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A hypervirial JWKB calculation

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Abstract. By a combination of mathematical analysis and microcomputer experiment it is shown that the hypervirial perturbation method can yield, not only the accurate quantum mechanical values, but also the zeroth-order JWKB values of E and $\langle x^2 \rangle$ for the case of a harmonic oscillator with a λx^4 perturbation.

1. Introduction

The hypervirial perturbation method (Swenson and Danforth 1972, Killingbeck 1981) makes possible the calculation to high orders of the Rayleigh-Schrödinger perturbation series for various model problems. In particular, it enables calculation of the series for the energy E and the expectation values $\langle x^N \rangle$ associated with the eigenstates of the much-treated Schrödinger equation

$$-\alpha D^2\psi + \beta x^2\psi + \lambda x^4\psi = E\psi. \quad (1)$$

The resulting series for this problem diverge, so it is necessary to perform some kind of transformation of the series in order to get a reasonable numerical result. Most of the methods used (e.g. Simon 1970, Caswell 1979) first produce the series and then transform it. This tends to produce computational problems with overflow and loss of accuracy, because of the divergent nature of the initial series. Killingbeck (1981) pointed out that the inclusion of a suitable variable (renormalisation) parameter K in the Schrödinger equation (1) permits construction of an algorithm which folds into one stage the production and transformation of the series. The result is a renormalised series which has comparatively small terms and gives semi-convergence to a perturbed energy. The present work is intended to point out two features which have not previously been noted. First, for $\beta \geq 0$ and $\lambda \geq 0$ the method can be made extremely accurate, subject only to the limitations of the computer used. Second, the method can be used to produce the traditional (i.e. zeroth-order) JWKB values for the energy and for the expectation values $\langle x^N \rangle$. Section 2 briefly reviews those parts of the hypervirial perturbation method which are needed to put into proper perspective the material of the later sections. Section 3 reports the results of computer experiments which explored the use of the renormalisation parameter K . Section 4 uses the Hellmann-Feynman theorem and classical hypervirial theorems to indicate how the hypervirial method can give JWKB results as well as accurate quantum mechanical results. Section 5 gives some specimen results which permit the estimation of a correction term to the JWKB formulae for the potential λx^4 .

2. The hypervirial method

For the Schrödinger equation (1) the hypervirial theorem which relates the various $\langle x^N \rangle$ can be written in the form

$$\frac{1}{2}\alpha N(N^2-1)\langle x^{N-2} \rangle = -(2N+2)E\langle x^N \rangle + (2N+4)\beta\langle x^{N+2} \rangle + (2N+6)\lambda\langle x^{N+4} \rangle. \quad (2)$$

The renormalised series approach (Killingbeck 1981) proceeds by setting β equal to $\mu - \lambda K$, with K variable, and then using the power series expansions

$$E = \sum E(M)\lambda^M \quad \langle x^N \rangle = \sum X(N, M)\lambda^M. \quad (3)$$

Making the appropriate substitutions in (2) and comparing coefficients of powers of λ produces a recurrence relation which can be rearranged to take the form

$$\begin{aligned} (2N+4)\mu X(N+2, M) &= \frac{1}{2}\alpha N(N^2-1)X(N-2, M) + (2N+4)KX(N+2, M-1) \\ &\quad - (2N+6)X(N+4, M-1) \\ &\quad + (2N+2)\sum_0^M E(P)X(N, M-P). \end{aligned} \quad (4)$$

This equation allows the sequential calculation of the $X(N, M)$ coefficients when it is used with the initial values $X(0, M) = \delta_{0,M}$ and $E(0) = (2n+1)(\mu\alpha)^{1/2}$ where n is the state number (0, 1, 2, etc). The energy coefficients at each order are found from the equation

$$(M+1)E(M+1) = X(4, M) - KX(2, M) \quad (5)$$

which follows from the Hellmann-Feynman theorem (Killingbeck 1985a).

3. Use of the parameter K

It is clear from equation (1) that if β and λ are fixed and μ and K vary according to the law $\mu = \beta + K\lambda$, then the resulting calculation is a perturbation theory analogue of a variational calculation using scaled harmonic oscillator functions as a basis set. The perturbation theory, however, uses neither explicit wavefunctions nor matrix elements. Setting $K = 0$ in the perturbation calculation gives the traditional Rayleigh-Schrödinger series for the problem. These series are divergent alternating ones, but as K is increased from zero (with λ positive) the perturbation series begin to give useful results; they give sums which converge to several decimal digits before the series ultimately diverge. In the earlier work on renormalised series, which only went up to tenth order or so, a 'plateau criterion' was used (Killingbeck 1981, Austin and Killingbeck 1982). The K (or μ) value was chosen to render the perturbation sum to some fixed order stationary with respect to variation of K (or μ). This was done because the *exact* E and $\langle x^N \rangle$ must be independent of the dummy parameters K and μ . However, with modern microcomputers it is possible to go to very high orders, and so the traditional way of dealing with asymptotic series (i.e. summing to the smallest term) can be used. We have performed a series of computations which revealed the following regularity: as K increases the sums of the perturbation series converge to

Table 1. Some results for the Hamiltonian $-D^2 + x^2 + \lambda x^4$ with $n = 10$ (i.e. ninth excited state). The order was held at 20 and K increased until at the K value shown the results had converged to the values shown.

λ	K	E	$\langle x^2 \rangle$
1	11	53.449 102	3.147 282 7
5	7	87.821 861	1.875 604 5
10	6	109.772 57	1.494 103 2
20	5	137.607 39	1.188 598 3
30	5	157.198 72	1.039 299 6
40	4	172.819 90	0.944 758 41

more and more digits before divergence ultimately sets in. However, the best converged result is reached at an order which also increases with K , so that the ultimate accuracy attainable is computer dependent. Table 1 shows some typical results obtained by holding the order at twenty and increasing K until well converged results were attained at or before order twenty. The results show that the use of the K parameter allows very accurate numerical calculations to be made for the Schrödinger equation (1) without the need for Padé approximants or other summation methods, and without the laborious (and sometimes fruitless) search for a plateau. That the Padé approximants for the $K = 0$ series should converge to the perturbed energies has been proved by analysis (Loeffel *et al* 1969). So far as we know there are no convergence theorems yet for the $K \neq 0$ series, which can be regarded as referring to a harmonic oscillator perturbed by a sum of potential terms of x^2 and x^4 type.

4. JWKB expectation values

For the Schrödinger equation (1) with β and λ values which give a single-well potential $V(x)$ the JWKB formula for the energy levels is

$$(n + \frac{1}{2})\pi\alpha^{1/2} = \int_L^U (E - \beta x^2 - \lambda x^4)^{1/2} dx \quad (6)$$

where U and L are the x values of the classical turning points. With $\lambda = 0$ the formula (6) correctly leads to the exact unperturbed energies for equation (1), whereas with $\lambda \neq 0$ the JWKB energy levels obtained using (6) will not be the exact quantum mechanical energy levels. To find a JWKB estimate of $\langle x^2 \rangle$ we can use a definition of expectation values which is based on energies (Killingbeck 1985a). For the Schrödinger equation (1) the Hellmann-Feynman theorem gives the result

$$\langle x^2 \rangle = \partial E / \partial \beta. \quad (7)$$

In numerical work (7) can be used to compute $\langle x^2 \rangle$ directly without computing detailed wavefunctions (Killingbeck 1985b). Dagens (1969) was apparently the first worker to use such an approach in the JWKB formalism. For the present problem we proceed by differentiating equation (6) with respect to β . The left-hand side gives zero. The boundary terms on the right give zero, since the integrand is zero at the turning points. Only the derivative of the integrand with respect to β gives a non-zero contribution,

and we finally obtain the result

$$\frac{\partial E}{\partial \beta} = \frac{\int_L^U x^2 (E - \beta x^2 - \lambda x^4)^{-1/2} dx}{(\int_L^U (E - \beta x^2 - \lambda x^4)^{-1/2} dx)}. \tag{8}$$

When evaluating (8) the E value on the right must equal the JWKB eigenvalue. If we interpret the quantity (8) as $\langle x^2 \rangle$ by using equation (7) then we find that the JWKB value for $\langle x^2 \rangle$ equals the time average of x^2 for a classical particle oscillating between the turning points, as may be seen by noting that the integrand in the denominator is proportional to the reciprocal of the classical velocity. The JWKB expectation value of any function $f(x)$ is obtained by using $f(x)$ instead of x^2 as the first factor of the first integral in (8).

We now look for a classical analogue of the quantum mechanical hypervirial relation (2). We start by considering a particle of mass m undergoing oscillations in a single-well potential $V(x)$ and study the product $x^{N+1}p$, where p is the momentum. We find

$$(d/dt)(x^{N+1}p) = x^{N+1}F + (N+1)x^N p^2 m^{-1} \tag{9}$$

where F is the force. Because of the periodic nature of the motion we can assert that the quantity in (9) must have a zero time average over one cycle. For the case $V = \beta x^2 + \lambda x^4$ we have $F = -2\beta x - 4\lambda x^3$ and also have the classical conservation of energy result $p^2 = 2m(E - V)$. Inserting these values of V, F and p^2 in (9), we find that the equation which asserts that the right-hand side of (9) must have zero time average looks like equation (2), except that it has $\alpha = 0$ on the left and refers to classical time averages instead of exact quantum mechanical expectation values. However, we have just seen that JWKB expectation values equal the classical time averages; the derivations also showed that the Hellmann-Feynman theorem gives the link between energies and expectation values in both the JWKB theory and the exact quantum mechanical theory. This suggests that using the hypervirial perturbation method of § 2 with $\alpha = 0$ should lead to some form of JWKB result for the energies and $\langle x^N \rangle$ values, and this is what was found to happen in microcomputer numerical experiments. The results of the analysis agree with our usual intuition about the semiclassical approximation, since α is usually presented in the form $\hbar^2/2m$; letting $\alpha \rightarrow 0$ thus corresponds to letting $\hbar \rightarrow 0$ or $m \rightarrow \infty$. The JWKB results for some particular α are obtained by setting $\alpha = 0$ in the recurrence relation (4) but retaining the full α value in the expression for the unperturbed energy $E(0)$.

5. Some numerical results

For the test case of the potential $V = \lambda x^4$ the integrals which appear in the JWKB theory can be evaluated numerically (Killingbeck 1985a) and the energy levels show a simple dependence on λ . We obtained the following JWKB results from the integrals:

$$E_n = 2.185\ 0693\ \lambda^{1/3} \alpha^{2/3} (n + \frac{1}{2})^{4/3} \tag{10}$$

$$\langle x^2 \rangle_n = 0.675\ 457\ 31\ \lambda^{-1/3} \alpha^{1/3} (n + \frac{1}{2})^{2/3} \tag{11}$$

$$\langle x^4 \rangle_n = 0.728\ 356\ 40\ \lambda^{-2/3} \alpha^{2/3} (n + \frac{1}{2})^{4/3}. \tag{12}$$

We note that the JWKB results obey the virial theorem, $E = 3\lambda \langle x^4 \rangle$. To treat the potential λx^4 by the hypervirial method we set $\beta = 0$ with $\mu = K\lambda$ and so treat the potential as consisting of an unperturbed part $K\lambda x^2$ plus a perturbing part $\lambda(x^4 - Kx^2)$. Table 2

shows some results at $\alpha = 0$ and $\alpha = 1$, with $\beta = 0, \lambda = 1$. As expected, the error of the JWKB numerical results decreases as the quantum number n increases and the JWKB results given by the perturbation series agree with those given by the above equations. This agreement provides a check on the accuracy of the $\alpha = 0$ results, while those for $\alpha = 1$ were checked against results from other methods. The present calculation, however, allows one technique to produce both sets of results.

If the factor $(n + \frac{1}{2})$ on the left-hand side of the JWKB equation (8) is replaced by the series

$$n + \frac{1}{2} + \sum_1^{\infty} A(k)n^{-k} \tag{13}$$

then the analysis of Titchmarsh (1961) implies that the coefficients $A(k)$ can be chosen so as to make equation (8) produce the correct quantum mechanical energies. This idea was used by Hioe *et al* (1976) in their numerical work on the perturbed harmonic oscillator. If we suppose that using (13) in (8) would give the correct energy, whereas using $(n + \frac{1}{2})$ gives the JWKB energy, a little algebra shows that as n tends to infinity we have

$$\Delta E/E \rightarrow \frac{4}{3} A(1)n^{-2} \tag{14}$$

where ΔE is the difference between the exact and wkb energies for the λx^4 potential. The numerical results of table 2 do show this kind of limiting behaviour and lead to the numerical estimate $A(1) = 0.0265$; using this $A(1)$ in equation (10) markedly improves the accuracy of the energy estimates. A different value, $A(1) = 0.0090$, was found to be appropriate for the $\langle x^2 \rangle$ formula (11). The difference between the two $A(1)$ values indicates that $A(1)$ in the energy equation varies with the coefficient β in the potential; if $A(1)$ in the energy equation (8) were potential independent then the argument of § 4 would lead to the conclusion that the $A(1)$ for equations (10) and (11) are the same.

It is clearly advantageous when using the methods of this paper to have a guiding rule to indicate how K or μ should depend on the potential parameters. Applying the test that the $E(0)$ value should roughly equal the actual perturbed energy leads to

Table 2. Results for the Hamiltonian $-D^2 + \lambda x^4$, at $\lambda = 1$, for a sequence of states with increasing n . The $\alpha = 0$ rows give the JWKB values. Note the remarkable accuracy of the JWKB values for $\langle x^2 \rangle$. In the $E(0)$ formula $\alpha = 1$ throughout.

n	K	α	E	$\langle x^2 \rangle$
0	6	1	1.060 3621	0.362 022
0	2	0	0.867 1453	0.425 512
10	11	1	50.256 255	3.239 008
10	10	0	50.240 152	3.238 8505
20	16	1	122.604 64	5.059 4824
20	16	0	122.594 32	5.059 4186
40	23	1	303.912 07	7.965 9233
40	23	0	303.905 51	7.965 8977
80	36	1	759.501 72	12.592 993
80	36	1	759.497 57	12.592 983
160	55	1	1905.896 0	19.948 710
160	55	0	1905.893 4	19.948 706

the theoretical result that μ should vary as $\alpha^{1/3} \lambda^{2/3} (n + \frac{1}{2})^{2/3}$ for the potential λx^4 . This result will also be valid for cases in which β is non-zero but λ and n are comparatively large. The results of tables 1 and 2 are in good accord with this theoretical estimate when the relationship $\mu = \beta + K\lambda$ is used to relate K and μ . In the limit $\lambda \rightarrow 0$, however, the μ value should approach β linearly in λ (according to first-order perturbation theory), so that the best K will have a positive non-zero value for $\lambda \rightarrow 0$. Theory indicates that K should vary roughly as $n\alpha^{1/2}\beta^{-1/2}$ as $\lambda \rightarrow 0$ for excited states. This agrees with the results of our microcomputer experiments.

As this work was about to be submitted a paper dealing with the Schrödinger equation (1) was published by Sanchez and Bejarano (1986). They obtained their JWKB energy levels from a formalism involving elliptic integrals and took their quantum mechanical energies from finite difference calculations. We have checked their results for the (β, λ) combinations (1, -0.02), (-1, 0.05), (-1, 1) and (-1, 5) and obtain fair agreement, except that our calculation shows their finite difference energies for excited states to be wrong in the last one or two digits quoted. Our method apparently fails for the negative-energy bound states in the double-well potential ($\beta < 0, \lambda > 0$), but for positive-energy bound states it clearly provides a uniform and accurate way of obtaining JWKB and exact values for both energies and $\langle x^N \rangle$ values.

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References

- Austin E J and Killingbeck J 1982 *J. Phys. A: Math. Gen.* **15** L443
 Caswell W E 1979 *Ann. Phys., NY* **123** 153
 Dagens L 1969 *J. Physique* **30** 593
 Hioe F T, MacMillen D and Montroll E W 1976 *J. Math. Phys.* **17** 1320
 Killingbeck J 1981 *J. Phys. A: Math. Gen.* **14** 1005
 — 1985a *Microcomputer Quantum Mechanics* (Bristol: Adam Hilger)
 — 1985b *J. Phys. A: Math. Gen.* **18** 245
 Loeffel J J, Martin S, Simon B and Wightman A S 1969 *Phys. Lett.* **30B** 656
 Sanchez A M and Bejarano J D 1986 *J. Phys. A: Math. Gen.* **19** 887
 Simon B 1970 *Ann. Phys., NY* **58** 76
 Swenson R J and Danforth S H 1972 *J. Chem. Phys.* **57** 1734
 Titchmarsh E C 1961 *Eigenfunction Expansions* vol 1 (Oxford: Oxford University Press)