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A Generalized Hill-Wheeler Ansatz

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The Hill-Wheeler ansatz for the total wave function, within the Generator Coordinate Method framework, is generalized by recourse to the theory of distributions. The ensuing approach allows one to obtain a basis that spans the collective subspace, without having to deal explicitly with the eigenvectors and eigenvalues of the overlap kernel. Applications to an exactly soluble model and anharmonic vibrations illustrate the present treatment.

1. Introduction

The generator coordinate method (GCM) is a technique of great physical appeal that has been developed [1, 2] to describe collective oscillations in nuclei. The flexibility of the method is firmly established and its applications to problems of physical interest are manyfold. A very small (and no by means representative) sample is that of [3-7]. In the GCM one makes the following ansatz for the total wave function

$$|\psi\rangle = \int da\, f(a)|\Phi(a)\rangle, \tag{1.1}$$

where $|\Phi(a)\rangle$, the generating functions, are in general (although not necessarily) Slater determinants which supposedly give a rough description of the intrinsic dynamics of the fermion system.
The a-parameter(s) refer to a collective coordinate which describes the particular nuclear motion one is interested in. The weight function $f(a)$ is determined by the variational principle

$$\delta \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = 0, \tag{1.2}$$

the expectation value of the hamiltonian H being given, in terms of the "hamiltonian overlap kernel" (h.o.k.)

$$h(a,b) = \langle\Phi(a)|\hat{H}|\Phi(b)\rangle, \tag{1.3}$$

as

$$\langle\Phi|\hat{H}|\Phi\rangle = \int da\, f^*(a) \int db\, f(b) h(a,b), \tag{1.4}$$

while, correspondingly, the denominator $\langle\psi|\psi\rangle$ is represented in terms of the "generator overlap kernel" (g.o.k.)

$$n(a,b) = \langle\Phi(a)|\Phi(b)\rangle, \tag{1.5}$$

by

$$\langle\psi|\psi\rangle = \int da\, f^*(a) \int db\, f(b) n(a,b). \tag{1.6}$$

The variational principle [1, 2] leads to the celebrated Hill-Wheeler (HW) equations (s)

$$\int da\, f(a)\{h(b,a) - e\, n(b,a)\} = 0, \tag{1.7}$$

which can be solved by recourse to well-established techniques [8]. Of these, three approaches should be singled out as the most important ones, namely:

i) The Gaussian Overlap Approximation (GOA). This approximation uses special properties of the overlap kernels $h(a,b)$ and $n(a,b)$, which are often sharply peaked at $a=b$. Exploiting this property one can transform the HW equation into a second order differential equation [3, 8, 9].

ii) Discretization of the Integrals in the Generator Coordinate a. This is the most frequently employed

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approach and leads to a diagonalization problem of the form

$$(A-Be)f=0, \tag{1.8}$$

where A and B stand, respectively, for those matrices which, after discretization, arise out of the kernels h and k (see for example, Ref. [6]).

iii) Expansion in Natural States [10]. These are orthogonal states that can be constructed out of the eigenvectors and eigenvalues of the g.o.k. $n(a,b)$ and span a sub Hilbert space S_c, the so-called "collective subspace", which is the smallest Hilbert space the contains all the generating states $|\Phi(a)\rangle$ [8, 10]. In some physical problems it is possible to deal with generating functions that allow for an analytical solution of the eigenvalue problem

$$\int da\, n(b,a)\, U_k(a)=N_k\, U_k(b), \tag{1.9}$$

so that an expansion in natural states can be carried out, the approximation being now that of cutting the expansion after a finite number of natural states, which once again leads to an eigenvalue problem.

There is a certain degree of arbitrariness inherent to method *ii)*. The way in which the discretization is to be accomplished is not prescribed *a priori* by a well-defined and unique procedure and a lot of freedom exits in the selection of the corresponding mesh points. Method *iii)* is a much more elegant one, but is marred by the fact that one needs *analytical* solutions to (1.9).

Deep studies into the mathematical foundations of the GCM [10–14] have shown that the structure of the GCM representation (1.1) i.e., the *kinematics* of theory [13, 14], is completely determined by the structure of the collective subspace S_c, which points towards method *iii)* as the most appropriate one. However, in addition to the already mentioned difficulty (i.e. solving [1.9]), one encounters also the problem that there are vectors in S_c that cannot be represented as HW states of the form (1.1) [13, 14].

As for the *dynamics* of the GCM ansatz, we can expect to obtain wave functions $|\psi\rangle$ which resemble the "exact" ones if, to a good approximation, $\hat{H}$ commutes with the projector operator $\hat{P}_c$ into the collective subspace [8]

$$[\hat{H},\hat{P}_c]=0, \tag{1.10}$$

which once more points towards the importance of appropiately dealing with S_c.

The purpose of the present effort is to present a *systematic* method of working within the collective subspace while *avoiding* the difficult problem posed by [1.9]. In other words, we wish to implement method *iii)* without having to face its main pitfalls. Our central idea is that of exploiting (and generalizing) a well-known fact connected with the application of the GCM to the one-dimensional harmonic oscillator. In this case it is found that, for certain values of the oscillator length, the corresponding solution has the character of a distribution [8]. This suggests a generalization of the GCM ansatz which is presented in Sect. 2.1, while the connection with S_c is discussed in Sect. 2.2. Sections 3 and 4 deal with illustrative examples of our technique and conclusions are drawn in Sect. 5.

2. Present Formalism

2.1. A Generalized GHW Ansatz

In view of the fact that there are vectors in the collective Hilbert subspace S_c that cannot be represented as Hill-Wheeler states of the form

$$|\psi\rangle=\int da\, f(a)|\Phi(a)\rangle, \tag{2.1}$$

we propose here a generalization of the ansatz (2.1). Instead of restricting the weight $f(a)$ to the class of "well-behaved" (square integrable) functions of the variable(s) a, we would suggest to give $f(a)$ the character of a distribution [15–17]

$$f(a)=\sum_{n=0}^{k} f_n(a_0)(-1)^n\delta^{(n)}(a-a_0), \tag{2.2}$$

so that, after the introduction of what we will hereafter refer to as "m-states"

$$\begin{aligned}|m,a_0\rangle&=\int(-1)^m\delta^{(m)}(a-a_0)|\Phi(a)\rangle da\\&=\frac{d^m}{da^m}|\Phi(a)\rangle|_{a=a_0}\end{aligned} \tag{2.3}$$

the following generalized GHW ansatz would ensue

$$|\psi_G\rangle=\sum_{m=0}^{k} f_m(a_0)|m,a_0\rangle. \tag{2.4}$$

It will be shown in the next sub-section that the m-states, i.e., the vectors $|m,a_0\rangle$, provide us with a basis of the collective subspace S_c. With this result, the variational principle

$$\delta\frac{\langle\psi_G|\hat{H}|\psi_G\rangle}{\langle\psi_G|\psi_G\rangle}=0, \tag{2.5}$$

leads to an eigenvalue problem for the "moments" $f_m(a_0)$ of the distribution (2.2)

$$\sum_n[H_{mn}(a_0)-eO_{mn}(a_0)]f_n(a_0)=0, \tag{2.6}$$

with the hamiltonian matrix

$$H_{mn}(a_0)=\langle m,a_0|\hat{H}|n,a_0\rangle, \tag{2.7}$$

and the overlap matrix

$$O_{mn}(a_0)=\langle m,a_0|n,a_0\rangle, \tag{2.8}$$

which can be solved by applying well-known techniques.

Notice that (2.6) does not arise here (as it does within the ordinary GHW framework) *as a result of approximating the integral (2.1) by a finite sum.* On the contrary, no approximations are involved in writing down (2.6), except possibly in what refers to the selection of k (cf. Eq. (2.2)), which will be discussed presently. Moreover, we are free to select the distribution point support (an isolated point) a_0 so as to actually minimize the ground state energy (notice that (2.5) entails only stationarity)*. Finally, in what respects to the choice of k, one should here follow the usual procedure; namely, when faced with an eigenvalue problem of the type (1.8) one must be sure that the overlap matrix B has no zero eigenvalues. The size of k is then limited by the requirement that no eigenvalue of B should be smaller than a given positive constant ε. Of course, *a posteriori* (and rather obvious) criterium would be that of cutting the number of moments $f_m(a_0)$ when one sees by inspection that "convergence" has been achieved (this will illustrated below).

2.2. The "m-States" Span the Collective Subspace

In order to prove that the "m-states" provide us with a basis of the collective subspace S_c, we have to consider diagonalizing the overlap (hermitian) kernel

$$n(a,a')=\langle\Phi(a)|\Phi(a')\rangle, \tag{2.9}$$

and obtain its eigenvectors $U_k(a)$ (and eigenvalues N_k)

$$\int da'\, n(a,a')\,U_k(a')=N_k\,U_k(a), \tag{2.10}$$

that form a complete orthogonalized set [8]

$$\sum_k U_k(a)\,U_k^*(a')=\delta(a-a'),$$
$$\int da\, U_k^*(a)\,U_{k'}(a)=\delta_{kk'}. \tag{2.11}$$

The spectrum N_k $(k=1,2,\ldots)$ is guaranteed to be discrete if $n(a,a')$ is of the Hilbert-Schmid type [8]. Should one face a situation in which the g.o.k is not of such a kind, recourse can be made to clever methods devised by Toledo-Piza et al. [12, 13] and by Lathouwers [10] in order to transform the given $n(a,a')$ into one of the Hilbert-Schmidt sort. The so-called "natural states", that one can build with the help of the eigenvectors and eigenvalues of the g.o.k. [10]

$$|k\rangle=\frac{1}{\sqrt{N_k}}\int U_k(a)|\Phi(a)\rangle da;\qquad N_k\neq 0, \tag{2.12}$$

can be shown to span the collective subspace S_c [8].

The proof that follows rests upon the assumption that the generating functions are analytical in a given region. Consequently, they can be Taylor-expanded within that region (and moreover, uniform convergence is guaranteed there). Assuming that a_0, the distribution point support, is located within this region, we can then Taylor-expand the function $|\Phi(a)\rangle$ in the neighbourhood of a_0 (cf. Eq. (2.2))

$$|\Phi(a)\rangle=\sum_m\left(\frac{d^m\Phi(a)}{da^m}\bigg|_{a=a_0}\right)\frac{(a-a_0)^m}{m!}$$
$$=\sum_m\frac{(a-a_0)^m}{m!}|m,a_0\rangle, \tag{2.13}$$

which, if introduced into (2.12) yields

$$|k\rangle=\sum_m B_{mk}(a_0)|m,a_0\rangle, \tag{2.14}$$

with

$$B_{mk}(a_0)=\frac{1}{m!\sqrt{N_k}}\int U_k(a)(a-a_0)^m da. \tag{2.15}$$

Equation (2.14) is tantamount to asserting that the natural states admit of expantions in terms of the m-states. If the latter span a subspace M, then

$$S_c\subset M. \tag{2.16}$$

Conversely, if we expand the generating functions in terms of the natural states

$$|\Phi(a)\rangle=\sum_k\langle k|\,\Phi(a)\rangle|k\rangle$$
$$=\sum_k C_k(a)|k\rangle, \tag{2.17}$$

and introduce this expansion into the definition (2.3) we are lead to

$$|m,a_0\rangle=\sum_k D_{km}(a_0)|k\rangle, \tag{2.18}$$

with

$$D_{km}(a_0)=\frac{d^m C_k(a)}{da^m}\bigg|_{a=a_0}. \tag{2.19}$$

* See, however, Sects. 4 and 5

It follows from (2.18) that

$$M \subset S_c, \tag{2.20}$$

which together with (2.16) completes our proof.
Notice that we have employed the eigenvectors and eigenvalues of the g.o.k. *only* to show that the *m*-states provide us with a basis of S_c. Of course, this in no ways entails the need for actually *using* the $U_k(a)$ and N_k in a given practical problem.

3. An Exactly Soluble $SU(2)$ Model

As a first application we shall consider an exactly soluble model (e.s.m.) of the Lipkin type [18] proposed by Abecasis et al. [19]. One deals in this e.s.m. with two N-fold degenerate single-particle (s.p.) levels, separated by the s.p. energy ε, and N identical fermions. Two quantum numbers characterize a given s.p. state. One of them adopts the values -1 (lowest level) and 1 (upper level). The other, which may be called the *p*-spin, singles out a state within the N-fold degeneracy. The model of [19] has been introduced in order to obtain an e.s.m. for which the Hartree-Fock (HF) state is never the trivial one provided by the unperturbed ground state. This does happen in the Lipkin model because the interaction is there unable to produce $1p-1h$ excitations. The idea of Abecasis et al. is, consequently, to modify Lipkin's hamiltonian so as to introduce a monopole force which can produce forward scattering. As the treatment of the Lipkin model within the GCM context has been exhaustively discussed [8], it may be of some interest to illustrate the formalism of Sect. 2 within the slightly different context of [19]. In order to write down the corresponding hamiltonian we introduce first the celebrated quasi-spin operators [18]

$$\hat{J}_+ = \hat{J}_-^\dagger = \sum_{p=1}^{N} C_{p+}^\dagger C_{p-},$$

$$\hat{J}_z = \tfrac{1}{2} \sum_{p=1}^{N} \sum_{\sigma=-1} \sigma C_{p\sigma}^\dagger C_{p\sigma}, \tag{3.1}$$

which fulfill the $SU(2)$ angular momentum commutation rules. With the energy given in units of the s.p. energy ε the hamiltonians reads

$$\hat{H} = J_z + \tfrac{1}{2} v \{\hat{J}^2 - \hat{J}_x^2 + \hat{J}_x\}, \tag{3.2}$$

with

$$\hat{J}_x = \tfrac{1}{2}(\hat{J}_+ + \hat{J}_-),$$
$$\hat{J}^2 = \hat{J}_z^2 + \tfrac{1}{2}(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+). \tag{3.3}$$

As in the Lipkin model, H commutes with J^2 and thus the exact solution is found by diagonalization within the (ground-state) multiplet $J = N/2$. One has to emphasize that the structure of these e.s.m. is very simple. In both cases [18, 19] there exists a collective subspace which coincides with the space spanned by the HW representation (1.1). This space is finite and, due to the quasi-spin symmetry, it decouples exactly from the rest of Hilbert space [8] (the optimal situation for the application of the method). For illustrative purposes, however, these e.s.m. provide one with an excellent testing ground, which has proved to be quite useful in trying new many-body techniques [8].
As the generator coordinate we shall select that angle ϕ (defining rotations in quasi-spin space) introduced by Agassi et al. [20] in constructing the HF solution for the Lipkin model, which is tantamount to adopting generating functions of the form

$$|\Phi(\phi)\rangle = \cos^N(\phi/2) \exp[\mathrm{tg}(\phi/2)\, \hat{J}_+]|0\rangle, \tag{3.4}$$

i.e., our generating functions resemble the coherent states of the Lipkin model, as discussed by Gilmore and Feng [21–23] and Kan et al. [24]. In (3.4) $|0\rangle$ denotes the unperturbed ground state

$$|0\rangle = \prod_{p=1}^{N} C_{p-}^\dagger |\text{particle vacuum}\rangle, \tag{3.5}$$

i.e., the lowest-lying eigenvector of $\hat{H}$ when the coupling constant v vanishes. The states (3.4) can also be written in terms of the eigenstates of $\hat{J}^2$ and $\hat{J}_z$ as [21–25]

$$|\Phi(\phi)\rangle = \sum_{M=-J}^{J} \binom{2J}{J+M}^{\frac{1}{2}} \cdot \left(\sin\frac{\phi}{2}\right)^{J+M} \left(\cos\frac{\phi}{2}\right)^{J-M} |JM\rangle, \tag{3.6}$$

an expression that immediately yields our "*m*-states", which within the present context read

$$|m, \phi_0\rangle = \sum_{M=-J}^{J} \binom{N}{J+M}^{\frac{1}{2}} F_{Mm}^{(J)}(\phi_0)|JM\rangle, \tag{3.7}$$

with

$$F_{Mm}^{(J)}(\phi_0) = \frac{d^m}{d\phi^m} \left\{ \left(\sin\frac{\phi}{2}\right)^{J+M} \left(\cos\frac{\phi}{2}\right)^{J-M} \right\}\Bigg|_{\phi=\phi_0} \tag{3.8}$$

We see now that the corresponding overlap matrix is independent of the distribution point support ϕ_0,

Table 1. The ratio (Approximate g.s. energy/Exact g.s. energy) is displayed, for the A.F.P. model [19], in the case $N=20$ and several values of the coupling constant v. The critical coupling constant [25] is attained at $v=0.025$. The number of moments employed in obtaining the different approximate solutions is indicated by a superscript. The last column gives the exact energies in units of the single particle energy

v	E^1_G/E_{exact}	E^3_G/E_{exact}	E^5_G/E_{exact}	E^7_G/E_{exact}	E^9_G/E_{exact}	$E_{\text{exact}}/\varepsilon$
0.1	0.9985263	0.9999757	0.9999997	1.0000000	1.0000000	−7.9148887
0.013	0.9970961	0.9999092	0.9999982	1.0000000	1.0000000	−7.2978635
0.015	0.9956945	0.9998064	0.9999944	0.9999999	1.0000000	−6.8901010
0.017	0.9938286	0.9996159	0.9999843	0.9999996	1.0000000	−6.4862530
0.021	0.9885648	0.9987614	0.9999670	0.9999957	0.9999999	−5.6968243
0.024	0.9847567	0.9977246	0.9997423	0.9999820	0.9999992	−5.1330449
0.026	0.9841631	0.9973427	0.9996146	0.9999646	0.9999981	−4.7810156
0.03	0.9873703	0.9982495	0.9996905	0.9999537	0.9999958	−4.1648255
0.035	0.9916015	0.9994189	0.9999344	0.9999896	0.9999984	−3.5713947
0.04	0.9940274	0.9997913	0.9999765	0.9999988	0.9999998	−3.1249994
0.05	0.9964684	0.9999579	0.9999992	1.0000000	1.0000000	−2.4999999

Table 2. Moments f_n evaluated at the distribution point support. The second column exhibits figures corresponding to the A.F.P. model and the third one those for the λx^4 anharmonic oscillator

Convergence of the distribution moments				
	A.F.P. Model $N=20$, $v=0.025$ $\psi_0=-0.1594662$		Anharmonic oscillator $\lambda=1$ $\alpha_0=1.6475659$	
f_0	1.2225035		0.9896210	
f_1	−0.1428172		−0.9009049	
f_2	0.819399	10^{-1}	0.3380986	
f_3	−0.44244	10^{-2}	−0.625560	10^{-1}
f_4	0.19159	10^{-2}	0.35321	10^{-2}
f_5	−0.451	10^{-4}	0.3505	10^{-3}
f_6	0.207	10^{-4}	0.2273	10^{-3}
f_7	−0.2	10^{-6}	−0.140	10^{-4}
f_8	0.8	10^{-7}	0.3	10^{-6}

namely

$$O_{mn}=\begin{cases}1 & \text{for } m=n\\ 0 & \text{for } m+n \text{ odd}\\ (-1)^{m+n}\sum_{k=0}\dfrac{\binom{N}{k}(T-k)^{m+n}}{2^{n+m+N-1}}, & \end{cases} \tag{3.9}$$

where T stands for $N/2$ and k for $T+M$. The hamiltonian matrix reads

$$H_{mn}(\phi_0)=\sum_{k=0}^{N}\left\{\binom{N}{k}[(k-T)+V(2T^2+T+k^2+2Tk)]\right.$$
$$\cdot F^{(T)}_{kn}(\phi_0)F^{(T)}_{km}(\phi_0)+V\binom{N}{k+1}(k+1)[F^{(T)}_{k+1m}(\phi_0)$$
$$\cdot F^{(T)}_{kn}(\phi_0)+F^{(T)}_{km}(\phi_0)F^{(T)}_{k+1n}(\phi_0)]-\frac{V}{2}\binom{N}{k+2}(k+2)(k+1)$$
$$\left.\cdot[F^{(T)}_{k+2m}(\phi_0)F^{(T)}_{kn}(\phi_0)+F^{(T)}_{km}(\phi_0)F^{(T)}_{k+2n}(\phi_0)]\right\}. \tag{3.10}$$

Some typical results are exhibited in Table 1. We show there the degree of agreement between the exact ground state energy and the approximate one, evaluated with different numbers of "moments" (cf. Eqs. (2.1)–(2.6)). It is to be seen that convergence is quite rapidly achieved, long before the number of moments equals $(2J+1)$, where our treatment will, of course, yield the exact solution.

This rapid convergence is the most salient fact to be commented, as it points towards the feasibility of the present approach in realistic calculations, and is also illustrated in Table 2 (second column) where, for the case $N=20$ and $v=0.025$, we show how the f_m become rapidly smaller as m grows.

4. The One-Dimensional Anharmonic Oscillator

In the case of a continuous generator coordinate, one faces, in trying to implement the GCM prescriptions, difficulties which demand some degree of caution [8]. This can already be seen in the GCM treatment of the one-dimensional harmonic oscillator [8], of great importance in the theory of collective motion. We shall, in the present section, tackle a slightly more involved (but related) problem, i.e., that of the anharmonicity in collective exitations at low energy, assuming, for the sake of simplicity, only one degree of freedom and an x^4-anharmonic term.

The anharmonic oscillator poses a problem which has been the subject of much work both from the analytical and the numerical point of view. During the last years the corresponding literature has been greatly enriched, a very small sample being the set of [26–36]. The interest in this subject arises in diverse fields in addition to the one referred to above, such as molecular physics or field theory

[26–36]. Here it will serve as a rather severe test of the formalism presented in Sect. 2. Moreover, as this is really a one-body problem and not a many-body one, it will make sense to interpret the eigenvalues of (2.6) as approximations not only to the ground-state (g.s.) but to the excited states also, on account of the theorem of separation (of eigenvalues [37]).
By employing suitable units one can cast the relevant hamiltonian in the form

$$\hat{H} = -\frac{d^2}{dx^2} + x^2 + \lambda x^4, \tag{4.1}$$

and we shall use as generating functions the (x-representation of the) harmonic oscillator wave functions corresponding to the g.s. (in order to look for approximations to both the g.s. and exited states of even parity)

$$\psi_0(\alpha, x) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2}, \tag{4.2}$$

and to the first excited state (to be employed so as to construct approximations to excited states of odd parity)

$$\psi_1(\alpha, x) = 2\left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \alpha^{\frac{1}{2}} x e^{-\alpha x^2}. \tag{4.3}$$

The (x-representations $\langle x|m, \alpha_0\rangle$ of the) m-states are easily seen to be

$$\mu_{0m}(\alpha_0, x) = \left(\frac{2\alpha_0}{\pi}\right)^{\frac{1}{4}} \sum_{k=0}^{m} C_{mk} \Phi^{(1)}_{m-k}(\alpha_0, x)\, \alpha_0^{-k}, \tag{4.4}$$

and

$$\mu_{1m}(\alpha_0, x) = 2\alpha_0^{\frac{1}{2}} \left(\frac{2\alpha_0}{\pi}\right)^{\frac{1}{4}} \sum_{k=0}^{m} D_{mk} \Phi^{(2)}_{m-k}(\alpha_0, x)\, \alpha_0^{-k}, \tag{4.5}$$

with

$$\Phi^{(1)}_{m-k}(\alpha_0, x) = (-1)^{m-k} x^{2(m-k)} e^{-\alpha_0 x^2}, \tag{4.6}$$

$$\Phi^{(2)}_{n-k}(\alpha_0, x) = \Phi^{(1)}_{m-k}(\alpha_0, x), \tag{4.7}$$

$$C_{nk+1} = -\frac{(4k-1)(n-k)}{4(k-1)} C_{nk}; \quad k = 1, 2, \ldots, n, \tag{4.8}$$

$$D_{nk+1} = -\frac{(4k-3)(n-k)}{4(k-1)} D_{nk}; \quad k = 1, 2, \ldots, n, \tag{4.9}$$

$$C_{n0} = 1 \quad \text{for all } n, \tag{4.10}$$

$$D_{n0} = 1 \quad \text{for all } n, \tag{4.11}$$

The corresponding overlap and hamiltonian matrices are, respectively (the superscript 1(2) refers to a state of even (odd) parity)

$$\begin{Bmatrix} H^1_{nm}(\alpha_0) \\ H^2_{nm}(\alpha_0) \end{Bmatrix} = \left(\frac{2\alpha_0}{\pi}\right)^{\frac{1}{2}} \begin{Bmatrix} 1 \\ 4\alpha_0 \end{Bmatrix} \sum_{k=0}^{n} \sum_{l=0}^{m} \begin{Bmatrix} C_{nk} & C_{ml} \\ D_{nk} & D_{ml} \end{Bmatrix} \times \frac{\langle \Phi^{(2)}_{n-k} | \hat{H} | \Phi^{(2)}_{m-l} \rangle}{\alpha_0^{k+l}}, \tag{4.12}$$

$$\begin{Bmatrix} O^1_{nm}(\alpha_0) \\ O^2_{nm}(\alpha_0) \end{Bmatrix} = \left(\frac{2\alpha_0}{\pi}\right)^{\frac{1}{2}} \begin{Bmatrix} 1 \\ 4\alpha_0 \end{Bmatrix} \sum_{k=0}^{n} \sum_{l=0}^{m} \begin{Bmatrix} C_{nk} & C_{ml} \\ D_{nk} & D_{ml} \end{Bmatrix} \times \frac{\langle \Phi^{(2)}_{n-k} | \Phi^{(2)}_{m-l} \rangle}{\alpha_0^{k+l}}, \tag{4.13}$$

with

$$\langle \Phi^{(1)}_N | \Phi^{(1)}_M \rangle = (-1)^{N+M} \left(\frac{\pi}{2\alpha_0}\right)^{\frac{1}{2}} \frac{[2(N+M)-1]!!}{(4\alpha_0)^{N+M}}, \tag{4.14}$$

$$\langle \Phi^{(1)}_N | \hat{H} | \Phi^{(1)}_M \rangle = \langle \Phi^{(1)}_N | \Phi^{(1)}_M \rangle \left\{ \left[\frac{8NM}{2(N+M)+1} + 1 \right] 2\alpha_0 + \frac{(1-4\alpha_0^2)}{4\alpha_0} [2(N+M)+1] + \lambda \frac{[2(N+M)+3]!!}{[2(N+M)-1]!!} \frac{1}{(4\alpha_0)^2} \right\}, \tag{4.15}$$

$$\langle \Phi^{(2)}_N | \Phi^{(2)}_M \rangle = -\langle \Phi^{(1)}_{N+\frac{1}{2}} | \Phi^{(1)}_{M+\frac{1}{2}} \rangle, \tag{4.16}$$

$$\langle \Phi^{(2)}_N | \hat{H} | \Phi^{(2)}_M \rangle = -\langle \Phi^{(1)}_{N+\frac{1}{2}} | \hat{H} | \Phi^{(1)}_{M+\frac{1}{2}} \rangle. \tag{4.17}$$

Some typical results are exhibited in Table 3 for $\lambda = 1$ (a rather large anharmonicity). We compare, for different numbers of "moments" n (cf. Eqs. (2.1)–(2.6)), our results with the (almost) exact ones of Biswas et al. [36]. The latter are obtained by recourse to the Hill-determinant method and involve dealing with matrices of the order of 40×40 [36]. The rather excellent agreement between our figures and those of [36], which are obtained with just a few (say, 6) moments, should give an idea of the power of the present approach.
Within the present context our results are strongly dependent upon the value chosen for the distribution point support α_0. This is to be expected, as S_c is infinite here, and illustrates the assertion made in Sect. 2.1: it is possible to take advantage of the fact that α_0 is a free parameter in order to truly minimize the g.s. energy.
Finally, a glance at the third column of Table 2 (cf. Sect. 3) should convince the reader that the $f_m(\alpha_0)$ diminish rather rapidly as m grows.

Table 3. Ratio of approximate energies to those obtained in [36], for, respectively, the ground state, and the 2nd, 4th and 6th excited ones. The corresponding number of moments, n, is given in the first column, while the last row displays the energy values reported in [36]

The λx^4 anharmonic oscillator				
n	$E_0/E^{(0)}_{\text{Biswas}}$	$E_2/E^{(2)}_{\text{Biswas}}$	$E_4/E^{(4)}_{\text{Biswas}}$	$E_6/E^{(6)}_{\text{Biswas}}$
2	1.000346538	1.0291993		
3	1.000024321	1.0026793	1.0715371	
4	1.000002131	1.0002705	1.0120754	1.1175670
5	1.000000213	1.0000291	1.0019383	1.0294024
6	1.000000006	1.0000009	1.0000664	1.0008184
7	1.000000001	1.0000001	1.0000065	1.0001351
8	1.000000000	1.0000000	1.0000004	1.0000084
9	1.000000000	1.0000000	1.0000000	1.0000005
E_{Biswas}	1.392351641	8.6550499	18.0575574	28.8353384

5. Conclusions

A generalization of the HW ansatz has been developed which allows one to exploit the properties of the collective subspace, as suggested by the pioneer work of Wong [11], Lathouwers [10] and de Toledo-Piza et al. [13, 14], *without having to diagonalize the generator overlap kernel* (1.5). Since this diagonalization is feasible only in very special cases, the main result of the present paper is seen to be the introduction of a *practical* method that allows for implementing the powerful ideas of Refs. [10–14] in a rather simple fashion.

The examples discussed in Sects. 3 and 4 show that our approach works satisfactorily both in a finite (discrete) case and in a continuous one. It should be pointed out that *these* examples, although simple, have *not* been tackled before (as far as we know) within the GCM scheme. Of course, related problems have been exhaustively discussed before [8].

The HW equations emerge from the variational principle, and, in solving them within any approximate scheme, one is guaranteed to obtain upper bounds to the g.s. energy. Our generalized HW ansatz provides us, *additionally*, with a free parameter (the distribution point support α_0) that allows for improving this upper bound. Of course, this will be of practical usefulness only in the continuous case, when we are *forced* adopt a truncation scheme, or in finite problems of such a dimension that any *exact* diagonalization becomes prohibitive.

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