J Math Chem (2012) 50:2648–2658
DOI 10.1007/s10910-012-0053-3

ORIGINAL PAPER

# A simple Hill-series approach to the linear potential

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Received: 25 April 2012 / Accepted: 10 July 2012 / Published online: 22 July 2012


**Abstract** A simple Hill-series method is shown to yield accurate energy levels and expectation values for the linear potential for any angular momentum L and confinement radius R. The numerical results are verified by comparison with those from two hypervirial perturbation methods which are specially constructed to give accurate results at $L = 0$ for small R values and at $L > 1$ for $R = \infty$.

**Keywords** Quantum mechanics · Eigenvalues · Expectation values · Perturbation theory

## 1 Introduction

The energy levels of the radial Schrodinger equation with a linear potential have been calculated by many different methods [e.g. 1–5]. It is well known that if the angular momentum L is zero and the coordinate r ranges from zero to infinity then the energy eigenvalues of the Schrodinger equation

$$H\Psi = \left[-D^2 + V(1)r + L(L+1)r^{-2}\right]\Psi = E\Psi \tag{1}$$

are determined by the zeros of appropriate Airy functions. The zeros which directly give the energy eigenvalues for the special parameter values $L = 0$ and $V(1) = 1$ and

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for confinement radius $R = \infty$ are tabulated to varying numbers of decimal digits in several works [e.g. 6,7]. For those special parameter values the authors of [8] have shown that it is possible to do a type of inverse calculation in which some sums of powers of the Airy function zeros can be deduced from a knowledge of the energy levels. Extending the Airy function formalism to deal with more general parameter values for the linear potential involves complicated algebra and leads to lengthy and unwieldy summations when numerical results are required [9,10]. In Sects. 2 and 3 we describe the main features of the Hill-series method, which can treat the bounded or unbounded linear potential for any angular momentum. Sections 4 and 5 show how hypervirial relations can be used to relate various numerical results and also to permit a perturbation approach to the $L = 0$ states of the linear potential problem for small R values. Section 6 describes a different hypervirial perturbation method which works for higher L values and for $R = \infty$. Section 7 gives specimen calculated results, comparing some of them with the perturbation theory results. Section 8 gives a brief conclusion. The special features of the Hill-series approach which makes it particularly effective are that it has very small memory storage requirements and that it can yield expectation values for each state along with the energy eigenvalue.

## 2 The family of recurrence relations

The Hill-series method incorporates a factor $\exp(-\beta r)$ into the wavefunction, where the parameter $\beta$ is varied to optimize the results. The method has previously been applied to the potential $-Zr^{-1} + V(1)r$, usually for the case $Z = 1$. This potential (the Cornell potential) has been used to describe the charmonium system in elementary particle theory [11] and also to describe the so-called radial Stark effect for the hydrogen atom [12]. For the hydrogen atom problem with a small positive V(1) value the Hill-series method with real $\beta$ values gives the perturbed bound state energies. For a small negative V(1) value the use of a complex $\beta$ produces the complex resonant state energies [13]. What we are exploring in the present work is how well the method works if we entirely remove the background Coulomb potential and so take the originally perturbing V(1)r term as the full potential. Numerical tests have shown that the renormalized hypervirial perturbation method [14], which works very well for the case in which Z equals 1 and V(1) is small, loses many decimal digits of accuracy for the $L = 0$ states if Z is set equal to zero, since the necessary strong unperturbed Coulomb potential has then been removed. The non-perturbative Hill-series method suffers no corresponding loss of accuracy and so can give much better results.

Adding an extra Coulomb term $-Zr^{-1}$ into the Hamiltonian in (1) and then postulating a solution for the Schrodinger equation $H\Psi = E\Psi$ of the form

$$\Psi = \exp(-\beta r) r^{L+1} \Sigma_0 W(N) r^N \tag{2}$$

leads to a recurrence relation for the coefficients W(N):

$$\begin{aligned}(N+2)\,(N+2L+3)\,W(N+2) = {} & [2\beta(N+L+2) - Z]\,W(N+1) \\ & -(E+\beta^2)W(N) + V(1)\,W(N-1)\end{aligned} \tag{3}$$

We note that it is permissible to use the exponential decay factor in the postulated wavefunction, since we are using only the positive r region. We can formally differentiate (3) with respect to any parameter which it contains, such as E, V(1) or Z and then use the obvious notation WE(N), WV(N) or WZ(N) for the coefficients in the series representing the appropriate derivatives. We conclude that the sets of derivative coefficients obey the same recurrence relation (3) as the W(N) but with one extra term added on the right hand side. This term arises from taking the derivative of a product in (3). It can easily be seen that for the WE recurrence relation it is $-$W(N), for the WV recurrence relation it is $+$W(N $-$ 1) while for the WZ recurrence relation it is $-$W(N $+$ 1). There is thus a one-way coupling between the derivative coefficients and the W coefficients.

It is necessary to stress an important feature of the calculation which is of particular relevance for the present calculation. Even when the actual PHYSICAL Z value is zero the WZ recurrence relation can still be used to find the expectation value of $r^{-1}$ (as explained below). We are taking the derivative at zero with respect to any parameter which has an actual zero numerical value in the Hamiltonian (and so becomes essentially a dummy parameter). This notion of a dummy (ie zero) potential term indicates how to find the expectation value of $r^2$ directly. All that is required is to think of a dummy term V(2)W(N $-$ 2) in (3) to see that we simply use the different extra term $+$W(N $-$ 2) instead of $+$W(N $-$ 1) in the WV recurrence relation (and so on for higher powers of r). Besides this direct approach, which would have to be applied in turn to each successive power of r, there are also hypervirial relations which permit a chain of $\langle r^N \rangle$ to be calculated from the known E and $\langle r \rangle$. This alternative approach is discussed in Sect. 4.

## 3 The calculation of energies and expectation values

The first step in the energy calculation is to set a radius r $=$ R at which to impose the Dirichlet boundary condition that the wavefunction must be zero. In a naïve direct approach (3) and (2) would be used together, taking a sufficient number of terms in the series (2) to give a converged value for the wavefunction at r $=$ R for some trial value of E. The trial E would than be varied so as to yield a zero wavefunction value at the boundary and the resulting E would be an eigenvalue. In the Hill-series approach this calculation is considerably simplified by using one uniform formalism for every possible R, including the case of infinite R at which the results of the traditional Hill determinant approach are obtained. In effect the Hill-series method imbeds the Hill determinant method within the power series method.

From (2) we see that, for a fixed r value r $=$ R, taking the sum of terms in the series up to the $r^M$ term will yield a wavefunction from which we can extract a factor equal to $\exp(-\beta R)\, R^{M+L+1}$ which is INDEPENDENT OF E. Thus we can take the remaining factor, which we denote by S(M), as the actual representative quantity which is to be rendered zero as E varies. This remaining factor can be written as a series in the reciprocal coordinate Y $=$ 1/R:

$$S(M) = W(0)Y^M + W(1)Y^{M-1} + \cdots\cdots\cdots + W(M) \tag{4}$$

On adding one more term in the series we will again have a common E-independent first factor (which is simply multiplied by R) while studying the new representative function S(M+1) shows that it obeys the simple recurrence relation

$$S(M+1) = S(M)Y + W(M+1) \tag{5}$$

Differentiating with respect to E, V(1) or Z shows that (5) has partner recurrence relations such as, for example

$$SE(M+1) = SE(M)Y + WE(M+1) \tag{6}$$

with analogous equations for SV and SZ.

This particular formalism has the advantage that it makes the increments of S and SE easily calculable as we travel along the recurrence relations for the coefficients, whereas traditional nested multiplication (proceeding "backwards" by adding a higher power term to the present sum of a series) would be more cumbersome. By extracting the factor S(M) from the sum (2) we arrive at a much more simple type of "forwards" nested multiplication. For the infinite space limit of R we set the reciprocal coordinate Y equal to zero in (5) and (6). This then requires us simply to study the latest coefficient in the wavefunction series rather than the full sum of the series. This "zero coefficient test" is equivalent to that of the Hill determinant approach and was noted by Ginsberg [15] as well as by later authors [16,17].

The calculational procedure using the several recurrence relations is straightforward. All initial coefficients and sums are set equal to zero, except W(0) and S(0), which are set equal to 1. For some trial E value the recurrence relations are used "in parallel" up to some suitably high M value MU (M upper) and a corrected E value E + DE is found by using the Newton's method equation

$$DE = -S(MU)/SE(MU) \tag{7}$$

After a few cycles the E value will converge to an eigenvalue, which will be the one closest to the initial trial energy, provided that we impose an upper limit on the magnitude of DE to avoid the large formal DE values which can arise if the initial value happens to be close to an extremum of the function for which a zero is being sought. By manipulating partial derivatives we also find that the expectation value of r is given by

$$\langle r \rangle = \partial E/\partial V(1) = -SV(MU)/SE(MU) \tag{8}$$

and that of $r^{-1}$ by

$$\langle r^{-1} \rangle = -\partial E/\partial Z = SZ(MU)/SE(MU) \tag{9}$$

Increasing the value of MU leads to stable values for the calculated values of the energy and the expectation values.

## 4 Scaling and the use of hypervirial relations

Inspection of the basic equations of the method shows that the recurrence relation (3) for the W coefficients and the partner ones for the derivative coefficients only use four terms at a time, while the Eqs. (7)–(9) only use the ratios of quantities.

It is thus possible to make an enormous saving in memory requirements and at the same time avoid any possible problems due to numerical overflow or underflow. The way to do this is to replace the indices $N+2$ down to $N-1$ by the indices 4 down to 1 and then to move along the elements at each step by using the replacement

$$W(J) = W(J+1)F \quad (J = 1 \text{ to } 3) \tag{10}$$

where F is a scaling factor which is usually chosen to be the reciprocal of the absolute value of W(4). By simultaneously scaling by the same factor F all the other quantities (S, SE, SV, SZ, WE, WV, WZ) we keep the ratios of all the quantities invariant and so Eqs. (7)–(9) remain valid. However, in making this reduction in the number of stored elements we must decide how much information needs to be retained in order to calculate expectation values. Thus, for example, to find $\langle r^2 \rangle$ we need to have the extra term $W(N-2)$, as explained in the preceding section. To ensure that this element is retained the compact numbering can be modified by replacing the labels $N+2$ down to $N-2$ by the labels 5 down to 1, with the shift of Eq. (10) being adjusted to go from 1 to 4.

In the discussion so far we have shown how to calculate directly a few expectation values of type $\langle r^N \rangle$ for low N values and so the question arises of how to simplify the numerical calculation of the $\langle r^N \rangle$ for higher N, particularly in the case in which a finite confinement radius R is being used. For the case $Z = 0$, where we have only the linear term $V(1)r$ and the angular momentum term $L(L+1)r^{-2}$ in the Hamiltonian, the traditional virial theorem acquires a boundary term [18] and becomes

$$2E - 3V(1)\langle r \rangle = -R(dE/dR) \tag{11}$$

so that the value of dE/dR can be found from the calculations. Equation (11) makes physical sense, since as we decrease R we expect the energy to rise and the average radius to decrease, making the difference on the left hand side positive, which is consistent with the negative value of dE/dR. As R tends to infinity this energy derivative tends to zero and we obtain the traditional infinite space virial theorem. We note that the angular momentum term makes no contribution, although it does appear in higher order hypervirial equations. Thus for example the next order hypervirial equation is

$$4E\langle r \rangle = 5V(1)\langle r^2 \rangle + 2L(L+1)\langle r^{-1} \rangle - R^2\,(dE/dR) \tag{12}$$

This shows that $\langle r^2 \rangle$ is in principle calculable from $\langle r \rangle$, $\langle r^{-1} \rangle$ and E (or $\langle r \rangle$ and E for the case $L = 0$) and subsequently all the higher $\langle r^N \rangle$ can also be found for the special case of the linear potential (for any confinement radius and for any angular momentum).

## 5 Perturbation theory for small R values at L = 0

The work of Fernandez and Castro [19] showed that the use of a confinement radius R adds a boundary term to each traditional hypervirial equation, so that the general hypervirial equation for the Hamiltonian $-\alpha D^2+\alpha L(L+1)r^{-2}+\lambda r$ takes the modified form

$$(\alpha/2)N\left[\left(N^2-1\right)-4L(L+1)\right]\langle r^{N-2}\rangle+(2N+2)\,E\langle r^N\rangle = (2N+3)\,\lambda\langle r^{N+1}\rangle - R^{N+1}dE/dR \tag{13}$$

In our calculations we take the coordinate r to extend from 0 to R. However, for the special case L = 0, if we consider the origin to be at the central point r = R/2 then we can see that a special simplification arises. The central point is also a centre of symmetry for the region and the unperturbed "particle in a box" wavefunctions all have a definite even or odd parity about that centre. Thus at that central origin the perturbation series for the case of a perturbing linear potential λr will have NO ODD POWERS of λ in it. On noting that the linear potential about the origin at r = 0 is simply the potential about the origin at r = R/2 plus the constant term λR/2 we conclude that the energy perturbation series for L = 0 and for the origin at r = 0 must take the form

$$E = n^2\pi^2R^{-2}+\lambda R/2+E_2\lambda^2R^4+E_4\lambda^4R^{10}+\cdots\cdots \tag{14}$$

with all the $E_N$ zero for odd N values <1. The explicit algebraic expressions for the $E_N$ up to $E_6$ given in [20] as a function of n do yield a zero $E_3$ and $E_5$ but the argument given above shows that all the odd $E_N$ are zero, except for the term $E_1 = R/2$ which arises from the shift of origin just described. To use hypervirial perturbation theory to work out the energy series it is more simple to drop the obvious powers of R in (14) and to consider the formal case R = 1. All the hypervirial equations then acquire the SAME term—dE/dR on the right hand side and this term becomes $2E-3\lambda\langle r\rangle$ on using (11). The family of hypervirial equations then involves only E and the various $\langle r^N\rangle$, which suffices to produce a closed system when perturbation series in λ are introduced for E and for the $\langle r^N\rangle$. We have written a short program which can work out the non-zero terms up to $E_{20}$ in the energy series and then sum the series by setting λ = 1 and inserting the correct powers of R into each term in the sum (14). Using the Wynn algorithm to sum the series for difficult cases it is possible to obtain high precision results for the states with L = 0 up to a value of about R = 3 for the ground state and to higher R values for excited states. (since by contrast with most perturbation problems the effects of the perturbation become weaker the higher the state.) These perturbation results provide an alternative check on the results of the non-perturbative Hill-series method for the special case L = 0. We note that the sign of each $E_N$ can vary with the state number n, so that for a given n the energy perturbation series is not necessarily an alternating series. The numerical $E_N$ for low N values can be estimated by calculations for several low R values using the Hill-series method and the results obtained in this manner are consistent with those found from the hypervirial perturbation method. For

states with high n values the perturbation results become very accurate; for example for n = 10 and R = 8 the perturbation result is E = 19.50678773209972, which is reproduced exactly by the Hill-series method by taking 200 terms with $\beta = 10$.

## 6 A perturbation approach for higher L values at R = ∞

The potential $V(r) = Ar^{-2} + Br$, with A and B both positive, has a minimum at $r = r_0$, where $r_0^3 = (2A/B)$. Differentiating V twice shows that it obeys the differential equation

$$r^2 V^{(2)} + 2rV^{(1)} = 2V \tag{15}$$

Introducing the coordinate $X = r - r_0$ and the series expansion

$$V(X) = \Sigma_0 V_N X^N \tag{16}$$

for the potential about the origin at $r = r_0$ we find from the differential equation that the potential coefficients $V_N$ obey the recurrence relation

$$(N+2)(N+1)\, r_0^2 V_{N+2} + 2(N+1)^2\, r_0 V_{N+1} = [2 - N(N+1)]V_N \tag{17}$$

where the values $V_1 = 0$ and $V_0 = V(r_0)$ suffice to initiate the recurrence calculation.

The resulting potential coefficients can then be used in a hypervirial perturbation calculation based on the unperturbed oscillator potential $V_0 + V_2X^2$. We found that the perturbation calculation gave accurate results for L = 2 and for higher L values.

It will directly give quantities such as $\langle r \rangle$ if desired and can also be used with non-integer values of L, so that it can be used to calculate $\langle r^{-2} \rangle$ by means of the numerical differencing approach described in the following section. The method of this section can be used for any two-term potential with a single well structure.

## 7 Some numerical results using a variable L value

Given the vast range of L and R values which can be treated it is only possible to give a selection of typical numerical results which will suffice to demonstrate the simplicity and accuracy of the Hill-series method for the linear potential problem. A feature of the method which is particularly useful is that it can be applied to arbitrary angular momentum values rather than just to the traditional integer values 0, 1, 2, etc.

The equations of the method permit this and to ensure that they can be used in a fully flexible manner it is necessary to ensure that L is treated as a double precision variable in any computer program used to implement the Hill-series calculation. In some computer languages it thus might be necessary to use the symbol XL rather than L to ensure this double precision status. This fully variable L gives two computational advantages. First, it allows the calculation to be carried out in several different dimensions, by using the well-known rule

$$XL = L + (D - 3)/2 \tag{18}$$

which relates an effective angular momentum XL in D dimensions to a general angular momentum L in a theory which uses the form $L(L+1)r^{-2}$ for the angular momentum term in its Hamiltonian. Thus, for example, a fully isotropic state in 3 dimensions would have $L = 0$. To find the equivalent fully isotropic states in 2 or 4 dimensions we see from (18) that we should use $XL = -1/2$ and $XL = 1/2$, respectively. These effective XL values can be used in the equations of the Hill-series method. The angular momentum term does not contribute a term in the virial equation and so we expect the virial equality $3V(1)\ \langle r\rangle = 2E$ to be obeyed in any number of dimensions for $R = \infty$. The accurate Hill-series results confirm this.

The second advantage in using continuously variable double precision L is that it makes it possible to find the energy of a particular level for two L values with a very small difference and so to find the expectation value $\langle r^{-2}\rangle$ for the corresponding state by using the equation

$$\langle r^{-2}\rangle = (2L + 1)^{-1}\,(\partial E/\partial L) \tag{19}$$

**Table 1** Perturbation coefficients to be used in Eq. (14) for the lowest four states of the linear potential, obtained by the hypervirial perturbation method

| | n = 1 | n = 2 |
|---|---|---|
| 2 | −1.097261462040153(−3) | 3.272070322253722(−4) |
| 4 | 2.221011078473665(−8) | −2.150741261249757(−8) |
| 6 | −1.092195094614907(−12) | 1.107159340063149(−12) |
| 8 | 6.926039859041837(−17) | −6.956039376683489(−17) |
| 10 | −4.961426561642162(−21) | 4.964560952146264(−21) |
| 12 | 3.753912756358222(−25) | −3.820371853095012(−25) |
| 14 | 4.061285789963617(−28) | 3.086189993734866(−29) |
| 16 | −3.567076886989357(−29) | −2.580201485976520(−33) |
| 18 | 3.367340080496691(−30) | 2.213477552302674(−37) |
| 20 | −3.028992967436031(−31) | −1.937359137799854(−41) |
| | n = 3 | n = 4 |
| 2 | 1.949333639302401(−4) | 1.193969079148062(−4) |
| 4 | −6.893974944048785(−10) | −2.760331908978424(−11) |
| 6 | −1.423626361190433(−14) | −6.753590987699282(−16) |
| 8 | 3.010872442263473(−19) | −9.814040135375797(−22) |
| 10 | −3.030742377872721(−24) | 2.327353563628991(−26) |
| 12 | 1.542709870521132(−30) | −8.347153278334914(−32) |
| 14 | 6.059367571343992(−34) | −7.333781422300249(−38) |
| 16 | −1.297400465395865(−38) | 1.310136997524794(−42) |
| 18 | 1.299914418663105(−43) | 1.366942119162146(−48) |
| 20 | 4.760158787456087(−49) | −5.397128960531323(−53) |

**Table 2** Infinite space (Y = 0) values of E, $\langle r \rangle$ and $\langle r^{-1} \rangle$ for the linear potential Z = 0 and V(1) = 1 as obtained by the Hill-series method

| E | $\langle r \rangle$ | $\langle r^{-1} \rangle$ |
|---|---|---|
| (L = −1/2) | | |
| 1.73721779087141 | 1.158145193914 | 1.397391920560 |
| 3.67023475587568 | 2.446823170584 | 0.8168085663077 |
| 5.16974219890423 | 3.446494799269 | 0.6295725335977 |
| 6.47400287721096 | 4.316009118141 | 0.5287594119475 |
| (L = 0) | | |
| 2.33810741045977 | 1.558738273640 | 0.8348669951779 |
| 4.08794944413097 | 2.725299629421 | 0.5821686958008 |
| 5.52055982809555 | 3.680373218730 | 0.4723119378752 |
| 6.78670809007176 | 4.524472060048 | 0.4071451153096 |
| (L = 1/2) | | |
| 2.87209773747121 | 1.914731824981 | 0.6259166799268 |
| 4.49301821878074 | 2.995345479187 | 0.4763738428621 |
| 5.86711681461815 | 3.911411209745 | 0.3994272027587 |
| 7.09776506793562 | 4.731843378624 | 0.3505089375132 |

MU ranges from 100 to 200 and $\beta = 5$ for all the results. The L values used correspond to those for the ground state in 2, 3 and 4 dimensions. The L = 0 results agree with the double precision zeros of the Airy function as given in [7]

**Table 3** The L = 0, V(1) = 1 groundstate energy as a function of the confinement radius R

| R | E | −dE/dR |
|---|---|---|
| 8.0 | 2.33810741549581 | 2.39452(−8) |
| 7.0 | 2.33810788078093 | 2.02773(−6) |
| 6.0 | 2.33813490033196 | 1.04853(−4) |
| 5.0 | (2.339)04933491280 | 3.05057(−3) |
| 4.0 | (2.355495)22653490 | 4.49760(−2) |
| 3.5 | (2.39665422)127899 | 1.33249(−1) |
| 3.0 | (2.509011068)19905 | 3.45450(−1) |
| 2.5 | (2.786484236164)80 | 8.31057(−1) |
| 2.0 | (3.49986758874422) | 2.00240(0) |
| 1.5 | (5.13093723880705) | 5.36346(0) |
| 1.0 | (10.3685071618363) | 1.92436(1) |

$\beta = 5$ and MU = 100 sufficed to obtain the results. The dE/dR values are found from the virial theorem [Eq. (11)]. The results from the perturbation series based on the coefficients of Table 1 are shown in brackets. The dE/dR values are severely truncated

To find $\langle r^{-2} \rangle$ by the direct implicit differentiation methods of Sect. 3 would be quite complicated, since the parameter L appears in terms on both the left and the right sides of the recurrence relation (3).

**Table 4** Hill-series energies for L = 2 and L = 3 (with R = $\infty$, $\beta = 5$, NU = 200)

| L = 2 | L = 3 |
|---|---|
| (4.248182257)15379 | (5.05092563492)817 |
| (5.629708376)69592 | (6.3321153747)1175 |
| (6.86888268)940316 | (7.504645642)06895 |
| (8.0097029)2267897 | (8.597117011)90232 |
| (9.077003)05076353 | (9.62726701)324443 |

The results from the perturbation method of Sect. 6 are shown in brackets

Table 1 gives the perturbation coefficients $E_N$ in the expansion (14) for the lowest four states of the linear potential with confinement radius R and angular momentum zero. Table 2 gives the energies and some expectation values for the lowest four states of the linear potential as found by the Hill-series method for R = $\infty$ (i.e Y = 0). The angular momentum values used correspond to the isotropic states in 2, 3 and 4 dimensions. The energies for the lowest four states with L = 0 agree with the corresponding double precision zeros of the Airy functions as given in [7]. Table 3 shows the Hill-series energy of the L = 0 ground state of the linear potential as the confinement radius R varies. The results for small R values agree with those found by using the hypervirial perturbation coefficients which are shown in Table 1. Table 4 shows the lowest five state energies for L = 2 and L = 3, comparing the Hill-series results with those from the hypervirial perturbation method described in Sect. 6.

## 8 Conclusion

The Airy function approach for the linear potential is easy to apply only for the special case in which L = 0 and R = $\infty$. The Hill-series method is applicable for any real value of L and can yield energies and expectation values for states of the linear potential with variable confinement radius R and variable dimension D. The implicit differentiation procedure used in the method directly produces expectation values without any quadrature and without the need for wavefunction storage.

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