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Abstract. Hypervirial theorems are applied in order to obtain easily perturbation series (PS) for eigenenergies and expected values of power of the radial coordinate of a general D-dimensional isotropic anharmonic oscillator ($IAO(D)$). In the next step the renormalisation method is introduced to obtain renormalised PS allowing the eigenenergies of $IAO(D)$ to be calculated with a high accuracy in a whole range of quantum numbers n, l and for high anharmonic constants.

1. Introduction

The study of quantum $IAO(D)$ is of considerable interest, not only for purely theoretical considerations, but also from the point of view of practical applications in chemical physics and nuclear physics. In these applications accurate and simple computation methods are needed.

The literature available on higher-dimensional IAO is, however, rather limited. Bell *et al* (1970a, b) have computed the energy levels of two- and three-dimensional quartic oscillators for quantum numbers $n < 50$ and $l < 10$ by numerical diagonalisation of matrices of large dimensions.

Pasupathy and Singh (1981) have formulated the exact quantisation condition generalising the WKB condition for any isotropic potential, but its applicability is limited to states with $l = 0$ only. Lakshmanan and Kaliappan (1980) have adopted the semi-classical Bohr–Sommerfeld quantisation method but their analytical formula is expected to be satisfactory only for a large quantum number n.

Recently, Seetharaman *et al* (1982) have derived a formula for $IAO(3)$ with potential $V = \frac{1}{2}(\omega r)^2 + \lambda r^4$ for energy levels via the WKB method. For the same potential Mathews *et al* (1982) have presented a very simple and accurate analytic formula for the energies of $IAO(D)$, $D \leq 3$.

In this work we derive PS for the energy and expected values of powers of the radial variable by employing the hypervirial relations (Hirschfelder 1960) for $IAO(D)$ with potential:

$$V(\lambda x) = \sum_{k=0}^{M} \lambda^k V_k x^{2(k+1)} = \hbar \omega_0 \sum_{k=0}^{M} \lambda^k v_k r^{2(k+1)},$$

$$x^2 = \sum_{k=0}^{D} x_i^2,$$

(1)

where λ is a perturbation parameter,

$$r = (m\omega_0/\hbar)^{1/2}x, \qquad \omega_0 = (2V_0/m)^{1/2}, \qquad v_k = (\hbar/m\omega_0)^{(k+1)}V_k/\omega_0\hbar$$

and m is a mass of the oscillator.

We also introduce a resummation of PS grounded on the Caswell (1979) approach and use it to combine the perturbation and WKB techniques.

This allows us to obtain a simple method for generating formulae for eigenenergies of a general IAO(D).

2. Perturbation series for IAO(D)

The Schrödinger equation for IAO(D) after introducing hyperspherical coordinates (Smith 1960) can be separated into hyper-radial and hyper-angular parts:

$$(H - E)R(r) = 0$$

where

$$H = -\tfrac{1}{2}(d^2/dr^2 + [(D-1)/r]d/dr - \Lambda^2(\Omega)/r^2) + V(\lambda r), \tag{2a}$$

$$(\Lambda^2(\Omega) - \Lambda^2)Y(\Omega) = 0, \qquad \Lambda^2 = \begin{cases} 0 & \text{for } D = 1, \\ L(L+D-2) & \text{for } D > 1, \end{cases} \tag{2b}$$

where

$$\psi(r) = R(r)Y(\Omega).$$

The Hamiltonian H obeys the commutation relations:

$$[r^j, H] = \tfrac{1}{2}j((j+D+2)r^{j-2} + 2r^{j-1}d/dr), \tag{3a}$$

$$[d/dr, H] = dV/dr + [(D-1)/2r]d/dr. \tag{3b}$$

The hypervirial theorems require that $\langle[W, H]\rangle$ vanish for solutions of equation (2a), where

$$\langle(\ldots)\rangle = \int_0^\infty (\ldots)R^2(r)r^{D-1}\,dr.$$

From equations (3a,b) and using $W = r^j\,d/dr$, the hypervirial relations which generalise those for $D = 1$ (Swenson and Danforth 1972, Lai and Lin 1982) are

$$E\langle r^j\rangle = \langle r^jV\rangle + \tfrac{1}{2}(j+1)^{-1}\langle r^{j+1}\,dV/dr\rangle - \tfrac{1}{8}(j+1)^{-1}j(j^2 - (D-2)^2)\langle r^{j-2}\rangle. \tag{4}$$

For the potential of the form (1) these relations give the following equations:

$$\langle r^{j+2}\rangle = B_j E\langle r^j\rangle + A_{j-2}\langle r^{j-2}\rangle - \sum_{k>0}\lambda^k C_{j+2}^{(k)}v_k\langle r^{j+2(k+1)}\rangle \tag{5a}$$

where

$$A_j = \tfrac{1}{4}(j+4)^{-1}(j+2)[(j+D)(j+4-D) - 4\Lambda^2],$$

$$B_j = 2(j+2)^{-1}(j+1), \qquad C_j^{(k)} = 2 + 2k/j. \tag{5b}$$

Now, if we expand E and $\langle r^j\rangle$ in the PS with respect to the parameter λ:

$$E = \sum_{k\geq 0}\lambda^k E_k, \qquad \langle r^j\rangle = \sum_{k\geq 0}\lambda^k R_k(j), \tag{6}$$

then applying the Hellmann–Feynman theorem, we find (Grant and Lai 1979)

$$E_k = \frac{1}{k} \sum_{m=1}^{k} m v_m R_{k-m}(2m+2). \tag{7}$$

Taking into account equations (4) and (5*a,b*) we obtain recursion relations for the coefficients $R_k(j)$:

$$R_k(j+2) = E_0 B_j R_k(j) + A_{j-2} R_k(j-2)$$

$$+ \sum_{m=1}^{k} (E_m B_j R_{k-m}(j) - C_{j+2}^{(m)} v_m R_{k-m}(j+2m+2)). \tag{8}$$

The above equations together with the initial conditions $R_k(0) = \delta_{k,0}$ are sufficient to generate the coefficients E_k of the PS and further coefficients $\mathscr{E}_n$ of the energy series in terms of $u_k \equiv \lambda^k v_k$:

$$E = \mathscr{E}_0 + \mathscr{E}_1 u_1 + \mathscr{E}_{01} u_2 + \mathscr{E}_2 u_1^2 + \mathscr{E}_{02} u_2^2 + \mathscr{E}_{11} u_1 u_2 + \ldots$$

$$= \sum_n \mathscr{E}_n \prod_k u_k^{n_k} \tag{9}$$

where

$$n \equiv (n_1 n_2 \ldots n_M), \qquad (n_1 n_2 \ldots n_k 0 \ldots 0) \equiv (n_1 n_2 \ldots n_k).$$

Some of the first $\mathscr{E}_n$ for $D = 1$ are given by the following

$$\begin{aligned} &\mathscr{E}_0 = E_0 \equiv \tfrac{1}{2}\varepsilon, & &\mathscr{E}_{11} = -\tfrac{15}{128}(63 + 118\varepsilon^2 + 11\varepsilon^4), \\ &\mathscr{E}_1 = \tfrac{3}{8}(1 + \varepsilon^2), & &\mathscr{E}_2 = -\tfrac{1}{32}(67 + 17\varepsilon^2)\varepsilon, \\ &\mathscr{E}_{01} = \tfrac{5}{16}(5 + \varepsilon^2)\varepsilon, & &\mathscr{E}_{02} = -\tfrac{1}{512}(19277 + 8290\varepsilon^2 + 393\varepsilon^4)\varepsilon. \end{aligned} \tag{10}$$

3. Renormalisation of perturbation series

3.1. The choice of renormalisation parameter for the quadratic–quartic oscillator

Usually the Schrödinger PS is only an asymptotic series, however we use a rearrangement of the terms in the potential $V(\lambda r)$ to improve the asymptotic properties of the PS. The new PS is still divergent but its divergence begins to be important only for very high terms. So, truncation after a finite number of terms gives reasonable energy values which can be optimised by choosing a proper partitioning of the Hamiltonian. In order to illustrate this technique we start with the specific example of the quadratic–quartic oscillator for which we can write:

$$V = \tfrac{1}{2}r^2 + u r^4 = \tfrac{1}{2}(\omega r)^2 + u(r^4 + (1-\omega^2)r^2/2u)$$

where ω is some parameter.

If we now introduce, independent of u, a parameter β by the definition

$$\omega^2 = 1 + \beta u \omega^{-1} \tag{11}$$

and transform the variable r into $\rho \omega^{-1/2}$ we obtain

$$V(\rho) = \omega[\tfrac{1}{2}\rho^2 + w(\rho^4 - \beta\rho^2)]$$

where

$$w = u\omega^{-3}.$$

Knowing the PS in terms of u, we can generate the PS in terms of w because taking into account the form of $V(\rho)$ we have

$$\omega \sum_n \mathcal{E}'_n w_k^n = \sum_n \mathcal{E}_n u^n. \tag{12}$$

Expanding $\omega = (1 - \beta w)^{-1/2}$ and $u^n = w^n (1 - \beta w)^{3n/2}$ in power series and equating both sides of equation (12) we obtain the coefficients $\mathcal{E}'_n$ as functions of the β (some of the first coefficients $\mathcal{E}'_n$ are given by equations (18b) in § 3.2). The improvement the convergence of PS depends on the proper choice of β parameter. In order to consider the possible ways of the determination of β, let us calculate the first-order energy

$$E^{(1)} = \omega(\mathcal{E}_0 + \omega^{-3} u(\mathcal{E}_1 - \tfrac{1}{2}\beta\mathcal{E}_0)). \tag{13}$$

The exact energy E is lower than $E^{(1)}$ since $E^{(1)}$ is the functional of energy $\langle \phi(\omega) H \phi(\omega) \rangle$, where $\phi(\omega)$ is the eigenfunction of a harmonic oscillator of a frequency ω. Thus, the optimum value of ω can be chosen from the condition

$$dE^{(1)}/d\omega = 0, \tag{14a}$$

implying the equation for ω:

$$\omega^3 = \omega + (4\mathcal{E}_1/\mathcal{E}_0)u.$$

This result means that $\beta = 4\mathcal{E}_1/\mathcal{E}_0$ (see equation (11)). The same result is obtained from the condition proposed by Killingbeck (1981)

$$dE^{(1)}/d\beta = 0. \tag{14b}$$

It is interesting that an identical value of β is obtained (see Caswell 1979) from the following equation

$$d\tilde{E}^{(1)}/d\beta = 0 \tag{14c}$$

where

$$\tilde{E}^{(1)} = \lim_{u \to \infty} (E^{(1)} u^{-1/3}) \tag{14}$$

is the first-order energy of quartic oscillator ($V = r^4$). The optimum value of β obtained for the limit $u \to \infty$ determines the optimum β for an arbitrary u. This result is valid also when we calculate β for Nth-order energy $E^{(N)}$ of the IAO(D) with the potential $V = \tfrac{1}{2}r^2 + ur^{2M}$.

The determination of β from equation (14c) is the simplest because $\tilde{E}^{(N)}$, defined analogously to $\tilde{E}^{(1)}$, is independent of u. Let us note, however, that equations (14a)–(14c) for $E^{(N)}$ can have no real solutions if $N > 1$ as $E^{(N)}$ and also $\tilde{E}^{(N)}$ are not the functionals of energy, for example the equation

$$d\tilde{E}^{(2)}/d\beta = (5\mathcal{E}_2 + 4\beta\mathcal{E}_1 - \tfrac{3}{8}\beta^2\mathcal{E}_0)/\mathcal{E}_0 = 0$$

has no real solutions for the states with the quantum number $n = 0, 1$. In such cases we propose to determine β under the condition that $\tilde{E}^{(N)}$ would differ as little as

possible from $E(4)$ i.e.

$$(d/d\beta)(\tilde{E}^{(N)} - E(4))^2 = (\tilde{E}^{(N)} - E(4))d\tilde{E}^{(N)}/d\beta = 0 \qquad (15)$$

where $E(4)$ is the exact eigenvalue of the quartic oscillator. If equation (14c) for $\tilde{E}^{(N)}$ has no solutions, we find β values from the condition

$$\tilde{E}^{(N)} = E(4). \qquad (16)$$

For $N > 1$, equations (14c) and (16) have many solutions but we must choose those which introduce the minimum errors in $E^{(N)}(u)$. We have proved that the solutions of equation (16), if they exist, give much more accurate values of $E^{(N)}(u)$ than the solutions of equation (14c) in the whole range of u and n values. The important fact is that the method of renormalisation of PS presented above (equation (16)) also provides the convergence of PS for $u \to \infty$, in the sense that $E^{(N)}(u)$ approaches the exact value of energy i.e. $E^{(N)}(u) \to u^{1/3}E(4)$. Such convergence has not been provided by the method of Killingbeck (1981) (see equation (14b)) or by the method proposed by Dmitrieva and Plindov (1979, 1980a, b which is referred to as I). Their method of calculation of energy is equivalent to the renormalisation of PS. Indeed, formula (12) for the energy $\bar{E}$ given in I can be obtained by expressing $\bar{E}$ in the form of renormalised PS

$$\bar{E} = \mathcal{E}_0' + u\mathcal{E}_1' + u^2\mathcal{E}_2' + \dots$$

with $u \equiv \frac{1}{2}Z$ and the renormalisation parameter $\beta \equiv 2A = 4\mathcal{E}_1/\mathcal{E}_0$ (equation (6) in I). However, with such a parameter β, which is independent of the order N, rather low accuracy for the energy is obtained. The relative errors in energy values obtained by this method with the additional Padé approximants applied are 8×10^{-4} for $N = 5$, while the corresponding errors obtained with our method, without any resummation procedure, are of the order 5×10^{-7} (these results will be published elsewhere).

3.2. The choice of renormalisation parameters for the quadratic–quartic–sextic oscillator

The method of renormalisation of PS in a general case will be illustrated in the following example.

Let us consider IAO(1) with the potential

$$V = \frac{1}{2}x^2 + u_1 x^4 + u_2 x^6, \qquad u_1^2 = 2u_2(1 + 3(2u_2)^{1/2})$$

for which the energy of the ground state can be exactly determined (Singh *et al* 1980)

$$E = \frac{1}{2}u_1(2u_2)^{-1/2}.$$

We can rewrite the above potential in the form

$$V = \frac{1}{2}\omega^2 x^2 + \tilde{u}_1(x^4 + (1 - \omega^2)x^2/2\tilde{u}_1) + u_2(x^6 + (u_1 - \tilde{u}_1)x^4/u_2).$$

If we introduce the coefficients β_1 and β_2 by the definitions

$$\omega^2 = 1 + \beta_1\tilde{u}_1\omega^{-1}, \qquad \tilde{u}_1 = u_1 + \beta_2 u_2(\omega\beta_1)^{-1} \qquad (17a, b)$$

then we can generate, in a similar way to that of § 3.1, the PS in terms of $w_k = u_k\omega^{-(k+2)}$:

$$E = \omega \sum_n \mathcal{E}_n' \prod_k w_k^{n_k}. \qquad (18a)$$

Some of the first coefficients $\mathscr{E}'_n$ are given below:

$$\mathscr{E}'_0 = \mathscr{E}_0, \qquad\qquad \mathscr{E}'_{11} = \mathscr{E}_{11} + \tfrac{3}{2}\beta_1\mathscr{E}_{01} + \beta_2\mathscr{E}_1 - \tfrac{1}{4}\beta_1\beta_2\mathscr{E}_0,$$

$$\mathscr{E}'_1 = \mathscr{E}_1 - \tfrac{1}{2}\beta_1\mathscr{E}_0, \qquad \mathscr{E}'_2 = \mathscr{E}_2 + \beta_1\mathscr{E}_1 - \tfrac{1}{8}\beta_1^2\mathscr{E}_0, \qquad (18b)$$

$$\mathscr{E}'_{01} = \mathscr{E}_{01} - \tfrac{1}{2}\beta_2\mathscr{E}_0, \qquad \mathscr{E}'_{02} = \mathscr{E}_{02} + \tfrac{3}{2}\beta_2\mathscr{E}_{01} - \tfrac{1}{8}\beta_2^2\mathscr{E}_0.$$

Let us calculate the first-order energy:

$$E^{(1)} = \omega(\mathscr{E}_0 + w_1\mathscr{E}'_1 + w_2\mathscr{E}'_{01})$$

and the second-order energy with respect to w_1 and w_2:

$$E^{(2)} = E^{(1)} + \omega(w_1^2\mathscr{E}'_2 + w_2^2\mathscr{E}'_{02} + w_1 w_2\mathscr{E}'_{11}).$$

From the equations $(\partial/\partial\beta_k)E^{(N)} = 0$ generalising equation $(14b)$, we obtain:

$$u_1(\beta_1 - 4\mathscr{E}_1/\mathscr{E}_0) + u_2(\beta_2 - 6\mathscr{E}_{01}/\mathscr{E}_0) = 0 \qquad \text{for } N = 1, \qquad (19a)$$

$$A = (\omega u_1)^2 A_1 + u_2^2 A_2 + \omega u_1 u_2 A_{11} = 0 \qquad \text{for } N = 2, \qquad (19b)$$

where

$$A_1 = (5\mathscr{E}_2 + 4\beta_1\mathscr{E}_1 - \tfrac{3}{8}\beta_1^2\mathscr{E}_0)/\mathscr{E}_0,$$

$$A_2 = (7\mathscr{E}_{02} + \tfrac{15}{2}\beta_2\mathscr{E}_{01} - \tfrac{3}{8}\beta_2^2\mathscr{E}_0)/\mathscr{E}_0,$$

$$A_{11} = (6\mathscr{E}_{11} + \tfrac{15}{2}\beta_1\mathscr{E}_{01} + 4\beta_2\mathscr{E}_1 - \tfrac{3}{4}\beta_1\beta_2\mathscr{E}_0)/\mathscr{E}_0.$$

Equation $(19a)$ has solutions for any u_1, u_2:

$$\beta_1^{(1)} = 4\mathscr{E}_1/\mathscr{E}_0, \qquad \beta_2^{(1)} = 6\mathscr{E}_{01}/\mathscr{E}_0.$$

Equation $(19b)$ in general cannot be fulfilled for any u_1 and u_2; however, if $u_k^2 \gg u_i^2$ we can determine β_k from the conditions

$$A_k = 0 \qquad\qquad\qquad\qquad (20a)$$

or

$$dA_k/d\beta_k = 0 \qquad\qquad\qquad\qquad (20b)$$

if equation $(20a)$ has no real roots. It is worth noticing that the above equations are equivalent to the equations

$$\left(\frac{\partial E^{(N)}}{\partial \beta_k}\right)_{u_i = u_k\delta_{i,k}} = 0. \qquad\qquad (21)$$

Let us calculate the β_k values for $n = 0$. From equation $(20b)$ we have

$$\beta_1^{(2)} = 16\mathscr{E}_1/(3\mathscr{E}_0) = 8, \qquad \beta_2^{(2)} = 10\mathscr{E}_{01}/\mathscr{E}_0 = 37.5.$$

They are close to β_k values obtained from the following conditions (compare equation (16)):

$$(\tilde{E}^{(2)})_{u_2=0} = E(4), \qquad \tilde{\beta}_1^{(2)} = 8.012$$

and

$$(\tilde{E}^{(2)})_{u_1=0} = E(6), \qquad \tilde{\beta}_2^{(2)} = 40.00.$$

The latter values give better results for the energy.

The values of the first- and second-order energy and their comparison with the exact energy are given in table 1. In order to show that the renormalisation of the constant $u_1 \rightarrow \tilde{u}_1$ essentially improves the convergence of PS, the table also includes the results for $\beta_2 = 0$ $(u_1 = \tilde{u}_1)$. This renormalisation is seen to increase the accuracy of results by one order of magnitude.

Table 1. The ground state energy E of IAO(1) with the potential $V = \frac{1}{2}x^2 + u_1 x^4 + u_2 x^6$ and the first-order $(E^{(1)})$ and second-order $(E^{(2)})$ energies of renormalised perturbation theory. The parenthesis includes the $\beta_2^{(2)}$ values.

u_2	0.01	0.1	1	10	100
u_1	0.1688	0.6844	3.2381	16.980	93.195
$E^{(1)}$	0.5997	0.7759	1.1713	1.9515	3.3931
$E^{(2)}(0)$	0.5962	0.7606	1.1264	1.8527	3.2038
$E^{(2)}(40)$	0.5966	0.7649	1.1444	1.8978	3.2938
E	0.5967	0.7651	1.1448	1.8984	3.2949

Generalisation of the above consideration to the general problem is straightforward. For the anharmonic potential with M constants $\{u_k\}$ we can introduce M coefficients $\{\beta_k\}$ by definition (17a) and:

$$\tilde{u}_{k-1} = u_{k-1} + \beta_k \tilde{u}_k (\omega \beta_{k-1})^{-1} \qquad \text{for } k = 2, 3, \ldots M,$$

$$\tilde{u}_M \equiv u_M.$$

(22)

Introducing the renormalised constants $w_k = u_k \omega^{-(k+2)}$ and taking into account the relation satisfied by ω,

$$\omega = \left(1 - \sum_k \beta_k w_k \right)^{-1/2},$$

(23)

we can generate the renormalised PS (18a) for IAO(D). We determine the renormalisation parameters β_k from the conditions

$$(\tilde{E}_k^{(N)})_{u_i = 0} = E(2k + 2), \qquad k \neq i$$

(24)

where

$$\tilde{E}_k^{(N)} = \lim_{u_k \to \infty} (E^{(N)} u_k^{-1/(k+1)}),$$

(25)

$E(2k + 2)$ is the eigenvalue of IAO(D) with potential $V = r^{2k+2}$, or from equation (21) if equation (24) has no solutions.

3.3. Renormalisation of a WKB type

The method of determination of parameters $\{\beta_k\}$ presented in § 3.2 is not the only possible one. For highly excited states with $n \gg 1$, we propose to employ another way of determining $\{\beta_k\}$ as equations (21) strictly only give the optimum $\{\beta_k\}$ values for $n = 0$ if $N \rightarrow \infty$. The method proposed below allows a higher accuracy of eigenenergy values to be determined; this is illustrated in the example which follows.

Let us calculate the first-order energy $\tilde{E}^{(1)}$ for a quartic oscillator. With this purpose in mind, we take in equations (14), (15b) the value of ω calculated from equation (11) for the limiting case when $u \to \infty$: $\omega_\infty = (\beta u)^{1/3}$. So we have

$$\tilde{E}^{(1)} = \beta^{1/3}(\tfrac{1}{2}\mathscr{E}_0 + \beta^{-1}\mathscr{E}_1) = C^{(1)}E_0^{4/3}(1 + 1/(4E_0^2))^{1/3}$$
$$= C^{(1)}E_0^{4/3}(1 + a^{(1)}E_0^{-2} + \ldots).$$

The expression obtained for $\tilde{E}^{(1)}$ has a form of WKB type expansion (Hioe and Montroll 1975) in which $C^{(1)} = 6^{1/3}(\tfrac{3}{4}) = 1.362\,84$ is replaced by $C = \pi^2 3^{4/3}(\Gamma(\tfrac{1}{4}))^{-8/3} = 1.376\,51$ and $a^{(1)} = \tfrac{1}{12}$ is replaced by

$$\delta_1 = 1/(9\pi) \qquad \text{for } D = 1.$$

In order for the renormalised PS to give good results for high states (similarly as WKB), it is sufficient to assume $\beta = E_0 x^{-3}$ with the parameter x depending only on an order of perturbation theory chosen so that $C^{(N)}(x) = C$. Then we obtain:

$$\tilde{E}^{(N)} = CE_0^{4/3}\left(1 + \sum_k^{N'} a_k^{(N)}E_0^{-2k}\right), \qquad N' = \begin{cases} N/2 & \text{for even } N \\ \tfrac{1}{2}(N+1) & \text{for odd } N \end{cases}.$$

The introduction of the parameter x gives an exact value of the WKB zero-order term and the higher WKB terms are produced by perturbation theory. The same type of expansion of $\tilde{E}^{(N)}$ is also obtained when $\beta^{-1}(E_0)$ is a function which can be expanded as a series:

$$\beta^{-1} = x^3 E_0^{-1}\left(1 + \sum_k b_k E_0^{-2k}\right). \tag{26}$$

Thus, the proper way of renormalisation of PS regulated by $\{b_k\}$ parameters combines the virtues of both the WKB and the perturbation methods. Let us take the simple function

$$\beta^{-1} = x^3 E_0^{-1}(1 + b(E_0^2 + gE_0^{-2})^{-1}) \tag{27}$$

which can be expanded as series (26).

The term gE_0^{-2} gives an essential contribution to β only for the lowest states and rapidly decreases with increasing E_0. In this way, the values of energy for $n \sim 1$ are improved while the values for $n \gg 1$, when the WKB method gives very good results, are not disturbed.

Let us define the parameter b such that $a_1^{(1)}(b) = \delta_1$. This assumption and equation (27) lead to the expression for the quartic oscillator energy when $g = 0$ obtained by Mathews *et al* (1982) as a result of the analysis of non-diagonal matrix elements of the Hamiltonian in the harmonic oscillator basis. Their approach is equivalent to the renormalised first-order perturbation theory.

The x values obtained from the condition $C^{(1)}(x) = C$ in the form

$$1 + 3x^3 = 2Cx$$

are

$$x_{(1)} = 0.607\,238, \qquad x_{(2)} = 0.497\,079$$

and the corresponding values of b:

$$b = (2C\delta_1 x - 9x^3/4)/(6x^3 - 1)$$

are

$$b_1 = -0.950\,372, \qquad b_2 = 0.498\,544.$$

Mathews *et al* have accepted the first solution. But we prefer the second since the least value of x in the Nth order of perturbation theory gives the most accurate results for $n \sim 1$. In table 2 we compare the first-order energies $\tilde{E}_n^{(1)}$ calculated with $\beta_p = 4\mathscr{E}_1/\mathscr{E}_0$ and with β_w determined by formula (27). The results are the illustration of the fact that β_p is the optimum only for $n \sim 1$, while β_w gives better results for $n \geq 2$. The introduction of the parameter $g = -0.45$ modifies β_w so that $\beta_w(g) \simeq \beta_p$ for $n \sim 1$ and due to this we obtain a good estimation of the energy for the whole range of the quantum number n.

Table 2. The first-order eigenenergies of a one-dimensional quartic oscillator calculated with the β_p (equation (14a)) and with the β_w (equation (27)).

n		0	1	2	4	10	20
β_p		6.00	10.00	15.60	27.33	63.14	123.07
β_w,	$g = 0$	1.36	10.00	18.85	35.76	85.10	166.71
β_w,	$g = -0.45$	6.00	9.82	18.835	35.76	85.10	166.71
$E(\beta_p)$		0.6814	2.4237	4.6850	10.1665	31.3587	76.477 95
$E(\beta_w)$,	$g = 0$	0.8881	2.4237	4.7033	10.2457	31.6596	77.236 11
$E(\beta_w)$,	$g = -0.45$	0.6814	2.4238	4.7031	10.2457	31.6596	77.236 11
		(680)	(3936)	(6968)	(33)	(5)	(08)

Higher accuracy of results can be obtained in a higher order and applying a longer expansion of β^{-1}. In the tables 3 and 4 we present the results for quartic one-dimensional and three-dimensional oscillators respectively, obtained with β^{-1} of the form

$$\beta^{-1} = x^3 E_0^{-1}(1 + (b_1 + e_1\Lambda^2)E_0^{-2} + (b_2 + e_2\Lambda^2)(E_0^4 + g_1 + g_2 E_0^{-2})^{-1}).$$

The values of the parameters x, b_1, b_2 are chosen from the conditions

$$C^{(2)}(x) = C, \qquad 8Cx = 3 + x^3(24 - 36x^3),$$

$$x = 0.395\,122\,788,$$

$$a_1^{(2)}(b_1) = \delta_1, \qquad b_1 = 3[16C\delta_1 x + x^3(67x^3 - 12)]/(8B),$$

$$b_1 = 0.388\,1968,$$

$$a_2^{(2)}(b_2) = \delta_2,$$

$$b_2 = 6[C\delta_2 x + b_1(x^3(b_1 - \tfrac{1}{2}) + \tfrac{1}{48}x^6(68b_1 + 335) - \tfrac{2}{9}Cb_1 x)],$$

$$b_2 = 0.408\,95,$$

where

$$B = x^3(18 - 51x^3) - 2Cx$$

(for the calculation of δ_2, see the appendix). The parameters g_1, g_2 are calculated from the conditions

$$\beta_w = \beta_p \text{ for } n = 0,1; \qquad g_1 = -4.761\,114, \qquad g_2 = 1.108\,314.$$

Table 3. The second-order eigenenergies of the one-dimensional quartic oscillator.

n	$E^{(2)}$
0	0.667 9862 (2)
1	2.393 6440 (0)
2	4.696 720 (95)
3	7.335 816 (730)
4	10.244 334 (08)
6	16.711 8950 (896)
8	23.889 9952 (36)
10	31.659 4571 (65)

Table 4. The second-order eigenenergies of quartic IAO(3).

n/l	0	2	4	6	8
0	2.393 644 (4)				
2	7.335 816 (730)	6.846 (30)			
4	13.379 348 (37)	13.010 (05)	12.163 (59)		
6	20.220 852 (48)	19.917 6 (60)	19.224 (18)	18.140 (52)	
8	27.706 394 (2)	27.445 96 (4)	26.848 (5)	25.923 (19)	24.658 (89)
10	35.740 316 (2)	35.510 3 (10)	34.980 21 (15)	34.160 (57)	33.051 (6)

n/l	1	3	5	7	9
1	4.496 (78)				
3	10.103 7 (0998)	9.412 (01)			
5	16.600 4 (5995)	16.053 (46)	15.078 (82)		
7	23.796 28(2)	23.333 8 (15)	22.516 6(10)	21.337 (58)	
9	31.577 8 (81)	31.173 55 (6)	30.457 8 (48)	29.436 25 (17)	28.094 (135)
11	39.868 65 (901)	39.507 3 (85)	38.865 61 (43)	37 951 6 (494)	36.763 (71)

To take account of a proper change in energy with the quantum number l we introduce parameters e_1, e_2 for $D = 3$ empirically (results for $l \neq 0$ are much less accurate than for $l = 0$). The accuracy of the second-order eigenenergies of the quartic IOA(D) for $l = 0$ is at least two decimal places higher when compared with the first-order (compare tables 3 and 4 with table 2 and also with tables 1 and 3 of Mathews *et al* 1982). For $n > 20$ our results are also much better than the numerical results of Bell *et al* (1970a, b) in which only eight significant figures are correct. We prove this fact by calculating the WKB fourth- and fifth-order eigenenergies (see appendix); they coincide with each other with an accuracy of ten significant figures.

4. Conclusions

Hypervirial theorems are applied to construct PS for energy and expected values of r^j for a general IAO(D). The transformation of the PS obtained is introduced to derive the renormalised PS. Two methods of determining the renormalisation parameters $\{\beta_k\}$ are proposed. One of them is based on searching for the minimum of $(\tilde{E}_k^{(N)} - E(2k+2))^2$ (see equations (15) and (21), (24)) and yields good results for the lowest

states with $n \sim 1$. The second method is based on employing the expansion of β_k^{-1} in series (26) and on the information given by the WKB approach. With this method, a high accuracy of results is obtained for $n \gg 1$.

A combination of the two approaches allows simple analytical formulae to be obtained for calculation of the eigenenergies of IAO(D) with high accuracy in the whole range of quantum numbers n, l and anharmonic constants $\{u_k\}$.

Acknowledgment

Appendix

We derive here an analytic expression for the higher-order WKB eigenenergies of the one-dimensional quartic oscillator. The WKB quantisation condition is

$$E_0 = \sum_k I_k$$

where for the potential $V = x^n$, and $\hbar/(2m)^{1/2} = 1$, following Kesarwani and Varshni (1981), we have

$$I_0 = \frac{1}{\pi} \int_{-x_0}^{x_0} (E - x^4)^{1/2}\, dx, \qquad x_0 = E^{1/4},$$

$$I_k = \sum_{m,n} A_{m,n}^{(k)} d^m J_n/dE^m, \qquad k = 1, 2, \ldots.$$

The integrals

$$J_n = \int_{-x_0}^{x_0} x^n (E - x^4)^{-1/2}\, dx$$

can be easily evaluated:

$$J_n = \tfrac{1}{2} E^{(n-1)/4} \Gamma^{-1}(\tfrac{1}{4}(n+3)) \Gamma(\tfrac{1}{4}(n+1)) \Gamma(\tfrac{1}{2}).$$

Now, the energy eigenvalues are determined from the equation

$$\mathscr{E} = \left(E_0 - \sum_{k=2}^{N} c_k \mathscr{E}^{3-2k} \right) \Big/ c_1, \qquad \mathscr{E} = E^{3/4}. \tag{A1}$$

Taking the $A_{m,n}^{(k)}$ coefficients from Kesarwani and Varshni (1981) we have (for $N = 5$)

$$c_1 = \tfrac{2}{3}(2\pi)^{-3/2} \Gamma^2(\tfrac{1}{4}), \qquad c_2 = -(12\pi c_1)^{-1},$$

$$c_3 = 22 \times 4^{-5} c, \qquad c_4 = -(4697/30)4^{-4} c. \qquad c_5 = -(1170\ 195/14)4^{-9} c_1. \tag{A2}$$

We solve equation (A1) by iteration, starting from $E = E_0$. As a result we obtain the analytic formula

$$E = C E_0^{4/3} \left(1 - \sum_{k=1}^{4} \delta_k E_0^{-2k} \right) \tag{A3}$$

where

$$C = c_1^{-4/3},$$

$$\delta_1 = \tfrac{4}{3}c_1c_2,$$

$$\delta_2 = \tfrac{2}{9}c_1^2(5c_2^2 + 6c_1c_3), \qquad\qquad (A4)$$

$$\delta_3 = (\tfrac{2}{9})c_1^3[11c_2(4c_2^2 + 9c_1c_3) + 27c_1^2c_4],$$

$$\delta_4 = \tfrac{1}{243}c_1^4[c_2^2(715c_2^2 + 3096c_1c_3) + 12c_1^2(126c_2c_4 + 81c_3^2) + 324c_1^3c_5].$$

Numerical values of these constants are given by the following

$$C = 2.185\,069\,300,$$

$$\delta_1 = -0.035\,367\,765, \qquad \delta_2 = 0.003\,527\,580,$$

$$\delta_3 = 0.001\,765\,731, \qquad \delta_4 = -0.004\,125\,822.$$

Formula (A3) approximates the solutions of equation (A1) with an error of less than 10^{-8} for $n \geqslant 3$. The accuracy of the eigenenergies calculated from (A3) improves rapidly with increasing n. For $n > 8$ an accuracy of ten significant figures is achieved.

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