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## Comment on the asymptotic iteration method for polynomial potentials

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### Abstract

It is shown that polynomial potentials can be treated by a method which cuts out most of the complications of the popular AIM approach. Several examples are given to show how expectation values and resonance energies can be calculated using the simplified approach.

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Several papers recently published in this journal have developed and applied a method called the asymptotic iteration method (AIM) [1–5]. A study of the basic equations of the method shows that for the case of a one-dimensional Schrödinger equation with the potential energy function  $V(r)$  or  $V(x)$  (depending on the problem) the AIM approach begins by incorporating some appropriate convergence factor in the wavefunction; it then develops two recurrence relations, one for the successive derivatives of the wavefunction  $\psi$  and the other for a quantity associated with  $V$ . The energy levels are found by means of a fairly complicated asymptotic analysis involving the output of both recurrence relations. The present author takes the view that for the case of a polynomial potential function the AIM method is in effect a roundabout approach to a much more simple power series technique, since the  $n$ th derivative of  $\psi$  divided by  $n!$  is simply a term in the local Taylor series expansion of the wavefunction. In the present paper, we give results for a few specimen calculations which use convergence factors similar to those used in AIM but which can give the energy levels more speedily and simply, as well as leading to some new results which it seems would be much more difficult to obtain by the roundabout AIM approach. Proponents of AIM might argue that it gives an approximate wavefunction as well as the energy for each level, thus permitting the calculation of integrals for expectation values. However, it has long been known how to calculate expectation values without doing any integrals and without even storing any wavefunction values [6]. For illustrative purposes, we treat the perturbed Coulomb problem with the Schrödinger equation

$$[-aD^2 + aL(L+1)r^{-2} - Zr^{-1} + V(1)r + V(2)r^2]\psi = E\psi. \quad (1)$$

This problem has a special interest, since it was at first concluded that a purely numerical form of AIM would not work for it and that a less accurate form of AIM which sums a perturbation series would be required [2]. The limited accuracy obtained in [2] is probably due to the low perturbative order used, since the original AIM perturbation theory [18] is in principle capable of high accuracy. However, a careful calculation by Amore and Fernandez [4] later made the direct numerical version of AIM work to high numerical accuracy for the Schrödinger equation (1), albeit by using a more complicated convergence factor than that which we use in this paper. Although we treat only the perturbed Coulomb problem here, we have also looked at the perturbed oscillator AIM calculation of [7] and found that it permits a similar simplification and extension to deal with both bound states and resonances for perturbed oscillator systems.

To apply the Hill-series approach, we first set

$$\psi = \exp(-Z_0 r) \sum_0^{\infty} A(N, E) r^N \quad (2)$$

in equation (1). This quickly leads to the recurrence relation

$$a(N+2)(N+2L+3)A(N+2, E) = [2aZ_0(L+N+2) - Z]A(N+1, E) - (E + aZ_0^2)A(N, E) + V(1)A(N-1, E) + V(2)A(N-2, E). \quad (3)$$

To apply this recurrence relation it might at first appear that the sum in equation (2) has to be worked out for some given radius  $R$  at which we require that  $\psi(R) = 0$ . However, it was shown long ago that the simple criterion  $A(N, E) = 0$  for sufficiently large  $N$  gives the energy levels in infinite space, because it turns out to be equivalent to the use of a Hill determinant approach [8–10]. An elegant modern approach to this equivalence by the method of moments has been developed in detail [11]. The energy criterion used here is visibly much more simple than the one used in the AIM approach. While it would be of formal interest to see whether the two different recurrence relations used in AIM could be transformed and combined to lead to the simple single criterion  $A(N, E) = 0$ , we confine ourselves to numerical examples in this paper. Equation (3) permits an extremely economical computation by using the numbering  $N+2 \rightarrow 5$  and so on, down to  $N-2 \rightarrow 1$ . Thus, only five  $A$  values are kept and at each cycle the values are moved along by 1 and are all simultaneously scaled by a numerical factor which keeps  $A(4)$  of order unity and thus avoids overflow or underflow. With this approach, an effective Hill determinant dimension of several hundreds is attainable simply by using an appropriate number of cycles of the recurrence relation. If equation (3) is written in the short but obvious notation

$$a(N+2)(N+2L+3)A(N+2, E) = F(A, E, N), \quad (4)$$

then differentiation with respect to  $E$  and to  $V(1)$  gives the partner recurrence relations

$$a(N+2)(N+2L+3)AE(N+2, E) = F(AE, E, N) - A(N, E) \quad (5)$$

$$a(N+2)(N+2L+3)AV(N+2, E) = F(AV, E, N) + A(N-1, E). \quad (6)$$

The three recurrence relations use the same numerical coefficients and so are very economical to propagate simultaneously. Three sets of five numbers are thus used. The Newton's method equation for correcting the initial energy estimate is

$$E \rightarrow E - A(5, E)/AE(5, E) \quad (7)$$

while the expectation value of  $r$  is given by

$$\langle r \rangle = -AV(5, E)/AE(5, E). \quad (8)$$

**Table 1.** Selected results for variable  $L$  and  $V(1)$ , with  $Z = 1$  and  $V(2) = 0$ .  $Z_0 = 3$  throughout and  $ND$  was varied from 100 to 200 to obtain convergence of the results. The results obtained have been truncated to 12 digits for ease of display.  $n$  is the state number for the associated value of  $L$ . The  $V(1)$  values are those used in [2].

$L$	$n$	$V(1)$	$E$	$\langle r \rangle$
0	1	0.096 20	1.094 896 999 108	2.202 293 139 307
0	0	0.574 62	0.292 563 392 451	0.940 389 386 472
1	1	0.009 69	1.564 999 106 376	2.740 935 246 790
1	0	0.362 98	1.235 850 586 455	1.700 472 410 298
2	1	-0.020 25	2.011 448 630 820	3.165 405 506 617
2	0	0.281 13	1.814 880 707 682	2.258 629 183 718
3	1	0.133 59	2.456 859 044 846	3.528 099 941 279
3	0	0.234 84	2.321 809 528 012	2.712 620 632 014

The basic theory is given in [6]. Differentiation with respect to  $Z$  or  $V(2)$  leads, of course, to  $\langle r^{-1} \rangle$  or  $\langle r^2 \rangle$ ; for a polynomial potential only one or two  $\langle r^N \rangle$  are needed, since they are all connected together by hypervirial relations [12]. To start off the three recurrence relations we simply set  $N = -1$  in them, with  $A(4, E) = 1$  and all other  $A, AE$  and  $AV$  coefficients zero, and then go up to some high value  $ND$  of  $N$  before using equations (7) and (8). An outer loop in the program can be used to increase the dimension  $ND$  gradually until a located energy value has stabilized to double precision. The  $ND$  value required depends on  $Z_0$  but for most cases a quick preliminary test can give a  $Z_0$  for which  $ND$  does not have to go beyond 300 to find  $E$ . The associated  $\langle r \rangle$  value indicates the region in which the wavefunction is localized in the case of a potential with two energy wells, for example when  $V(1)$  and  $V(2)$  have opposite signs. A crucial advantage of the formalism described above is that by writing the theory in terms of ratios (as in equations (7) and (8)) we can apply the same scaling to the  $A, AE$  and  $AV$  coefficients at each step and thus leave the final results unchanged while avoiding overflow or underflow problems. An analogous procedure makes it possible to perform forward finite difference shooting through an alternating sequence of classical and non-classical regions [13], something previously regarded as impossible. When the method described above is applied to the real energy levels calculated in [2] it easily gives between 12 and 16 decimal digits of accuracy for all the results displayed to 6 digit accuracy in tables 4–6 of [2] for a wide range of values of  $L, Z, V(1)$  and  $V(2)$ . Table 1 shows a few results, giving also the  $\langle r \rangle$  values which were not obtainable by the method of [2]. For the case  $a = \frac{1}{2}, Z = 8$  and with  $L$  chosen to make  $L(L + 1) = 5$ , the method with  $Z_0 = 16$  gives a ground-state energy of  $-1.447\ 656\ 821\ 925\ 36$ , in accord with the result given in [15] for a Dirichlet calculation with  $R \rightarrow \infty$ . A more interesting application of our technique is to the case  $a = \frac{1}{2}, Z = 1, V(1) = -2\lambda, V(2) = 2\lambda^2$ , with  $\lambda$  a small positive number [12]. The deviation of the lowest bound state 1s energy from the formal Rayleigh–Schrödinger value of  $-\frac{1}{2} - 3\lambda$  is a small term which is a non-analytic function of  $\lambda$ . It can be estimated by a form of linearized perturbation theory [12] but the method of this paper gives more precise numerical values. Table 2 shows some typical results and a numerical fitting analysis shows that the results fit very well to the non-analytic function

$$\Delta = A\lambda^B \exp(-C/\lambda) \tag{9}$$

with  $A = 7.503\ 5425, B = -1.928\ 7740, C = 0.504\ 091\ 32$ . The calculations also show that besides the 1s wavefunction concentrated near the origin there is also an outer wavefunction which has an energy close to  $-\frac{1}{2} - \lambda$  and which is centred on the potential minimum close

**Table 2.** Results for the non-analytic difference  $\Delta = E + 3\lambda + \frac{1}{2}$ , for the 1s state with  $Z = 1, L = 0, V(1) = -2\lambda, V(2) = 2\lambda^2$ . The variable number of digits in  $\Delta$  arises because  $E$  was only calculated to ordinary double precision (16 decimal digits).  $Z_0 = 3$  was used throughout.

$\lambda$	$\Delta$
0.015	6.272(-13)
0.020	1.606 9445(-9)
0.025	1.612 142 076(-7)
0.030	3.233 724 768(-6)
0.035	2.597 844 9826(-5)
0.040	1.181 971 822 924(-4)
0.045	3.695 786 240 296(-4)
0.050	8.931 019 480 76(-4)
0.055	1.798 584 059 8593(-3)
0.060	3.173 875 235 4203(-3)
0.070	7.546 639 486 534(-3)
0.080	1.421 216 899 3068(-2)
0.090	2.313 419 884 2273(-2)
0.100	3.417 309 603 7330(-2)

to  $r = \frac{1}{(2\lambda)}$ . The outer state is the lowest of a sequence of quasi-oscillator states which are centred on that minimum position. The  $\langle r \rangle$  values, of course, are important in establishing this property. Despite these interesting results for bound states, the method becomes really powerful (and presumably more difficult for the indirect AIM approach) when we allow  $Z_0, E$  and the coefficients  $A, AE$  and  $AV$  to become complex numbers, so that complex arithmetic has to be used in all the recurrence relations and equations given above. As a first calibratory test, we looked again at the 1s resonant state, treated in [14] by using complex hypervirial perturbation theory. The results agreed with those of table 4 of [12] for both  $r$  and  $r^2$  negative perturbations but also added several digits of accuracy to the resonance energies. For this case, the complex numbers produced by equation (8) are the complex derivatives of the resonance energy with respect to  $V(1)$  and so make it possible to predict the new resonance energy if  $V(1)$  is changed slightly. While checking the Hill-series method results against those in table 4 of [12], we performed some numerical analysis on the resonance energies. In particular, for  $a = \frac{1}{2}, Z = 1, V(1) = -\lambda, V(2) = 0$ , with  $\lambda$  small and positive we found that the imaginary part of  $E$  for the 1s state is well described by equation (9), with  $A = 0.007\ 16, B = -3.380\ 45, C = -0.6998$ . The WKB results in equations (45) and (46) of [16] appear to predict the values  $A = 0.025, B = -2, C = -\frac{1}{6}$  for EI, but these values give a very much worse fit to the calculated EI.

Since the method uses a Newton's method rootfinder, it functions best when it is given an approximate starting energy. For resonance calculations, the complex hypervirial method suffices to give these starting values and has the advantage that it indicates the precise 'zero-field' state associated with a perturbed level. As a novel resonance problem, we took the problem associated with table 2 but reversed the signs of the coefficients  $V(1)$  and  $V(2)$ , so that we have  $a = \frac{1}{2}, Z = 1, V(1) = 2\lambda, V(2) = -2\lambda^2$ , for small positive  $\lambda$ . The  $r^2$  term is tending to produce a resonance while the  $r$  term is tending to inhibit that resonance, so that the resonance width is much less than it would be in the absence of the  $r$  term. Table 3 shows some results for the 1s resonance. Complex hypervirial theory also worked quite well for this new problem and so gave good initial energies which were then improved by the method of this paper. As a further application of the Hill-series technique to resonant states

**Table 3.** The 1s state resonance energies for the case  $Z = 1$ ,  $V(1) = 2\lambda$ ,  $V(2) = -2\lambda^2$ .  $Z_0$  is held at the complex value (3, 1) throughout. ER has been truncated down to 12 significant digits.

$\lambda$	ER	EI
0.08	-0.372 260 539 195	2.094 85(-11)
0.09	-0.292 657 958 935	7.92133(-10)
0.10	-0.275 192 333 308	1.391 8965(-8)
0.11	-0.258 625 504 752	1.403 485 49(-7)
0.12	-0.268 487 922 979	5.046 982 587(-6)
0.13	-0.228 119 877 601	4.521 147 14(-6)
0.14	-0.214 170 320 986	1.703 590 088(-5)
0.15	-0.201 101 987 760	5.253 545 303(-5)
0.16	-0.188 931 690 247	1.376 034 564(-4)
0.17	-0.177 678 415 428	3.148 988 552 09(-4)
0.18	-0.167 354 799 437	6.436 713 155 94
0.19	-0.157 959 539 447	1.196 186 881 108(-3)
0.20	-0.149 472 402 587	2.050 704 784 01(-3)

**Table 4.** A sequence of s state resonances for the case  $a = \frac{1}{2}$ ,  $z = 1$ ,  $V(2) = 0$ ,  $V(1) = -0.05$ .  $Z_0$  is held at the complex value (1, 2) throughout.  $n$  is the principal quantum number of the associated zero-field state. Both ER and EI have been truncated down to 12 significant digits. The results are listed in an order of decreasing ER.

$n$	ER	EI
2	-0.407 608 248 504	1.344 564 372 48(-1)
3	-0.432 751 536 575	3.151 092 160 06(-1)
4	-0.475 527 770 448	4.621 165 679 06(-1)
5	-0.522 497 587 072	5.896 812 096 89(-1)
6	-0.570 099 656 811	7.046 178 932 39(-1)
1	-0.580 316 157 388	1.484 786 159 30(-4)
7	-0.617 187 038 890	8.105 772 813 04(-1)
8	-0.663 366 789 612	9.097 440 847 89(-1)
9	-0.708 520 882 894	1.003 537 979 97(0)
10	-0.752 640 429 138	1.092 939 949 78(0)
11	-0.795 760 909 908	1.178 660 462 70(0)
12	-0.837 934 782 146	1.261 233 411 11(0)

we looked at an interesting phenomenon which does not seem to have been treated in detail or even remarked on in the previous literature, although it is occasionally implicit in published numerical results. The vast majority of the works which have dealt with the problem of a Coulomb potential with a negative linear perturbation have treated only the resonance arising from the 1s state, taking it to be the ‘lowest’ resonance. For the bound state problem and for the case of small positive  $V(1)$  and  $V(2)$ , we expect the repulsive coupling effect between the levels to maintain the original 1s, 2s, 3s, . . . order for the perturbed s states. This ordering effect is lost for the complex variable resonant state case. Table 4 shows a sequence of resonant states for the case  $V(1) = -0.05$ ,  $V(2) = 0$ . The complex energies were first found by using complex hypervirial perturbation theory, since it actually identifies the initial unperturbed state from which the perturbed state arises. Three digit accuracy was obtained from the preliminary perturbation results and then the Hill-series method refined this to many more digits. The 1s resonance is seen to be much narrower than the others but is sixth in the list if the resonant

states are ranked according to descending ER. The numerical values of ER seem to continue downwards throughout the negative real axis. We followed them down to  $n = 24$  and found that the spacing of the successive ER values was decreasing only very slowly with  $n$ . We should note, however, that in our view it is stretching terminology somewhat to describe as a resonance a perturbed state with a very large EI. While the complex energy might have some meaning in terms of formal spectral theory for such a state, the usual physical interpretation involving the lifetime of an initially localized wavefunction is completely lost. The range of examples given in this short paper should serve to illustrate that a direct approach to the calculation of the coefficients  $A(N, E)$  is in some cases more accurate and more flexible than the complicated and indirect analysis adopted in the AIM approach.

*Note added in proof.* The method of this paper can give the results of tables 1–3 of the recent AIM work [19] to double precision. For example, for the case  $Z = 1$ ,  $V(1) = 1$ , and taking account of the unorthodox  $L$  values used in [19], we find the following energies for the lowest three 5 states, with the results of [19] in brackets: (2.36071239)1032495, (4.112290)914683557, (5.55207)8937241668.

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