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Hypervirial treatment of multidimensional isotropic bounded oscillators

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A method derived earlier to analyze one-dimensional systems is applied to the study of multidimensional isotropic bounded oscillators. The problem is reduced to a one-dimensional one in order to take advantage of several earlier results. The application of the method to the harmonic-oscillator model shows that the results so obtained are excellent.

I. INTRODUCTION

Owing to its great usefulness in different astronomy and physics fields, the bounded-harmonic-oscillator model has received great interest for many years.[1-14] Among the applications of this sort of model, we can mention the following:

(a) study of the fundamental mass-radius relation of the white dwarf theory[2];
(b) determination of the rate of escape of stars from galactic and globular clusters[3];
(c) specific heat of solids[5];
(d) phase transitions of second order[6];
(e) the magnetic properties of a system of electrons contained within a cylinder.[7]

Some works related to the isotropic harmonic oscillator have been presented[7,9] but the greatest number of them are devoted to the one-dimensional case. The mathematical methods employed in the analysis of this problem, in a direct or indirect way, are the confluent hypergeometric function[1,4,8-11] in the majority of cases. Unfortunately, this sets a limitation on the possible bounded systems to be studied, and so only the harmonic oscillator and the hydrogen atom have been studied so far. Even general methods, like the WKB approximation,[11] were only applied to the harmonic oscillator.

Recently, we have developed a powerful and general method[13-16] which allows the analysis of any one-dimensional bounded system whose potential energy has the form

$$V(x)=cx^k\ ,\quad k>0\ .$$

Through a particular way of combining the hypervirial theorems with the perturbation theory, we deduced a method which permits the treatment of symmetric oscillators as well as shifted oscillators under different boundary conditions. In another paper[17] we have generalized such a method in order to be suitable for multidimensional systems. The purpose of this paper is to apply this new methodology to multidimensional isotropic bounded oscillators (MIBO). Hence these models can be studied without further difficulty with our generalized method.[17] We do so by a reduction of the multidimensional problem to a one-dimensional one, in order to take advantage of several previously published results.[13-16]

The present paper is organized as follows. Section II introduces, in general terms, the method to be used. In Sec. III we deduce the general formulas which allow us to obtain the eigenvalue for any MIBO. Finally, Sec. IV deals with the application to the harmonic oscillator model, and Sec. V gives a concluding assessment.

II. METHOD

Let us consider the one-dimensional eigenvalue equation

$$H\phi=E\phi\ , \tag{1}$$

$$H=-\frac{D^2}{2}+V(x)\quad D\equiv\frac{d}{dx}\ , \tag{2}$$

whose eigenfunctions must satisfy the Dirichlet boundary conditions in the extreme points of the finite closed interval [0,*b*], i.e.,

$$\phi(0)=\phi(b)=0 . \quad (3)$$

The functions $x^N\phi'(x)$ do not belong to the domain of H because of the boundary conditions (3), so that hypervirial relationships[18] adopt a different expression with regard to the usual ones[13–16]

$$\langle [H,x^N D]\rangle=\tfrac{1}{2}b^N|\phi'(b)|^2 , \quad (4)$$

where $\langle\phi|\phi\rangle=1$.

From Eq. (1) it can be deduced at once that $\phi'(b)$ is related to the derivative of E in a very simple way

$$\frac{\partial E}{\partial b}=-\tfrac{1}{2}|\phi'(b)|^2 . \quad (5)$$

Then

$$\langle [H,x^N D]\rangle=-b^N\frac{\partial E}{\partial b} . \quad (6)$$

The calculation of the commutator $[H,x^N D]$, the elimination of the D^2 terms from Eq. (1), and the removal of the D terms by application of the trivial hypervirial relations

$$\langle [H,x^{N-1}]\rangle=0 \quad (7)$$

leads to the formula

$$\tfrac{1}{4}N(N-1)(N-2)\langle x^{N-3}\rangle+2NE\langle x^{N-1}\rangle -2N\langle x^{N-1}V\rangle-\langle x^N V'\rangle=-b^N\frac{\partial E}{\partial b} . \quad (8)$$

When the potential energy possesses the form

$$V(x)=cx^k+\frac{t^2}{2x^2} , \quad (9)$$

Eq. (8) shows a relationship for the derivative of the eigenvalues as a function of the average values $\langle x^N\rangle$,

$$2NEA^{N-1}+(N-1)(\tfrac{1}{4}N(N-2)-t^2)A^{N-3} -c(2N+k)A^{N+k-1}=-b^N\frac{\partial E}{\partial b} , \quad (10)$$

where

$$A^N\equiv\langle x^N\rangle .$$

From the power-series expansion in c for A^N and E

$$E=\sum_{s=0}^{\infty}E^s c^s , \quad A^N=\sum_{s=0}^{\infty}A_s^N c^s , \quad (11)$$

the application of the virial theorem

$$2E-c(k+2)A^k=-b\frac{\partial E}{\partial b} , \quad (12)$$

and the Hellmann-Feynman theorem

$$\frac{\partial E}{\partial c}=A^k , \quad (13)$$

we arrive at an expression which shows the connection between E^s and b.

$$E^s(b)=K_s b^{(k+2)s-2} ,$$

$$K_0=E^0(b=1) , \qquad s>0 , \quad (14)$$

$$K_s=E^s(b=1)=\frac{A_{s-1}^k(b=1)}{s} ,$$

The previous formulas assure us that it is only necessary to calculate those terms of series (11) for $b=1$.

It is possible to get a recurrence relation which allows the computation of the whole set $\{A_s^N\}$ (and consequently of $\{E^s\}$) if $\partial E/\partial b$ is removed from (10) and (12), and then expansions (11) are replaced in the resultant equation

$$A_s^N=b^N\frac{2-(k+2)s}{2(N+1)sE^0}A_{s-1}^k-\frac{N}{2(N+1)E^0}[\tfrac{1}{4}(N^2-1)-t^2]A_s^{N-2}+\frac{2N+k+2}{2(N+1)E^0}A_{s-1}^{N+K} -\frac{1}{E^0}\sum_{j=1}^{s}\frac{A_{j-1}^k A_{s-j}}{j} , \quad s>0 \quad (15)$$

$$A_0^N=\frac{b^N}{N+1}-\frac{N}{2(N+1)E^0}[\tfrac{1}{4}(N^2-1)-t^2]A_0^{N-2} . \quad (16)$$

In order to calculate the matrix elements A_s^N through the recurrence relationship, it is necessary to know only E^0 and to take into account the normalization condition

$$A_s^0=\delta_{s0} .$$

III. ANALYSIS OF THE MIBO

The Schrödinger equation for an M-dimensional isotropic oscillator is

$$-\frac{\hbar^2}{2m}\Delta\phi(\vec{r})+cc_0r^k\phi(\vec{r})=E\phi(\vec{r}) ,$$
$$\vec{r}=(x_1,x_2,\ldots,x_M) , \quad \Delta=\sum_{i=1}^{M}\frac{\partial^2}{\partial x_i^2} , \tag{17}$$

where c (perturbation parameter) is a scalar and c_0r^k has energy units. Defining the new dimensionless quantites $\vec{q}$ and W

$$\vec{r}=\left[\frac{\hbar^2}{mc_0}\right]^{1/(k+2)}\vec{q} ,$$
$$W=\left[\frac{1}{c_0}\right]^{2/(k+2)}\left[\frac{m}{\hbar^2}\right]^{k/(k+2)}E , \tag{18}$$

Eq. (17) transforms into

$$-\tfrac{1}{2}\Delta\phi(\vec{q})+cq^k\phi(\vec{q})=W\phi(\vec{q}) . \tag{19}$$

If the oscillator is confined within the limits of a sphere with radius r_0, it is necessary that solutions of Eq. (19) satisfy the Dirichlet boundary conditions over a spherical surface of radius q_0,

$$\phi(\vec{q})=0 \quad \text{for } q\geq q_0 ,$$
$$q_0=(mc_0\hbar^2)^{1/(k+2)}r_0 . \tag{20}$$

Applying M-dimensional spherical coordinates, Eq. (19) may be transformed into a one-dimensional equation[19,20]

$$-\frac{1}{2}\left[\frac{\partial^2}{\partial q^2}+\frac{M-1}{q}\frac{\partial}{\partial q}-\frac{l(l+M-2)}{q^2}\right]f_{nl}(q)+cq^kf_{nl}(q)=W_{nl}f_{nl}(q) , \quad f_{nl}(q_0)=0 . \tag{21}$$

As usual, n and l represent the radial quantum number and one of the $M-1$ angular quantum numbers, respectively. From now on in order to simplify the notation, we will omit the use of the subindices n and l.

The definition of the new function $g(q)$

$$g(q)=q^{(M-1)/2}f(q) \tag{22}$$

permits us to write Eq. (21) in a similar way to that employed in Sec. II:

$$-\tfrac{1}{2}g''+U(q)=Wg , \tag{23}$$

$$U(q)=cq^k+\frac{t^2}{2q^2} ,$$
$$t^2=l(l+M-2)+\frac{(M-1)^2}{2}-\frac{M^2-1}{4} . \tag{24}$$

$g(q)$ satisfies the Dirichlet boundary conditions

$$g(0)=g(q_0)=0 , \tag{25}$$

and therefore we can make use of the results given in the preceding section to solve Eq. (23). Equations (15) and (16), with $b\equiv q_0$, $A^N\equiv\langle q^N\rangle$, and $E^0=W^0$, permit us to obtain the eigenvalues and average values of q^N as a power series of c (or q_0). First we solve Eq. (23) for $c=0$ in order to get W^0 and to be able to make the necessary calculations. The change of variables

$$x=(2W^0)^{1/2}q$$

transforms Eq. (23) into

$$y''+\left[1-\frac{t^2}{x^2}\right]y=0 , \tag{26}$$

whose solution is closely related to the Bessel function $J_a(x)$:

$$y(x)=x^{1/2}J_a(x) , \quad a(l)=(0.25+t^2)^{1/2} . \tag{27}$$

Denoting the nth zero of $J_a(x)$ with x_{nl}, we have

$$W_{nl}^0=x_{nl}^2/2q_0^2 . \tag{28}$$

Consequently, the problem is reduced to a search for the roots of the Bessel functions and then to employ Eqs. (15) and (16).

IV. EXAMPLE: HARMONIC OSCILLATOR MODEL

We choose the harmonic oscillator model in order to illustrate the application of Eqs. (15) and (16). We pointed out in Sec. II that it is just necessary to make the calculation once for $b=q_0=1$. Equations (15) and (16) show the relationships

$$A_s^N=\frac{1-2s}{(N+1)se}A_{s-1}^2-\frac{N}{2(N+1)e}[\tfrac{1}{4}(N^2-1)-t^2]A_s^{N-2}+\frac{N+2}{(N+1)e}A_{s-1}^{N+2}-e^{-1}\sum_{j=1}^{s}\frac{A_{j-1}^2A_{s-j}^N}{j}\,,\quad s>0 \quad (29)$$

$$A_0^N=\frac{1}{N+1}-\frac{N}{2(N+1)e}[\tfrac{1}{4}(N^2-1)-t^2]A_0^{N-2}\,, \quad (30)$$

$$e=W_{nl}^0(q_0=1)=\frac{x_{nl}^2}{2}\,. \quad (31)$$

Solving for (29) and (30) in consecutive steps, we obtain the following results:

$$A_0^2(q_0=1)=\frac{1}{3}-\frac{1}{3e}(\tfrac{3}{4}-t^2)\,, \quad (32)$$

$$A_0^4(q_0=1)=\frac{1}{5}-\frac{2}{15e}(\tfrac{15}{4}-t^2)+\frac{2}{15e^2}(\tfrac{15}{4}-t^2)(\tfrac{3}{4}-t^2)\,, \quad (33)$$

$$A_1^2(q_0=1)=\frac{2}{45e}+[\tfrac{1}{3}(\tfrac{3}{4}-t^2)-\tfrac{8}{45}(\tfrac{15}{4}-t^2)]e^{-2}+[\tfrac{8}{45}(\tfrac{15}{4}-t^2)(\tfrac{3}{4}-t^2)-\tfrac{1}{9}(\tfrac{3}{4}-t^2)^2]e^{-3}\,. \quad (34)$$

With the help of these quantities we can express the dimensionless energy W, corrected up to the second order:

$$W=\frac{e}{q_0^2}+cA_0^2(q_0=1)q_0^2+\frac{c^2}{2}A_1^2(q_0=1)q_0^6\,. \quad (35)$$

We get for the eigenvalues of Eq. (17):

$$E_{nl}=\frac{\hbar^2x_{nl}^2}{2mr_0^2}+cA_0^2(n,l,q_0=1)c_0r_0^2+\frac{c^2}{2}A_1^2(n,l,q_0=1)\frac{mc_0^2}{\hbar^2}r_0^6\,. \quad (36)$$

The procedure can be continued to obtain any desired number of terms in the perturbational expansions (35) and (36).

For $M=2$ we have the plane oscillator, which was briefly discussed by Dingle[7] in his analysis of the magnetic properties of a system of electrons trapped in a cylinder. His perturbative study was made only for the first-order correction. Equation (32) gives for $M=2$

$$A_0^2(n,l,q_0)=\frac{q_0^2}{3}\left[1+\frac{2(l^2-1)}{x_{nl}^2}\right]\,, \quad (37)$$

which is coincident with that result obtained by Dingle through the application of the Schafheithin formula.[21]

Equation (35) is valid for relatively small q_0 values and its accuracy can be improved by adding new perturbative corrections. One of the main advantages of the present method rests upon the property that Eqs. (29) and (30) can be easily programmed, and it offers the possibility of obtaining the eigenvalues with extreme accuracy. In Table I I we show eigenvalues W_{10} corresponding to the three-dimensional bounded harmonic oscillator ($M=3$) for different choices for q_0 and with several perturbative degrees of approximation, when $c=0.5$:

$$W_{10}(s,q_0)=\frac{\pi^2}{2q_0^2}+\sum_{j=1}^{s}(0.5)^jK_jq_0^{4j-2}\,. \quad (38)$$

Results show a decrease of accuracy when q_0 increases, but the value $W_{10}(q_0=2.5)=1.552$ is near near enough to the asymptotic value $W_{10}(\infty)=1.5$.

TABLE I. Eigenvalues $W_{10}(s,q_0)$ for the three-dimensional bounded harmonic oscillator ($M=3$) calculated from Eq. (38).

s \ q_0	0.5	1.0	$(\frac{3}{2})^{1/2}$	1.5	2.0	2.5
1	19.774 543	5.076 138 6	3.501 872 7	2.511 252 2	1.799 046 0	1.672 92
2	19.774 534	5.075 580 7	3.499 909 0	2.504 897 6	1.763 341 3	1.536 72
3	19.774 534	5.075 582 0	3.499 999 0	2.504 973 7	1.764 792 9	1.549 31
4	19.774 534	5.075 582 0	3.500 000 0	2.504 976 3	1.764 838 2	1.552 61
5	19.774 534	5.075 582 0	3.500 000 0	2.504 976 1	1.764 816 8	1.551 42
6	19.774 534	5.075 582 0	3.500 000 0	2.504 976 1	1.764 808 3	1.551 54
7	19.774 534	5.075 582 0	3.500 000 0	2.504 976 1	1.764 808 7	1.551 67
8	19.774 534	5.075 582 0	3.500 000 0	2.504 976 1	1.764 808 7	1.551 66
9	19.774 534	5.075 582 0	3.500 000 0	2.504 976 1	1.764 808 7	1.551 65
10	19.774 534	5.075 582 0	3.500 000 0	2.504 976 1	1.764 808 7	1.551 65
11	19.774 534	5.075 582 0	3.500 000 0	2.504 976 1	1.764 808 7	1.551 66

When $q_0=(\frac{3}{2})^{1/2}$ (the root of the fourth Hermite polynomial) we obtain the exact result $W_{10}=3.5$. Furthermore, the approximate analytical expression (35) is applicable for q_0 values up to 2.5 with an error of less than 1%. In order to reach relatively good results in the whole q_0 interval of values, it is convenient to resort to the cothz method, presented by Vawter.[12] This author proposed the approximation of the perturbative polynomial

$$W=\sum_{s=0}^{\infty} p_s q_0^{4s-2}\ ,\quad p_s=c^s K_s \tag{39}$$

by way of the function

$$W=W(\infty)\coth f(q_0^2)\ , \tag{40}$$

where $W(\infty)$ represents the energy of the free oscillator ($q_0=\infty$), and

$$f(x)=\sum_{s=0}^{\infty} c_s x^{2s+1}\ . \tag{41}$$

The coefficients c_s can be obtained through the q_0 power-series expansion of $\coth f(q_0^2)$ and equalizing the coefficients in the series with those of (39):

$$p_s=W(\infty)\sum_{j=0}^{s}\frac{2^{2j}}{(2j)!}B_{2j}c_{s-j}^{2j-1}\ . \tag{42}$$

B_i's are the Bernoulli's numbers and c_i^j's are the coefficients of the polynomial $f(x)^j$.[12]

The first three coefficients are

$$c_0=W(\infty)/e\ , \tag{43}$$

$$c_1=c_0^3/3-p_1c_0^2/W(\infty)\ , \tag{44}$$

$$c_2=c_0^5/5-p_1c_0^4/W(\infty)-p_2c_o^2/W(\infty)$$
$$+p_1^2c_0^3/W(\infty)^2\ . \tag{45}$$

In Vawter's original method,[12] the coefficients p_s are obtained from the confluent hypergeometric function. It is a more troublesome procedure than the direct application of Eqs. (29) and (30). Moreover, Vawter's analysis is restricted to the unidimensional harmonic oscillator, while the present equations are valid irrespective of the dimension of the space.

In Table II we display the eigenvalue W_{10} when $M=3$, including 1, 2, and 3 coefficients in the function $f(q_0^2)$($W_{10}^{(1)}$, $W_{10}^{(2)}$, and $W_{10}^{(3)}$, respectively). For the purpose of making a direct comparison, the chosen q_0 values are coincident with those previously given in Table I. We can see that the obtainable accuracy with just three coefficients c_s is excellent within the range of validity of the perturbational polynomial. In order to get appropriate results in the interval of high q_0 values, one must restore the application of the first two coefficients c_s because $c_2<0$.

V. FURTHER COMMENTS

In our previous works on one-dimensional systems[13–16] we had taken into account only a potential function

$$V(x)=cx^k\ .$$

Then, results presented in Sec. II are a generalization of those ones. When $t=0$, Eqs. (15) and (16) are coincident with the odd solutions of the sym-

TABLE II. Eigenvalues $W_{10}^{(1)}$, $W_{10}^{(2)}$, and $W_{10}^{(3)}$ for the tridimensional bounded harmonic oscillator calculated from Eq. (40).

q_0	$W_{10}^{(1)}$	$W_{10}^{(2)}$	$W_{10}^{(3)}$
0.5	19.777 190	19.774 534	19.774 534
1.0	5.085 856	5.075 555	5.075 582
$(\frac{3}{2})^{1/2}$	3.514 743	3.499 913	3.499 999
1.5	2.524 995	2.504 708	2.504 969
2.0	1.789 065	1.763 747 3	1.764 743
2.5	1.568 680	1.549 552 0	1.551 204

metric models studied before. The particular case which was numerically analyzed ($n=1$, $l=0$, $M=3$) agree exactly with the second eigenvalue of the harmonic oscillator symmetrically bounded. An interesting feature regarding the virial theorem is that its mathematical expression is independent of t. It is owed to the fact that $t^2/2x^2$ is homogeneous of degree -2. In the one-dimensional case[13–16] as well as in the present case, our results are the most accurate which have been reported up to now.

We deem it necessary to point out that our method permits the treatment of any bounded oscillator with identical ease. One can include Eqs. (15) and (16) for any $k>0$ in a sole program. This property constitutes a striking difference with respect to other existing methods.[1,4,8–11,22] Besides, the recurrence relation (30) allows us to get a set of relationships which involve integrals of the Bessel functions. Such integrals have the form

$$\frac{\int_0^{x_{nl}} x^{N+1} J_a^2(x)dx}{\int_0^{x_{nl}} x J_a^2(x)dx} = x_{nl}^N A_0^N(q_0=1) \quad (46)$$

and for $N=2$ we obtain

$$\frac{\int_0^{x_{nl}} x^3 J_a^2(x)dx}{\int_0^{x_{nl}} x J_a^2(x)dx} = \frac{x_{nl}^2}{3} - \frac{2}{3}(\frac{3}{4}-t^2) . \quad (47)$$

We consider that this sort of integral relationship eventually could be of interest and value in other fields of physics.

At present, research on this subject is being done in our laboratory and future results are planned to be published elsewhere.

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