta = 0.03125$.

DISCUSSION

In this paper we have described two valuable methods for improving the efficiency of a numerical method we recently proposed for the numerical solution of Schrödinger's equation. We have derived an asymptotic error expansion for the method which not only allows one to get some estimate of the accuracy of the calculations, but also suggests several possible numerical procedures for obtaining very accurate results with only a relatively small computing time. Together with the harmonic oscillator approximation which can be employed to give considerably faster convergence, the approximate integral eigenvalue approach to the numerical solution of the Schrödinger equation provides a technique which is at least competitive to the standard numerical integration methods normally used, and in certain cases, a considerable improvement.

Although most of what has been described here has been applied particularly to the ground-state, a discussion of the errors for the higher bound states is quite analogous. Moreover, information about the higher angular-momentum states follows in a similar manner by noting the explicit form for the kernel given in [1, Eq. (6.2)]. The harmonic oscillator approximation can also be generalized to the higher energy states in a straightforward manner.

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