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Calculating probabilities without quadrature

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Abstract   It is shown that a direct method for bound states can give the integrated probability over a given region and also the normalised squared wavefunction at a given point without using any quadratures or wavefunction storage. The method is tested on a known example and is then applied to an asymmetric double well potential and also to find the probability of penetration of a particle into the non-classical region for a single well potential.

1 Introduction

In a recent study of quantum tunnelling effects and their relation to complex classical mechanics in the large energy limit Bender and Hook [1] studied two asymmetric double well potentials, for which they calculated the integrated probability to the right of the central peak in the potential for several bound states The method which was used to find these probabilities was a 9th order Runge–Kutta adaptive shooting method (as provided in Mathematica), with a facility to perform quadrature over selected regions. In the present work we treat one of the potentials of [1] as well as several other potentials and show that integrated probabilities over a region, as well as point values of the

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squared normalised wavefunction, are obtainable to high accuracy without storing the wavefunction. No quadrature is needed, either to find the probabilities or to calculate normalisation constants. The crucial step is to realize that the desired quantities are just the expectation values of Heaviside functions or delta functions and so can be found using a simple formalism which directly gives expectation value for a one dimensional potential [2].

In Sects. 2.1–2.4 we describe the most simple possible form of the method and then test it on some harmonic oscillator problems for which exact analytical results are known. Having demonstrated that the method is reliable we then apply it in Sect. 3 to a double well potential treated in [1], calculating the probabilities and also several extra expectation values which indicate the localisation of some of the eigenfunctions. We then apply the method in Sect. 4 to investigate a proposed law that the integrated probability over the non-classical region should vary as $(n + 1/2)^{-1/3}$ for bound states of high quantum number n in a single well potential. This result has only been established for the simple harmonic oscillator [3,4] (because of its exactly known analytical wavefunctions). The technique of this paper allows us to show that the law is also valid for other potentials (which suggests that it might ultimately be derivable by an approach based on JWKB theory). Section 5 gives a discussion of the method used and its relationship with other methods.

The present work has a dual purpose. It is intended to show in some detail HOW the computations are done and also to give sufficient mathematical background to explain WHY they work. We have thus adopted a hybrid (but easily understandable) notation. We keep the traditional = equality sign in the mathematical equations but in the specimen program segments we use the historic Algol symbol : = in the assignment statements. To condense several statements on to one line (for brevity) we use the : separator symbol of QBasic.

2.1 An incremental Hartree method

If we use the lowest order finite difference representation of the kinetic energy operator—$\alpha\,D^2$ in the Schrodinger equation then we obtain the result

$$\alpha\,D^2\Psi\,(x) = \alpha\,h^{-2}\,[\Psi\,(x+h) + \Psi\,(x-h) - 2\Psi\,(x)] = [V\,(x) - E]\,\Psi\,(x) \quad (1)$$

where h is the fixed steplength. Re-arranging (1) directly gives the traditional shooting recurrence relation (often named after Hartree [5]):

$$\Psi\,(x+h) = \left[2 + \left(h^2/\alpha\right)\,(\,V\,(x) - E)\right]\Psi\,(x) - \Psi\,(x-h) \quad (2)$$

It is clear that in the direct use of (2) the constant term 2 will tend to dominate the term involving h^2, particularly if we use a sequence of decreasing h values in order to apply Richardson extrapolation. To reduce the associated rounding errors for our accurate probability calculations we have produced a new incremental form of (2) by introducing the variable

$$G(x + h/2) = h^{-1} [\Psi(x + h) - \Psi(x)] \qquad (3)$$

which is a good estimate of the gradient of Ψ at the midpoint $(x + h/2)$. We then replace (2) by the pair of "leapfrog" equations (involving h rather than h^2):

$$G(x + h/2) = (h/\alpha)[V(x) - E]\Psi(x) + G(x - h/2) \qquad (4a)$$
$$\Psi(x + h) = \Psi(x) + hG(x + h/2) \qquad (4b)$$

2.2 Direct expectation values

The expectation value <U> of a function U(x) is traditionally defined to be the integral over all space of the product of U(x) and the squared normalised wavefunction. However, perturbation theory shows that <U> can be interpreted as a response coefficient. Adding a very small perturbation λU(x) to the potential V(x) gives the first order energy shift λ <U>, so that <U> can be found by calculating the resulting energy shift. This can be done directly within the same shooting process which finds the energy [2]. If we suppose that the small term λU(x) is added to V(x) then we can differentiate Eqs. (4a), (4b) with respect to E and with respect to λ, using the mnemonic symbols ΨE, ΨU,GE and GU for the derivatives involved (and also noting that the λU term is a "virtual" one, since the derivatives are formally to be taken at $\lambda = 0$). On performing the differentiations we see that the pairs $(\Psi E,GE)$ and $(\Psi U,GU)$ obey the Eqs. (4a), (4b), except for an extra term on the right in (4a) which arises from the derivative of the term involving h. Using all the recurrence relations simultaneously is not computationally expensive, since the term $(h/\alpha)(V - E)$ is common to all three.

Since we wish to show how simple the calculation is in practice and also to emphasize that only ONE value of each variable (the current value) is ever stored, we give the sets of equations in the form of assignment statements. Since Greek symbols are not available in most computer programming languages we have used W (for wavefunction) in place of Ψ and the symbols H and HA for h and h/α, with the standard symbol * to denote multiplication. At each step we use the current x to evaluate the quantity $T = HA*(V-E)$ and then use T in the set of recurrence relations as follows (where U is the function for which we seek <U>):

$$GE := T^*WE + GE + HA^*W \quad : \quad WE := WE + H^*GE \qquad (5a)$$
$$GU := T^*WU + GU + HA^*W^*U \quad : \quad WU := WU + H^*GU \qquad (5b)$$
$$G := T^*W + G \qquad\qquad\qquad : \quad W := W + H^*G \qquad (5c)$$

Note that since all new values depend on the previous W we must only update W to its new value as the last operation. To use the three recurrence relations to find an energy eigenvalue and the expectation value of U(x) we perform the shooting process for a trial E (using the the set of recurrence relations "in parallel"). If the wavefunction at the starting point $x = x_0$ is zero than we can initially set $x = x_0$, with W and the other four variables all set to zero and with G given the value 1 (or any positive value, because of subsequent scaling). Using the values of the variables at the upper boundary

x = L (where we require that the wavefunction shall be zero) we find a Newton's law correction for the trial E. The corrected energy and the estimated expectation value <U> (denoted by UX) are given by the assignment statements

$$E := E - W/WE \quad : \quad UX := -WU/WE \tag{6}$$

Some initial trial E must be chosen but after a few iterations using (6) the energy will reach a stable value E(h). If desired the WU recurrence relation need only be used to give the desired expectation value <U> (h) when the energy has finally converged. After performing the shooting process for several decreasing h values we can extract accurate values for both E and <U> by traditional Richardson extrapolation of the E(h) and <U> (h) sequences.

   Equation (6) involve only RATIOS of the variables at the endpoint. Overflow and underflow of numerical values during the shooting can thus be avoided by the simultaneous scaling of all six variables by the same positive factor. Dividing by the modulus of the current W value is the most simple way to perform the scaling. Despite the scaling, the points at which W and G change sign (if recorded for the smallest h used) will give accurate positions for the nodes and extrema of the wavefunction.

   Although to make the present work self-contained we have outlined some of the existing basic theory [3,6] in the preceding discussion, we have made an original blend of equations and assignment statements in order to stress how simple the actual computational implementation of that theory is. In particular, the application of our basic theoretical approach to an incremental Hartree equation appears for the first time in the present work, as does the "point source" derivation of the delta function operator U_1 in the following section.

2.3 The representation of the singular functions

There are various representations of the delta function at a point x_0 in terms of Gaussian or other functions with decreasing width and increasing height. However, rather than using such a family of continuous functions we found that it is better to consider the effect of a delta function point source at x_0 when regarded as a potential term in the Schrodinger equation with kinetic energy operator $-\alpha D^2$. A formal integration through the point x_0 gives the well—known result that the delta source produces a discontinuity with the magnitude $\alpha^{-1} \Psi(x_0)$ in the gradient of the wavefunction. To simulate this effect all we need to do is to use the isolated effective potential term V = 1/h at x = x_0, since this can be seen to produce exactly the same jump in the gradient of the wavefunction. This potential has the new characteristic that it varies with h. From another point of view we can regard it as representing a rectangle of width h and height 1/h which is centred on x_0 and has an area of 1. To simulate the Heaviside function H(x − x_0) seems to be simple, in that the potential function required would be 1 for x > x_0 and 0 for x < x_0 .However,this would leave an ambiguity at x = x_0. We have found that the appropriate finite difference procedure is to set the potential function equal to 1/2 at x = x_0, thus giving a linear ramp between the values 0 and 1. Since we are using a finite difference method with a steplength h we can suppose that

the coordinate value x = x_0 appears at a known lattice point N_0. Recalling that in the formalism U is the symbol for the function for which we are seeking <U>, we denote the effective delta and Heaviside potentials by U_1 and U_2, respectively. Our proposed potentials then have the following finite difference description:

$$
\begin{array}{lll}
(N < N_0) & U_1 = 0, & U_2 = 0 \\
(N = N_0) & U_1 = 1/h, & U_2 = 1/2 \\
(N > N_0) & U_1 = 0, & U_2 = 1
\end{array}
\tag{7}
$$

Once these effective potentials have been incorporated in the subroutine of a program which evaluates the potential function at a given x then it is possible to give any potential functions a limited (or even bounded) support by multiplying it by appropriately placed U_2 Heaviside functions. For example, if we multiply the Schrodinger equation by the first derivative $\Psi^{(1)}$ of Ψ and then integrate over x between X and infinity (where the wavefunction and its derivative are taken to be zero) the result can be written in the form

$$
<H(x - X) V^{(1)}> = \alpha \left[\Psi^{(1)}(X) \right]^2 + (E - V(X)) [\Psi(X)]^2
\tag{8}
$$

which relates the values of the wavefunction and its derivative at a point x = X to an expectation value of the gradient of the potential over the region from X to infinity.

In the mathematical derivation the expectation value on the left of (8) actually appears as the integral of the product $V^{(1)}[\Psi(x)]^2$ between X and infinity, where the wavefunction is supposed to be normalised over the FULL x axis. This example illustrates clearly the simplification introduced by interpreting expectation values as energy response coefficients.

2.4 Testing the singular potential terms

For the harmonic oscillator Hamiltonian $-D^2 + x^2$ the energy levels and their associated wavefunctions are known exactly and so provide test data for the proposed finite difference representations of the delta and Heaviside functions. For the two lowest states with $E_0 = 1$ and $E_1 = 3$ we have the analytical results

$$
[\Psi_0(0)]^2 = \pi^{-1/2} \quad \text{and} \quad \left[\Psi_1^{(1)}(0) \right]^2 = 2\pi^{-1/2}
\tag{9}
$$

Shooting over the interval $[-10, 10]$, with the wavefunction assumed to be zero at both ends and using the doubling sequence of five strip numbers from 100 to 1,600 our proposed U_1 potential gave (after Richardson extrapolation of the five $<U_1>$ values) the result $[\Psi_0(0)]^2 = 0.56418958354776$, which agrees to all digits with the exact analytical result. Calculating the expectation value $<H(x - 0)2x>$ using the Heaviside U_2 as the multiplier gave exactly the same numerical result, in accord with Eq. (8) above. To find the squared gradient of the wavefunction at the origin, since we do not have a direct version of an appropriate operator we are constrained to use

Table 1 The expectation values of U_1, representing $\Psi^2(0)$, and of $2xU_2$, representing $<H(x-0)V^{(1)}>$ for the Hamiltonian $-D^2 + x^2$

NS	$<U_1>$	$<2xU_2>$
100	0.5659711482830545	0.5588641758246479
200	0.5646314974960592	0.5628650314106558
400	0.5642998479183509	0.5638588645519439
800	0.5642171363072899	0.5641069298976592
1600	0.564196470905084	0.5641689217649956

The two quantities vary in opposite directions as the strip number NS varies but Richardson extrapolation gives the same h=0 limit of $\pi^{-1/2}$ for both columns. The shooting region is $[-10, 10]$
Richardson extrapolation of both columns gives 0.56418958354776

Eq. (8) and so use the multiplier U_2 in a calculation of $<H(x-0)2x>$ for the first excited state with the energy 3. Using the same parameters as for the first calculation we obtained the numerical result 1.12837916709551 for the expectation value, which agrees to all digits with the squared gradient of Ψ_1 at the origin given in (9). As a specimen set of results we show in Table 1 the five results obtained for the two different ways of calculating the squared groundstate wavefunction at the origin. As expected, the two numerical values differ at each h value but they are tending towards the same limiting value as h tends to zero, since in that limit we arrive at the equality (8) of exact calculus. The Richardson extrapolation process extracts those limiting values and shows that they are equal.

Having shown on this exact test problem that the proposed finite difference potentials U_1 and U_2 can give accurate results, we repeated the calculations for the potential x^4, for which there are no exact analytical results. The method worked just as easily as for the harmonic oscillator case and showed that the squared groundstate wavefunction at the origin has the numerical value 0.628751369372725, while the squared wavefunction gradient at the origin for the first excited state has the numerical value 2.04917066889810.

These double precision tests indicate that the potentials U_1 and U_2 do indeed give accurate finite difference simulations of the delta and Heaviside functions, respectively, so that we can now apply them with confidence to the two problems cited in the introduction.

3 An asymmetric double well problem

An asymmetric double well potential is given in factored form in Eq. (1) of [1]. On multiplying out the brackets we obtain the explicit polynomial potential

$$V(x) = 3.5\,x^4 - 5.39\,x^3 - 14.48825\,x^2 + 16.37825x \qquad (10)$$

The central maximum between the two wells appears at $x = X_0$, where X_0 does not seem to be any obvious simple number; the best that we can do is to quote its numerical

Table 2 The energies and P(x > X_0) values for the states 0–5 of the asymmetric double well potential of Eq. (10)

n	E	P(x > X_0)
0	−18.0182362094496	2.84560350738(−6)
1	−7.18785142638893	9.95933274498(−1)
2	−6.85945455860846	4.31559441706(−3)
3	1.68064155058050	5.97584214433(−1)
4	2.88446251290660	4.07688957353(−1)
5	8.33121546914676	5.07459041529(−1)

The computational parameters used are given in the text. The first six digits of the probabilities agree with the results given as percentages in [1] for the states 1–4. ([1] does not give results for the two states 0–5)

value as X_0 = 0.4884007905025242 to double precision. Nevertheless, this apparent complication does highlight a feature of the finite difference approach which will also play a role in the calculations of Sect. 4. The point is that we must ensure that X_0 falls at a lattice point for all h values used during the shooting process. One simple way to do this is to use a symmetric shooting interval [−XS, XS] in which XS (the shooting X) is an integer multiple of X_0. To ensure that the boundaries are in effect "at infinity" for the states which we study we have set XS = 20 X_0. This makes the potential so large at the boundaries that the calculated energies are unaffected by any boundary effects. By using a doubling sequence of strip numbers NS we ensure that the potential peak always falls on a lattice point. The N_0 value which corresponds to x = X_0 can be pre-calculated on each run, so that the singular U functions of Eq. (7) can be applied. Alternatively N_0 can be located by using the test that the quantity $2(x − X_0)/h$ has a modulus less than 1.

On applying the incremental Hartree shooting approach to the potential of Eq. (10) we obtained the results shown in Table 2. The probability results show that the lowest three states can be accurately described as "right" or "left" states with respect to the central peak, whereas the higher state wavefunctions (especially that of state number 5) are distributed in a more even manner about the peak. The expectation values <x> and <x^2> were also calculated for the lowest three states, thus yielding for each wavefunction the mean square width $\Delta = [<x^2> − <x>^2]^{1/2}$. The pairs (<x>, Δ) for the lowest three states (in an ascending order of energy) were calculated to be (−1.17106, 0.29601), (1.80014, 0.36056) and (−0.95978, 0.55978) (we give truncated numerical values).This shows that these states have wavefunctions which are well localized within the left hand well (at about x = −1.250) or the right hand well (at about x = 1.916).

We note that our direct method is well able to find the very small "right hand" probability for the lowest state, with a wavefunction which is strongly concentrated in the left hand well. This probability was not given in [1] and would be difficult to find with high accuracy by any method which has to store the widely varying wavefunction at all points, normalize it and then do an explicit quadrature over the region concerned.

4 Probabilities for the non-classical region

By a mixture of analytical and numerical methods the authors of [3,4] have arrived at the conclusion that for the high lying (i.e high n) states of the harmonic oscillator with $V(x) = x^2$ the probability P(ext) for the particle to be in the external non—classical region (where $V(x) > E$) varies asymptotically according to the law

$$P(ext) = A(n + 1/2)^{-1/3} + B(n + 1/2)^{-1/2} \tag{11}$$

Only the harmonic oscillator was treated in [3,4],since the knowledge of the exact wavefunctions simplified some of the calculations. The direct method of the present work would obviously allow other potentials to be investigated. However, there is a technical problem. In calculating the energy and other quantities for a high—lying state we shall need to know the precise quantum number n for the state. To undertake a node-counting approach to determine n would be extremely tedious for states of very high n. We resolved the problem by treating the special family of single well potentials of the form $\alpha x^2 + \beta x^4$ (with α and β both positive). As has been shown previously [7] hypervirial perturbation theory can give very accurate energy levels for such potentials AND also has a specific n value attached to that energy. Thus a preliminary perturbation calculation can provide both the n value and the target energy for the finite difference calculation, which can then be used for the specialised task of finding the required probability P(ext).

The probability can be calculated by using a full axis shooting calculation to find the probability P(int) associated with internal classical region, which is then subtracted from 1 to give the required P(ext). Alternatively, if we wish to treat only odd parity states, we can perform a half—axis shooting starting at the origin and so calculate P(ext) directly.

To check whether the law (11) applies to the potentials being studied we have adopted two approaches. Table 3 shows the P(int) and P(ext) values for a sequence of increasing n values for the specimen potentials x^2 and x^4 and we constructed similar tables for other potentials in the family of potentials being studied. The asymptotic power law dependence of P(ext) on $n + 1/2$ can be estimated by taking the logarithm of the ratio of the P(ext) values and dividing it by the logarithm of the ratio of the $(n + 1/2)$ values for the two results with the highest n values. For all the tables of results this ratio is very close to $-1/3$, thus suggesting that the same asymptotic inverse cube root law holds for all the potentials being studied. Having obtained this preliminary result we can then carry out a more detailed analysis which exploits the properties of the Richardson extrapolation procedure. Inspection of (11) suggests that there might be a longer series involved, in such a way that we can write

$$P(ext)(n + 1/2)^{1/3} = A + BY + CY^2 + \dots \tag{12}$$

with the variable Y being $(n + 1/2)^{-1/6}$. Thus if we tabulate the product on the left of (12) as a function of Y then the more general form of Richardson extrapolation (valid for an irregular sequence of Y values) should extract the value of A. If the sequence of extrapolated A values in the Richardson process tends smoothly towards a stable

Table 3 The calculated P(int), P(ext) values for the potentials x^2 and x^4, using state numbers n which have the constant ratio 3/2	n	P(int), P(ext) (x^2)	P(int), P(ext) (x^4)
	32	0.9583747991459	0.96787753696945
		4.16252008541(−2)	3.21224630306(−2)
	48	0.9635046349099	0.97174981514605
		3.64953650901(−2)	2.82501848540(−2)
	72	0.9680335815556	0.97519634310256
		3.19664184444(−2)	2.48036568974(−2)
	108	0.9720204555577	0.97824957590052
		2.79795444423(−2)	2.17504240995(−2)
	162	0.9755227903196	0.98094490065128
		2.44772096804(−2)	1.90550993487(−2)
The full -axis shooting was over the region $[-4X_t, 4X_t]$ where the turning point is at X_t	243	0.9785948147315	0.98331802170185
		2.14051852685(−2)	1.66819782982(−2)

Table 4 The parameters A and B (see Eq. (12) of the text) for some members of the family of perturbed oscillator potentials $\alpha x^2 + \beta x^4$	(α, β)	A	B
	1, 0	0.133974968	−0.0122517
	0, 1	0.104790443	−0.0245035
	1, 1	0.104790443	−0.0126884
	2, 1	0.104790444	−0.0008733
	3, 1	0.104790444	0.0109418

limit then we have shown that the asymptotic $(n+1/2)^{-1/3}$ law does hold, whereas an unstable or fluctuating A estimate would indicate that the law is invalid. (We should note here that two Richardson extrapolation calculations are involved : the first one to find P(ext) for a given n by using several h values and the second one to extract the value of A from the P(ext) values for several n).

The results showed that a stable A is indeed obtained and that re-analysing the data while knowing this value also enables a reasonable estimate of B to be obtained. Table 4 shows A and B for some specimen potentials. The results show that the A value is almost entirely determined by the stronger x^4 component in the potential (which, of course, will dominate the asymptotic behaviour of the wavefunction). As the x^2 coefficient α in the potential is increased (with $\beta = 1$) the A value remains almost constant but the B value changes sign for an α value close to 2.

5 Discussion

By incorporating the delta and Heaviside functions in a modified form of our previously established methods for expectation value calculation we have shown that the integrated probability for a bound state over a selected region can be found by a direct approach which avoids any quadratures. and (amusingly) that the square of the correctly normalised wavefunction at a point can be found without calculating a

normalisation integral and without even storing the wavefunction. By giving some computational details we hope to encourage other workers to make use of the direct approach for the two singular U functions discussed in this work (a few [9,10] have already made use of an earlier approach [2] which works for smooth U functions).

We should note that (in defiance of persistent folk—wisdom) the use of scaling (Sect. 2.2) renders simple forwards shooting stable and accurate, as was previously shown for a much more difficult many—well potential [8]. In the present work we have used an improved form of the most simple Hartree method, with a leading energy error of h^2 type in the E(h) obtained for a steplength h. When we boosted this error to h^4 type by adding another term in the initial Eq. (2) (following the procedure explained in [6]) we found that there is not an appreciable gain for the very specialised calculations of the present work, since the singular nature of the potentials U_1 and U_2 leads to their expectation values STILL having a leading h^2 error term (although the expectation values of x and x^2 do follow the energy and acquire an h^4 type behaviour).

The incremental Hartree method uses only a few mathematical operations per step and keeps the rounding error very small, even for the smallest (and most crucial) h value used. Using five h values with Richardson extrapolation gives what is effectively a tenth order method. By contrast, methods which set out to be directly of very high order require the evaluation of one or more complicated functions at every step of a shooting process. This tends to introduce considerable rounding error even for a single run and usually requires multiple precision calculations to alleviate this problem. The accurate results of the present work, using only very simple mathematical expressions, were obtained by using standard double precision.

Several of the works which apply the canonical function method [11,12] use only a large but fixed number of steps in their calculations, even though the method clearly uses ratios of functions at the endpoints. We suggest that the use of several steplengths, together with scaling and Richardson extrapolation, would be useful in increasing even further the accuracy of the canonical function method.

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