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Variational Application of the Group of Transformations

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The variational application of the group of transformationsis analysed for the three following cases: translations, deformations and rotations. The parameters introduced within these transformations are determined via hypervirial theorems. The method proposed is applied to severa1 anharmonic oscillators and results are compared with previous exact values.

A aplicação variacional do grupo de transformações é analisada para os três seguintes casos: translações, deformações e rotações. Os parâmetros introduzidos nessas transformações são determinados via teoremas hiperviriais. O método proposto é aplicado a vários osciladores anarmônicos e os resultados são comparados a valores exatos conhecidos.

1. INTRODUCTION

Variational determination of an approximate wavefunction for a physical system requires the insertion of a set of adjustable parameters (linear or not). Then, optimum values for them are calculated by utilizing extremum conditions for the energy functional. The evolution of the wavefunction in terms of such parameters has been previously studied within the fornalism of unitary operators[1] and by way of the analysis of induced transformation[2-3]. Under certain conditions, the introduction of a variational parameter constitutes a sufficient and necessary condition in order that a diagonal hypervirial theorem being satisfied. The relationship between corresponding hypervirial associ-

ated operators was set forth in both cases. Hirschfelder et al[2-3] have discussed the coordinate transformations

$$x \rightarrow \sigma(x,a)$$

with the specification

$$\sigma(x,0) = x$$

for rectilinear as well as for curvilinear coordinates, and where $\underline{a}$ is a variational parameter. However, this class of transformations have not been analysed and applied intensively from an unified point ofview, as far as we know.

The purpose of this communication is to analyse indepth such methodology via the group of transformations. As we will see later, it will carry us to a variational method which is associated to those groups in the following sense.

If G is a group of transformations and X is a set of variables, then

$$\sigma(\bar{a},X) = A(\bar{a})X \quad \forall A \in G$$

$\bar{a}$ being a set of variational parameters. We shall study three kind of transformations: rotations, deformations and translations. The later was utilized by Hurley for diatomic molecules. The plan of the paper is as follows.

In Section 2 the group of transformations are studied, and the most relevant results are given in connection with their subsequent application within the variational method. Unitary operators related to the transformations are analysed in Section 3. The proposed variational methods developed in Section 4.

Finally, some numerical applications are shown in Section 5 for coupled oscillators and anharmonic oscillators. Results obtained are compared with other numerical values, which are calculated from more elaborated methods. The effects of the transformations in the symmetry of the zero-order wavefunction are discussed too in this Section.

2. GROUP DE TRANSFORMATIONS

2.1. Orthogonal Groyps

We denote with $O(n)$ the group of matrices in R^{nxn} which have the property of being orthogonal. Then, $O(n) \subset R^{nxn}$ and

$$C \in O(n) \rightarrow C^{\dagger}C = CC^{\dagger} = I \tag{1}$$

$$\det C = \pm 1 \tag{2}$$

Rotations constitute a subgroup of $O(n)$. We designate such group with $R(n)$, whose elements satisfy the condition

$$C \in R(n) \longrightarrow \det C = +1$$

The number of independent coefficients in a matrix of $O(n)$ is equal to $n(n-1)/2 \equiv s$. We denote with $\bar{\theta} = (\theta_1, \theta_2, \ldots, \theta_s)$ the set of such parameters. From Eq.(1) we can immediately deduce that if $A_i = (\partial C/\partial \theta_i)C^{\dagger}$, then

$$\frac{\partial C}{\partial \theta_i} = A_i C \; ; \quad i = 1,2,\ldots,s \tag{3}$$

where $A_i^t = - A_i$.

2.2. Group of Pure Deformations

A pure deformation in R^n is defined by a diagonal matrix of R^{nxn}

$$\eta = (\eta_i \delta_{ij}) \; ; \quad \eta_i > 0 \; ; \quad i = 1,2,\ldots,n \tag{4}$$

We denote this group with $D(n)$.

2.3. Central Affinity

A central affinity τ is defined as a composition between a pure deformation and a orthogonal transformation, i.e

$$\tau = \eta C \tag{5}$$

where

$$\eta \in D(n) \quad \text{and} \quad C \in O(n)$$

The linear transformation τ defines a change of variables onto the column vector of coordinates X, in the form

$$\sigma = \tau X \; ; \; X, \sigma \in R^n \tag{6}$$

It can be deduced at once the following properties for r:

$$\tau\tau^{\dagger} = \eta^2 \tag{7}$$

$$\frac{\partial \tau}{\partial \theta_i} = \frac{\partial \eta}{\partial \eta_i} \; \eta^{-1} \; \tau \tag{8}$$

$$\frac{\partial \tau}{\partial \theta_i} = \eta \; A_i C = \eta \, A_i \, \eta^{-1} \; \tau \tag{9}$$

Let B_i be the matrix defined by

$$\frac{\partial \tau}{\partial \theta_i} \equiv B_i \tag{10}$$

Then $B_i = -B_i^t$, so Eq. (9) can be written in an alternative way by deriving Eq. (7) with respect to θ_i

$$\frac{\partial \tau}{\partial \theta_i} = B_i \, \eta^{-2} \; \tau = B_i \, \eta^{-1} \; C \tag{11}$$

Comparing Eqs. (11) and (9), the following relationship between A_i and B_i is obtained

$$A_i = \eta^{-1} \, B_i \, \eta^{-1} \tag{12}$$

The change of the new coordinate o with vari'ational parameters $\bar{\theta}$ and $\bar{\eta} = (\eta_1, \ldots, \eta_n)$ is got from Eq. (6)

$$\frac{\partial \sigma}{\partial \theta_i} = \frac{\partial \tau}{\partial \theta_i} X = B_i \, \eta^{-2} \, \sigma = \eta \, A_i \, \eta^{-1} \, \sigma$$

$$\frac{\partial \sigma}{\partial \eta_i} = \frac{\partial \eta}{\partial \eta_i} \eta^{-1} \sigma = \begin{pmatrix} 0 \\ \vdots \\ \sigma^i / \eta_i \\ \vdots \\ 0 \end{pmatrix} = \frac{\sigma^i}{\eta_i} \; I_{nx1} \tag{13}$$

Now we can analyse the Jacobian of the transformation and its effect in the metric:

$$X = \tau^{-1} \, \sigma = C^{\dagger} \, \eta^{-1} \, \sigma \tag{14}$$

$$\frac{\partial x^i}{\partial \sigma_j} = (\tau^{-1})^i_j \tag{15}$$

If (g_{ij}) is the metric tensor defined by X, and (g'_{ij}) is the metric tensor defined by o, then

$$g'_{ij} = (\tau^{-1})^k_i \, (\tau^{-1})^l_j \, g_{kl} = C^k_i \, \eta_i^{-1} \, C^l_j \, \eta_j^{-1} \, g_{kl} = C_{il} \, C^l_j \, \eta_i^{-1} \, \eta_j^{-1} \tag{16}$$

For X being a set of rectilinear coordinates, then $g_{ij} = \delta_{ij}$, so Eq. (16) is simplified to

$$g'_{ij} = \delta_{ij} \, \eta_i^{-1} \, \eta_j^{-1} \tag{17}$$

which shows us that the metric is not affected by C.

For example if $\tau \in R^{2x2}$, and C is a rotation by an angle a, we obtain

$$A_\alpha = \frac{\delta C}{\delta \alpha} C^{\dagger} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{18}$$

From Eq. (12)

$$B_\alpha = \begin{pmatrix} 0 & -\eta_1 & \eta_2 \\ \eta_1 & \eta_2 & 0 \end{pmatrix} \tag{19}$$

and, on account of

$$\sigma = \tau X \tag{20}$$

then

$$\frac{\partial \sigma}{\partial \alpha} = \begin{pmatrix} -\frac{\eta_1}{\eta_2} & \sigma_2 \\ \frac{\eta_2}{\eta_1} & \sigma_1 \end{pmatrix} \tag{21}$$

As a second example for the transformation in spherical coordinates, we have that if

$$\operatorname{tg} \phi = \frac{x^1}{x^2} \quad ; \quad \operatorname{tg} \phi' = \frac{\sigma^1}{\sigma^2} \tag{22}$$

then, the relation between ϕ and ϕ' is

$$\operatorname{tg} \phi' = \eta_2 \, \eta_1^{-1} \operatorname{tg} (\phi + \alpha) \tag{23}$$

2.4. Group of Translations

We indicate the group of translations in R^n with $T(R^n)$. If $T_a \in T(R^n)$, then

$$T_a X = X + a, \quad \text{with } X, a \in R^n \tag{24}$$

The Jacobian for this transformation is the identity, i.e

$$J_X^{\sigma} = \left(\frac{\partial \sigma^i}{\partial x^j} \right) = I \tag{25}$$

and, furthermore

$$J_a^{\sigma} = \left(\frac{\partial \sigma^i}{\partial a^j} \right) = I \tag{26}$$

2.5. Composition between a central affinity and a translation

For a composition between a central affinity and a translation, the resulting change of variables is

$$Y = \tau T_a X \; ; \quad \tau \in D(R^n) \; ; \quad C \in O(R^n) \; ; \quad T_a \in T(R^n) \tag{27}$$

$$Y = \tau(X + a) \tag{28}$$

The inverse transformation is

$$X = T_a^{-1}(\tau^{-1} Y) = \tau^{-1} Y - a \tag{29}$$

3. UNITARY OPERATORS IN $L^2(R^n)$ ASSOCIATED TO THE GROUP OF TRANSFORMATIORIS

3.1. Operators associated to $O(R^n)$

Defining the operator U_0 as an application of the space of functions $f(X)$ of integrable square onto itself

$$\begin{aligned} &U_0 : L^2(R^n) \longrightarrow L^2(R^n) \\ &U_0 \Psi(X) = \Psi(CX) \; ; \; \Psi \in L^2(R^n) \; ; \; X \in R^n ; \; C \in O(R^n) \end{aligned} \tag{1}$$

we can immediately that

$$\int \Psi_1^*(CX) \; \Psi_2(CX) \; dX = \int \Psi_1^*(X) \; \Psi_2(X) \; dX \tag{2}$$

or, equivalently

$$U_0^\dagger \; U_0 = U_0 \; U_0^\dagger = I$$

so, the operator U_0 defined by Eq (1) is unitary.

3.2. Opisrator associated to $D(R^n)$

After the fashion of the previous definition, we now define operator U_D as

$$U_D : L^2(R^n) \longrightarrow L^2(R^n)$$

$$U_D \Psi(X) = (\eta_1 \ldots . \eta_n)^{1/2} \Psi(\eta X) \; ; \; \Psi \in L^2(R^n); \; X \in R^n; \; \eta \in D(R^n) \tag{3}$$

and this operator results unitary too.

3.3. Operators associated to a central affinity

For the operator connected to a central affinity wehave that

$$U_\tau = U_D \, U_0 \tag{4}$$

$$U_\tau \, \Psi(X) = (\eta_1, \ldots, \eta_n)^{1/2} \, \Psi(\tau X) \tag{5}$$

where, obviously, U is unitary.

Previously defined operators satisfy the equalities

$$U_0^\dagger \, \Psi(X) = \Gamma(C^\dagger X) \tag{6}$$

$$U_D^\dagger \, \Psi(X) = (\eta_1, \ldots, \eta_n)^{-1/2} \, \Psi(\eta^{-1} X) \tag{7}$$

$$U_\tau^\dagger \, \Psi(X) = (\eta_1, \ldots, \eta_n)^{-1/2} \, \Psi(\tau^{-1} X) \tag{8}$$

3.4. Operators associated to $T(R^n)$

We define an operator U_{T_a} associated to a translation by way of

$$U_{T_a} \, \Psi(X) = \Psi(X + a) = \Psi(T_a \, X) \tag{9}$$

where

$$\int \Psi^*(X+a) \, \Psi(X+a) \, dX = 1 \tag{10}$$

Then

$$U_{T_a}^{\dagger} = U_{T_{-a}} = U_{T_a}^{-1} \tag{11}$$

$$U_{T_a}^{\dagger}\ \Psi(X) = \Psi(X-a) = \Psi(T_{-a}X) \tag{12}$$

4. VARIATIONAL METHOD

The present proposed method of application of scaling to a trial wavefunction consists in regarding in a variational way the parameters $\bar{\theta}$, $\bar{n}$, and $\bar{a}$. Firstly let us take $\Psi(X) \in L^2(R^n)$ and to study the central affinity for X rectilinear. The variational function is

$$U_\tau\ \Psi(X) = (\eta_1,\ldots,\eta_n)^{1/2}\ \Psi(\sigma) \tag{1}$$

with $a = \tau X$ and $\tau = \eta C$. The energy functional is

$$E(\bar{n},\bar{\theta}) = \langle U_\tau\ \Psi(X)\,|H|\,U_\tau\ \Psi(X)\rangle = \langle\Psi(X)\,|\tilde{H}|\,\Psi(X)\rangle \tag{2}$$

where

$$H = U_\tau^{\dagger}\ H\ U_\tau \tag{3}$$

$$\tilde{H}\ \Psi(X) = U_\tau^{\dagger}\ H(X)\ (\eta_1,\ldots,\eta_n)^{1/2}\ \Psi(\tau X) = H(\tau^{-1}\ X)\ \Psi(X) \tag{4}$$

$$H(\tau^{-1}X) = T(\tau^{-1}X) + V(\tau^{-1}X) = T(\bar{\theta},\bar{n},X) + V(\bar{\theta},\bar{n},X) \tag{5}$$

In this case the metric does not depend of θ, so does T too. Then

$$T = T(\bar{n},X) \tag{6}$$

or, equivalently

$$[T,U_0] = 0 \tag{7}$$

In this case

$$\frac{\partial E(\bar{\theta},\bar{\eta})}{\partial \theta_i} = \langle \Psi(X) | \partial V/\partial \theta_i | \Psi(X) \rangle \quad ; \quad i = 1,2,\ldots,s \tag{8}$$

We proceed now to analyse hypervirial operators corresponding to each class of parameter. From Eq. (2.13) we can obtain such operators, because

$$\frac{\partial U_\tau \Psi(X)}{\partial \eta_i} = \left\{ \frac{1}{2\eta_i} + \frac{\sigma^i}{\eta_i} \frac{\partial}{\partial \sigma^i} \right\} U_\tau \Psi(X) =$$

$$= \frac{1}{2\eta_i} \left\{ \sigma^i \frac{\partial}{\partial \sigma^i} + \frac{\partial}{\partial \sigma^i} \sigma^i \right\} U_\tau \Psi(X) = \frac{1}{2\eta_i} W_{\eta_i} U_\tau \Psi(X) \tag{9}$$

where W_{η_i} is the sought operator. The extremum condition of the functional E with respect to η_i, i.e

$$\frac{\partial E(\bar{\theta},\bar{\eta})}{\partial \eta_i} = 0 \quad ; \quad i = 1,2,\ldots,n \tag{10}$$

leads us to the well known diagonal hypervirial theorem[2-3]

$$\langle [H, W_{\eta_i}] \rangle = 0 \quad ; i = 1,2,\ldots,n \tag{11}$$

For the other set of parameters, we have

$$\frac{\partial U_\tau \Psi(X)}{\partial \theta_i} = (\eta A_i \eta^{-1} \sigma) \nabla_\sigma U_\tau \Psi(X) \quad ; \quad i = 1,2,\ldots,s \tag{12}$$

In this case, the hypervirial operators is given by

$$W_{\theta_i} = (\eta A_i \eta^{-1}) \sigma_0 \nabla_\sigma \tag{13}$$

where

$$\nabla_\sigma \equiv \sum_j e_j \frac{\partial}{\partial \sigma^j}$$

The condition of extremurn of E with regard to θ_i, i.e.

$$\frac{\partial E(\bar{\theta},\bar{\eta})}{\partial \theta_i} = 0 \quad ; \quad i = 1,2,\ldots,s \tag{14}$$

gives us

$$\langle [V, W_{\theta_i}] \rangle = 0 \tag{15}$$

because

$$[T, W_{\theta_i}] = 0 \tag{16}$$

Conserning translations we have that

$$U_{T_a} \Psi(X) = \exp(i a.p)\ \Psi(X) = \Psi(X+a) \tag{17}$$

with

$$U_{T_a} = \exp(i a.p) \quad , \quad \text{and} \quad U^{\dagger}_{T_a} = \exp(-i a.p) \tag{18}$$

The Hamiltonian operator transforms as

$$\tilde{H} = U^{\dagger}_{T_a} H U_{T_a} = \tilde{T} + \tilde{V} = T + \tilde{V} \tag{19}$$

where

$$\tilde{T} = U^{\dagger}_{T_a} T U_{T_a} = T \tag{20}$$

owing to

$$[T, U_{T_a}] = [T, p] = 0 \tag{21}$$

The depsndence of the energy functional with the vector associated to translation is given by

$$E(a) = \langle \Psi(T_a X) | H | \Psi(T_a X) \rangle = \langle \Psi(X) | \tilde{H} | \Psi(X) \rangle \tag{22}$$

$$\nabla_a E = \langle \Psi(X,a) | [\tilde{V}, \nabla_a] | \Psi(X,a) \rangle = - \langle \Psi(X,a) | \nabla_a V | \Psi(X,a) \rangle \tag{23}$$

$$\nabla_a E = \langle \Psi(X) | \nabla_a \tilde{V} | \Psi(X) \rangle \tag{24}$$

Then, the condition of extremum for E with respect to the translation is expressed by the following equation

$$\langle \Psi(X) | \nabla_a \tilde{V} | \Psi(X) \rangle = 0 \tag{25}$$

As we can clearly see, translation as well as rotation have not effect on the kinetic energy of the system and only influence the potential. Farther on, we shall see that orthogonal transformations and translations enables us to "adjust" trial wavefunctions so as to take into account the symmetry of the potential. Deformations allow the fulfilment of the virial theorem when the corresponding parameters are determined in a way such that energy is stationary with respect to them. In the present method we propose the minimization of the energy functional with respect to the parameters associated to the transformation

$$Y = \tau\, T_a\, X = \tau(X + a)$$

so the total number of such parameters is $n(n+3)/2$. The unitary operator U in $L^2(R^n)$ is

$$U = U_D\, U_0\, U_{T_a} \tag{26}$$

and hypervirial relations to be satisfied are those given by Eqs.(11), (15), and (25). We take as initial wavefunctions the eigenfunctions $\{\phi_n(X)\}$ of H^0, i.e

$$H^0\, \phi_n(X) = \varepsilon_n\, \phi_n(X) \tag{27}$$

where the Hamiltonian operator H corresponding to the system under study can be written

$$H = H^0 + H'$$

According to Bangudu and Robinson[5-7] we can determine which operators are whose mean values are corrected up to the first order Let

$$\sim (\,i\,\neq)\, U_D\, U_0\, U_{T_a} \quad ; \quad \dot{1} = (\bar{\theta}, \bar{\eta}, \bar{a}) \tag{28}$$

If

$$h(\bar{b}) = T + \{\varepsilon(\bar{b}) - (T\phi)/\phi\} \tag{29}$$

then

$$\langle \partial h/\partial b_i \rangle = \partial \varepsilon/\partial b_i \tag{30}$$

is corrected up to the first order. In this case the operator $h(\bar{b})$ is totally determined by the choice made through Eq. (27). According to it

$$H^0(\sigma)\ \phi(\sigma) = \varepsilon(\bar{b})\ \phi(\sigma)$$

and

$$h(\bar{b}) = H^0(a) \tag{31}$$

5. APPLICATIONS

5.1. Uniidimensional anharmonic oscillator

Let us analyse the unidimensional system whose Hamiltonian operator is

$$H = H^0 + H' \tag{1}$$

where

$$H^0 = -\frac{d^2}{dx^2} + v_2\ x^2\ ;\ H' = v_3\ x^3 + v_4\ x^4 \tag{2}$$

Accorditig to Eq. (1) and the final discussion in Sec.4, initial wave-functions are those corresponding to the unidimensional harmonic oscillator. If P_x is the inversion operator i.e

$$P_x f(x) = f(-x)$$

then

$$[H^0, P_x] = 0\ ;\quad \text{and}\quad P_x\ \phi_n^0(x) = \pm\ \phi_n^0(x) \tag{3}$$

Moreover

$$[H, P_x] = [H', P_x] \neq 0 \tag{4}$$

and

$$\langle \phi_n^0(x) | x^3 | \phi_n^0(x) \rangle = 0\ \forall\ n \tag{5}$$

Through the group of translations we can modify the symmetry of $\phi_n^0(x)$

in order to circumvent the reai difficulty expressed in Eq.(5). Then, we define the change of variables

$$\sigma = \eta x + b \; ; \quad \eta \neq 0 \tag{6}$$

so that

$$x = \eta^{-1} \sigma + a \; ; \; a = - b/\eta$$

and

$$U_{T_b} \; U_D \; \phi_n^0(x) = \phi_n(\sigma) \tag{7}$$

Furtherrnore

$$P_x \; \phi_n^0(\sigma) = \phi_n^0(\eta, b, -x) \neq \phi_n^0(\eta, b, x) \tag{8}$$

Following the steps indicated in Sec.4, results of Table 1 are obtained. According to the final analysis in the previous Section

a	b	E_0	E_1	E_2
$v_2 = v_4 = 1$, $v_3 = 0.5$				
0.	1.	1.75	6.75	14.75
-0.082007	0.60499	1.38496		
-0.10437	0.53008		4.6165	
-0.10946	0.46827			8.5508
$v_2 = v_3 = v_4 = 1$				
0.	1.	1.75	6.75	14.75
-0.17556	0.62741	1.32501		
-0.21558	0.54554		4.42150	
-0.225487	0.47875			8.25097

Table 1 - Energy rnean values for the first three states of the Unidimensional Anharmonic Oscillator with Hamiltonian Operator $H = - \frac{d^2}{dx^2} + + v_2 x^2 + v_3 x^3 + v_4 x^4$.

$$h(\eta,b) = \eta^2 T + \sigma^2/2 = \eta^2 T + \frac{1}{2}(\eta x + b)^2 \qquad (9)$$

$$\partial h/\partial b = \eta x + b \qquad (10)$$

which shows us that the introduction of the parameter b associated to translation, allows the calculation of $\langle x \rangle$ corrected up to the first order, as well as to obtain $\langle x^n \rangle$ (n odd). These results could not have been obtained without the utilization of a translation (due to Eq. (5)).

5.2. Bidimensional bi-harmonic oscillator

Now, as a bidimensional example, we choose a model which has been extensively studied[8-14]

$$H = H^0 + H' \; ; \; H' = h_1^0 + h_2^0 \; ; \; h_i^0 = T_i + v_i^0 \; ; \; i = 1,2 \qquad (11)$$

$$v_i^0 = w_i x_i^2/2 \; ; \; H' = \lambda(x_2^2 x_1 + \eta x_1^3) \qquad (12)$$

Let P_1 and P_2 be inversion operators corresponding to coordinates x_1 and x_2 respectively, i.e

$$P_i f(x_i,x_j) = f(-x_i,x_j) \; ; \; i,j = 1,2 \qquad (13)$$

Then

$$[H^0,P_i] = 0 \quad , \quad \text{and} \quad [P_1,P_2] = 0 \qquad (14)$$

If

$$\phi^0_{n_1,n_2}(x_1,x_2) = \phi^0_{n_1}(x_1)\phi^0_{n_2}(x_2) \qquad (15)$$

are eigenfunctions of H^0, then

$$P_i \phi^0_{n_1,n_2} = \pm \phi^0_{n_1,n_2} \; ; \; i = 1,2 \qquad (16)$$

and, furthermore

$$[H,P_1] = [H',P_1] \neq 0 \; ; \; [H,P_2] = 0 \; ; \; [H,P_1P_2] \neq 0 \qquad (17)$$

In such case, eigenfunctions of H only satisfy the equation

$$P_2 \phi_{n_1,n_2} = \pm \phi_{n_1,n_2} \tag{18}$$

That being so, we must "break" the symmetry associated to x_1, in close analogy to the previous case. Then, we define the following coordinate transformation

$$\sigma = U_{T_b} U_D X = \begin{pmatrix} \eta_1 & 0 \\ 0 & \eta_2 \end{pmatrix} X + \begin{pmatrix} b \\ 0 \end{pmatrix} \tag{19}$$

$$X = \begin{pmatrix} \eta_1^{-1} & 0 \\ 0 & \eta_2^{-1} \end{pmatrix} + \begin{pmatrix} a \\ 0 \end{pmatrix} \tag{20}$$

Making calculations as indicated in Section 4, results given in Table 2 are obtained. Besides

$$h(\eta_1,\eta_2,b) = \eta_1^2 T_1 + \eta_2^2 T_2 + \frac{1}{2}(\eta_1 x_1 + b) + \frac{1}{2}(\eta_2 x_2)^2 \tag{21}$$

$$\partial h/\partial b = \eta_1 x_1 + b \tag{22}$$

Then, the insertion of parameter b allows us to calculate non-zero mean values of odd moments associated with x_1, in a similar way as in the previous model. Several results are presented in Table 2 for different choices of the parameters A, η, w_1 and w_2, which are compared

A	η	w_1	w^2	Ref.(9)	Ref.(10)	Present Method	Exact
-0.1116	0.08414	0.29375	2.12581	0.9920	0.9925	0.9928	0.9916
-0.1600	0.16000	0.49000	1.69000	0.9836	0.9846	0.9853	0.9826
-0.2000	0.20000	0.49000	1.69000	0.9667	0.9661	0.9690	0.9621

Table 2 - Energy mean values for the ground state of the Bidimensional Bi-harmonic Oscillator with Hamiltonian operator $H = -\frac{d^2}{dx_1^2} + w_1 x_1^2/2 - \frac{d^2}{dx_2^2} + w_2 x_2^2/2 + (x_2^2 x_1 + x_1^3)$.

with other approximated methods as well as with the exacts ones. As we can see, a good agreement exists among different results. But we rnust point out that from a computational point of view, our variational method is similar than the others.

5.3. *Bidimensional* anharmonic oscillator

In order to analyse the effect of orthogonal groups, let us consider the model whose Hamiltonian operator is

$$H = H^0 + H'$$

with

$$H^0 = -\frac{1}{2}\Delta + \frac{1}{2} X^{\dagger} X\,, \quad X = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad ; \; H' = \alpha\, x_1\, x_2 \tag{23}$$

In this case

$$[H,P_1] \neq 0 \quad ; \quad [H,P_2] \neq 0 \quad ; \quad [H,P_1P_2] = 0 \tag{24}$$

and

$$\langle H' \rangle = 0 \tag{25}$$

In order to obtain a change in the symmetry of the wavefunction, we apply the following transforrnation

$$\sigma = \begin{pmatrix} \eta_1 & 0 \\ 0 & \eta_2 \end{pmatrix} \begin{pmatrix} \cos\theta & -\mathrm{sen}\theta \\ \mathrm{sen}\theta & \cos\theta \end{pmatrix} X \tag{26}$$

The application of extremum conditions gives us the following values

$$\mathrm{sen}\theta = \cos\theta = \frac{\sqrt{2}}{2}\,, \quad \eta_1 = \eta_2 = (1+\alpha)^{1/4}$$

which are precisely the exact results. Hypervirial operators associated to a rotation are, according to Eq. (3.13)

$$A_\theta = \frac{\partial C}{\partial \theta} C^{\dagger} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{27}$$

$$W_\theta = - \eta_1 \eta_2^{-1} \sigma_2 \frac{\partial}{\partial \sigma_1} + \eta_2 \eta_1^{-1} \sigma_1 \frac{\partial}{\partial \sigma_2} = - \xi_2 \frac{\partial}{\partial \xi_1} + \xi_1 \frac{\partial}{\partial \xi_2} \tag{28}$$

where

$$\xi_i = \eta_i^{-1} \sigma_i$$

This result was completely foreseen from analysis given in Section 3.

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