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Collective Hamiltonians in the generator coordinate method: Isoscalar monopole vibrations in light spherical nuclei

Diógenes Galetti
Instituto de Física Teórica, São Paulo, Brasil

A. F. R. de Toledo Piza
Instituto de Física da Universidade de São Paulo, São Paulo, Brasil

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A procedure for constructing a collective Hamiltonian for a given nuclear collective motion is developed from the generator coordinate method. The procedure is based on the construction of a collective subspace of the many-body Hilbert space, and this is achieved by the diagonalization of the generator coordinate method overlap kernel. The Weyl transformation makes the connection between nonlocal phase space Hamiltonian kernels, obtained from the generator coordinate method, and operators in the collective space. The Gaussian overlap approximation and monopole vibrations in light spherical nuclei are studied in this formalism.

[NUCLEAR STRUCTURE Generator coordinate method. Weyl transformation. Collective Hamiltonians. Application to the monopole giant resonance.]

I. INTRODUCTION

If we consider the dynamical behavior of a system which exhibits a collective motion to be basically described by some special degrees of freedom and not by all of the single particle coordinates, we are led, in practical cases, to a situation in which a certain amount of *a priori* knowledge must be used in order to single out those semiclassical parameters that are associated with the actual variables which describe the motion. This process is at the foundation of the generator coordinate method (GCM) (Refs. 1 and 2); we must be able to describe the collection motion by the use of conveniently chosen semiclassical parameters (or even one parameter). The generator coordinate ansatz uses some set of states, labeled by one parameter α (the extension to more parameters being, in principle, straightforward), to construct the many body state

$$|\Psi\rangle = \int f(\alpha)\,|\alpha\rangle d\alpha \ , \tag{1.1}$$

which is introduced in the Ritz variational principle to get the Griffin-Wheeler equation[2] for $f(\alpha)$

$$\int [\langle\alpha|H|\alpha'\rangle - E\langle\alpha|\alpha'\rangle] f(\alpha')d\alpha' = 0 \ . \tag{1.2}$$

This is the basic equation of this method. The conditions under which this equation has acceptable physical solutions, and also the relationship between (1.2) and a Schrödinger equation projected in a collective subspace of the full many-body Hilbert space, have been discussed many times.[3]

A new approach to the generator coordinate method has been developed more recently,[4–6] the aim of which is to construct explicitly, in terms of states $|\alpha\rangle$, a collective subspace of the full many-body Hilbert space; this subspace is identified as the specific collective subspace in which the collective motion is to be described. One is able to obtain the projection operator associated to this particular subspace and consequently one can also explicitly restrict the many-body dynamics to this subspace. One thus gets a Schrödinger equation for the collective motion[5]

$$\int [H(k,k') - E\delta(k-k')]g(k')dk' = 0 \ . \tag{1.3}$$

In this equation, k and k' refer to the diagonal representation of a collective variable naturally associated to the adopted semiclassical parameter of the GCM scheme. One has to deal with a Hamiltonian operator kernel which is, in general, nonlocal.

In this paper we will discuss a procedure to obtain, from that nonlocal operator kernel, a collective Hamiltonian operator defined in the collective subspace; such a collective Hamiltonian is written as a function of a natural pair of conjugated collective operators $\hat{q}$ and $\hat{p}$ and is obtained by the use of the Weyl transformation.[7–9] The crucial step in this procedure is a quasilocal expansion of the nonlocal Hamiltonian operator kernel and the inherent question of the convergence of this series. In fact, we will identify the first two terms of that series as collective potential and kinetic energy, respectively.

In Sec. II A we will briefly review the formalism proposed in Refs. 4–6. The Weyl transformation is reviewed in its main aspects in Sec. II B. The formal procedure to get the collective Hamiltonians is presented in Sec. III, and the whole procedure is carried out in two cases, namely the Gaussian overlap approximation and monopole nuclear vibrations in light spherical nuclei, in Sec. IV. Finally, conclusions are given in Sec. V.

II. BASIC CONCEPTS

A. The GCM and the collective subspace

As proposed in Refs. 4–6, the quantum GCM ansatz (1.1) can be used to construct a well defined quantum kinematics to describe the corresponding nuclear collective motion we are interested in. The starting point of this approach is the identification of the GCM overlap kernel

$$N(\alpha,\alpha') \equiv \langle \alpha \mid \alpha' \rangle$$

as an operator kernel, bounded and self-adjoint, in the space of the weight functions $f(\alpha)$. The procedure to construct the collective subspace consists then in the diagonalization of this operator. The diagonalization can be carried out, in principle at least, as guaranteed by the spectral theorem of functional calculus; i.e., one looks for a unitary transformation $U_k(\alpha)$ that takes the operator kernel $N(\alpha,\alpha')$ to a new representation in which it appears as a multiplication operator

$$\int d\alpha \int d\alpha' U_k^{\dagger}(\alpha)\langle \alpha \mid \alpha' \rangle U_{k'}(\alpha') = \Lambda(k)\delta(k-k') \ . \tag{2.1}$$

In this equation we are implicitly assuming that $\langle \alpha \mid \alpha' \rangle$ has a continuous spectrum. This is by no means necessary in general, and other cases can be handled by means of appropriate technical changes in the discussion to follow.

This allows us to formally write the set of states

$$|k\rangle = \int \frac{U_k(\alpha)}{\Lambda^{1/2}(k)} |\alpha\rangle d\alpha \tag{2.2}$$

as the base states in the collective subspace provided $\Lambda(k) \neq 0$.[5] This set of states exhibits orthonormality and completness properties

$$\langle k \mid k' \rangle = \delta(k-k') \ , \tag{2.3a}$$

$$\int dk \mid k \rangle\langle k \mid = \hat{1}_c \ , \tag{2.3b}$$

where $\hat{1}_c$ is the unity operator in this collective subspace. Collective operators $\hat{p}$ and $\hat{q}$ can now be defined as

$$\hat{p} \mid k \rangle = \hbar k \mid k \rangle \ , \tag{2.4a}$$

$$\hat{q} \mid k \rangle = i\frac{\partial}{\partial k} \mid k \rangle \ . \tag{2.4b}$$

It can easily be checked that $[\hat{q},\hat{p}] = i\hbar\hat{1}_c$.

With the help of that set of base states we can now write the many-body wave function generated by ansatz (1.1) in the form

$$g(k) \equiv \langle k \mid \Psi \rangle = \int \frac{U_k^{\dagger}(\alpha)}{\Lambda^{1/2}(k)} \langle \alpha \mid \Psi \rangle d\alpha = \Lambda^{1/2}(k) \int U_k^{\dagger}(\alpha) f(\alpha) d\alpha \ . \tag{2.5}$$

We can also obtain the formal expression for the Hamiltonian restricted to this subspace, in terms of the usual energy kernel of the GCM,

$$\langle k \mid H \mid k' \rangle = \int\int \frac{U_k^{\dagger}(\alpha)}{\Lambda^{1/2}(k)} \times \langle \alpha \mid H \mid \alpha' \rangle \frac{U_{k'}(\alpha')}{\Lambda^{1/2}(k')} d\alpha d\alpha' \ . \tag{2.6}$$

Using the above results, the basic equation (1.2) is reduced to the projected Schrödinger equation (1.3). In what follows we will implement this procedure in specific cases and also identify a collective Hamiltonian expressed in terms of the collective operators $\hat{q}$ and $\hat{p}$, introduced above. The basic tool for this purpose is the Weyl transformation.

B. Brief review of Weyl transformation

The Weyl transformation was introduced in 1927 (Ref. 7) with the purpose of obtaining a mapping of operators, associated to physical quantities and acting in a Hilbert space of state vectors, onto ordinary phase space functions. It is related to the so-called Wigner function,[10] which consists, particularly, in the mapping of the density operator on a certain phase space function. Thus it allows for an alternative description of quantum mechanics by using phase space functions instead of operators, and Wigner functions instead of state vectors.

More recently, the properties of Weyl transformation have been studied in a series of paper.[8] Here we will closely follow Ref. 9.

In order to introduce the Weyl transformation we need to assume the existence of a well defined quantum kinematics; this is precisely what we have introduced in Sec. II A through the definition of the collective subspace equations (2.3). Consequently, we are able to apply the procedure exposed in Ref. 9 to this collective subspace.

Momentum and coordinate operators satisfy the usual commutation relations (one dimension)

$$[\hat{p},\hat{p}]=[\hat{q},\hat{q}]=0\ ,\quad [\hat{q},\hat{p}]=i\hbar\hat{1}_c$$

and have eigenvectors and eigenvalues

$$\hat{p}\,|p\rangle=p\,|p\rangle\ ,\quad \hat{q}\,|x\rangle=q\,|x\rangle\ ,$$

where $p=\hbar k$. Furthermore, these eigenvectors satisfy the relations

$$\int dp\,|p\rangle\langle p\,|=\hat{1}_c\ ,\quad \int dx\,|x\rangle\langle x\,|=\hat{1}_c\ , \tag{2.7}$$

$$\langle p\,|p'\rangle=\delta(p-p')\ ,\quad \langle x\,|x'\rangle=\delta(x-x')\ , \tag{2.8}$$

$$\langle x\,|p\rangle=h^{-1/2}e^{ipx/\hbar}\ .$$

From the identity

$$\hat{A}=\int dx'dx''dp'dp''\,|x''\rangle\langle x''\,|p''\rangle\times\langle p''\,|\hat{A}\,|p'\rangle\langle p'\,|x'\rangle\langle x'|\ ,$$

with the help of the coordinate transformation

$$x''=q+\frac{\sigma}{2}\ ,\quad x'=q-\frac{\sigma}{2}\ ,$$

$$p''=p+\frac{u}{2}\ ,\quad p'=p-\frac{u}{2}\ ,$$

we obtain

$$\hat{A}=\frac{1}{h}\int dq\,dp\,a_w(q,p)\Delta(q,p)\ ,$$

where

$$a_w(q,p)=\int du\left\langle p+\frac{u}{2}\left|\hat{A}\right|p-\frac{u}{2}\right\rangle e^{iqu/\hbar} \tag{2.9}$$

is the Weyl transform of the operator $\hat{A}$, and

$$\Delta(q,p)=\frac{1}{h}\int d\sigma\left|q+\frac{\sigma}{2}\right\rangle\left\langle q-\frac{\sigma}{2}\right|e^{ip\sigma/\hbar} \tag{2.10}$$

is a Hermitian operator. This operator can be put in a more convenient form

$$\Delta(q,p)=h^{-1}\int d\sigma\,du\,\exp\{i[(q-\hat{q})u+(p-\hat{p})\sigma]/\hbar\}\ . \tag{2.11}$$

Obviously we could have, alternatively,

$$a_w(q,p)=\int d\sigma\left\langle q-\frac{\sigma}{2}\left|\hat{A}\right|q+\frac{\sigma}{2}\right\rangle e^{ip\sigma/\hbar}\ ,$$

$$\Delta(q,p)=\int du\left|p-\frac{u}{2}\right\rangle\left\langle p+\frac{u}{2}\right|e^{iqu/\hbar}\ .$$

It is possible, in principle, to recover the operator $\hat{A}$ from its Weyl transform and the corresponding expression for $\Delta(q,p)$. In fact, it is easy to show that

$$\hat{A}=\int dp\,dp\,\delta(q-\hat{q})\delta(p-\hat{p})a_0(q,p)\ , \tag{2.12}$$

where

$$a_0(q,p)\equiv\exp\left[\frac{\hbar}{2i}\frac{\partial}{\partial p}\frac{\partial}{\partial q}\right]a_w(q,p)\ .$$

This shows how to extract operator $\hat{A}$ from its Weyl transform $a_w(q,p)$, i.e., we firstly calculate $a_0(q,p)$ and then substitute the variables q and p by the operator $\hat{q}$ and $\hat{p}$, respectively, the coordinate operators always appearing on the left of the momentum operators. This procedure is particularly convenient if we have to deal with binomials in $\hat{p}$ and $\hat{q}$.

In this way, if we have operators having Weyl transforms of the form

$$a_w(q,p)=f(q)p^n\ ,$$

then

$$\hat{A}(\hat{p},\hat{q}) = \sum_{l=0}^{n} \begin{bmatrix} n \\ l \end{bmatrix} \left[\frac{\hbar}{2i}\right]^l \frac{d^l}{d\hat{q}^l} f(\hat{q})\hat{p}^{n-l} \ ,$$

or using the commutation relations for the $\hat{q} - \hat{p}$ operators,

$$\hat{A}(\hat{p},\hat{q}) = \frac{1}{2^n} \sum_{l=0}^{n} \begin{bmatrix} n \\ l \end{bmatrix} \hat{p}^{\,l} f(\hat{q})\hat{p}^{n-l} \ .$$

This result can also be written as

$$a_w(q,p) \rightleftarrows \frac{1}{2^n} \sum_{l=0}^{n} \begin{bmatrix} n \\ l \end{bmatrix} \hat{p}^{\,l} f(\hat{q})\hat{p}^{n-l} \ ,$$

where $\rightleftarrows$ stands for Weyl correspondence; we could have, alternatively,

$$f(q)p^n \rightleftarrows \frac{1}{2^n}\{\{\ldots\{f(\hat{q}),\hat{p}\},\hat{p}\}\ldots\hat{p}\}\ ,$$

n anticommutators , (2.13)

III. COLLECTIVE HAMILTONIANS

In the space of collective states $|k\rangle$ satisfying properties (2.3a) and (2.3b), the kernel of an operator H is given by $\langle k|H|k'\rangle$. We could already apply the Weyl transformation to this kernel, but in order to make clear the connection between the collective coordinate and the generator coordinate, as will be seen later, we will make a double Fourier transformation to consider alternatively the kernel $\langle x|H|x'\rangle$. If we now make the coordinate transformation

$$q = \frac{x + x'}{2}, \quad \sigma = x' - x \ ,$$

we can rewrite

$$\langle x|H|x'\rangle = \left\langle q - \frac{\sigma}{2}\middle|H\middle|q + \frac{\sigma}{2}\right\rangle \equiv H(q,\sigma) \tag{3.1}$$

and the Weyl transform of this operator is given by

$$h_w(q,p) = \int d\sigma \left\langle q - \frac{\sigma}{2}\middle|H\middle|q + \frac{\sigma}{2}\right\rangle e^{ip\sigma/\hbar} \ ,$$

which gives exactly the same result as that obtained from $\langle k|H|k'\rangle$.

In order to obtain a series expressing the collective Hamiltonian in terms of the collective operators $\hat{q}$ and $\hat{p}$, it is necessary to assume that the kernel associated to a microscopic Hamiltonian operator admits the quasilocal expansion

$$\left\langle q - \frac{\sigma}{2}\middle|H\middle|q + \frac{\sigma}{2}\right\rangle = \sum_{n=0}^{\infty} H^{(n)}(q)\delta^{(n)}(\sigma) \ , \tag{3.2}$$

where $\delta^{(n)}(\sigma)$ is the nth derivative of Dirac distribution and

$$H^{(n)}(q) = \frac{(-1)^n}{n!} \int d\sigma' \, H(q,\sigma')(\sigma')^n \ .$$

The validity of that assumption, and the convergence of the resulting series, as needed, will be assumed throughout this paper.

The Weyl transform of H is then written as

$$h_w(q,p) = \sum_{n=0}^{\infty} H^{(n)}(q) \int d\sigma \delta^{(n)}(\sigma) e^{ip\sigma/\hbar} \ .$$

We can now extract the collective Hamiltonian $H(\hat{q},\hat{p})$ by the use of (2.12)

$$H(\hat{q},\hat{p}) = \int dp\, dq\, \delta(q - \hat{q})\delta(p - \hat{p}) \exp\left[\frac{\hbar}{2i}\frac{\partial}{\partial p}\frac{\partial}{\partial q}\right] \sum_{n=0}^{\infty} (-1)^n H^{(n)}(q) \left[\frac{d^n}{d\sigma^n} e^{ip\sigma/\hbar}\right]_{\sigma=0} \ .$$

The final result may be cast in the form

$$H(\hat{q},\hat{p}) = H^{(0)}(\hat{q}) + \sum_{n=1}^{\infty} \frac{(-i)^n}{(2\hbar)^n}\{\{\ldots\{H^{(n)}(\hat{q}),\hat{p}\}\ldots\hat{p}\} \tag{3.3}$$

by the use of (2.13).

This Hamiltonian may be interpreted as follows. The term independent of $\hat{p}$, $H^{(0)}(\hat{q})$, will be considered a collective potential. Its expression is

$$V(\hat{q}) \equiv H^{(0)}(\hat{q}) = \int H(\hat{q},\sigma')d\sigma' \ . \tag{3.4}$$

By symmetry arguments only, we can show the vanishing of terms in odd powers of $\hat{p}$, i.e.,

$$H^{2n+1}(\hat{q}) = 0 \ .$$

The second order term

$$H^{(2)}(\hat{q}) = \tfrac{1}{2} \int H(\hat{q},\sigma')(\sigma')^2 d\sigma' \tag{3.5}$$

gives information about the inertia of the system.

In favorable cases the collective dynamics will be well described only by the two terms (3.4) and (3.5). However, it is important to note that we cannot consider the collective inertia and the collective potential to be defined unambigously by these expressions. In fact, canonical transformations from $\hat{q},\hat{p}$ to new variables in the collective subspace will change these objects while preserving the collective dynamics given by the collective Hamiltonian. But since our procedure clearly defines a collective coordinate, we will use it for defining our respresentation and consistently extract a collective potential and inertia parameter.

It is important to stress that quasilocal expansion of the energy and overlap kernels have already appeared in connection with the treatment of the Griffin-Wheeler equation (1.2), notably in the work of Brink and Banerjee[11]; in that work, however, divergences in the weight functions are not discussed, and the treatment can only be meaningful in the special case of narrow overlaps. In an earlier work by Giraud and Grammaticos,[12] the idea of a quasilocal expansion, very much in the spirit of the present one, is indicated in connection with an orthonormal representation of the collective space associated with an auxiliary "collective" variable introduced independently of the generator coordinate (GC) scheme, leading to a representation in the GC collective subspace which may be *a priori* unrelated to the adopted generator coordinate. Finally, it is interesting to point out the relationship between this present method of obtaining collective Hamiltonians and that of Klein.[13] Here we have shown that the Weyl transformation is a natural tool for treating the nonlocal energy kernel, even when this kernel is not expanded as in (3.2); however, under certain situations, the expansion is very convenient. The treatment presented in Ref. 13 makes use of the quasilocal expansion (3.2), and the extraction of the collective Hamiltonian proceeds from the integration in the σ variable of that expansion. The final result obtained by Klein coincides with expression (3.3), and has been used, in the form mentioned in Ref. 6, in a description of the Goldhaber-Teller dipole vibration[14] in ^{4}He.[15] There the result for the collective Hamiltonian can be exactly given in closed analytical form due to the fact that the series (3.2) naturally truncates.

IV. ILLUSTRATIVE EXAMPLES

In this section we intend to show how the above formal scheme works when we apply it to calculate collective parameters. We will consider, in what follows, a simple but already nontrivial case of translationally invariant GCM overlap kernels with one real generator coordinate α. Thus

$$N(\alpha,\alpha') = n(\alpha - \alpha') \ .$$

The spectrum in this case is immediately given by a Fourier transformation

$$\Lambda(K) = (2\pi)^{-1/2} \int d\alpha \, e^{iK\alpha} n(\alpha) \ , \tag{4.1}$$

which, under the cases to be treated below, does not exhibit a null space, but admits zero as a limit point when $|k| \to \infty$.

When the parameter α is associated to a coordinate, it is easily seen that the collective subspace is given in a "momentum" representation. We take a double Fourier transformation of (2.6), in order to work with a coordinate representation, as mentioned in Sec. III,

$$H(x,x') = \int\int \frac{e^{iKx}}{(2\pi)^{1/2}} \times \langle K | H | K' \rangle \frac{e^{-iK'x'}}{(2\pi)^{1/2}} dK \, dK' \ .$$

Making use of the transformation

$$K - K' = k \ , \quad \frac{K + K'}{2} = \bar{K} \ ,$$

$$x - x' = y \ , \quad \frac{x + x'}{2} = q \ ,$$

we have

$$H(q,y) = (2\pi)^{-1} \int\int e^{-ikq} e^{-i\bar{K}y} \left\langle \bar{K} + \frac{k}{2} \middle| H \middle| \bar{K} - \frac{k}{2} \right\rangle d\bar{K} \, dk \ . \tag{4.2}$$

Using (3.1) and (3.4) it is easy to verify that the collective potential is given by

$$H^{(0)}(q) = (2\pi)^{-1} \int\int\int e^{-ikq} \left\langle \bar{K} + \frac{k}{2} \middle| H \middle| \bar{K} - \frac{k}{2} \right\rangle e^{-i\bar{K}y} d\bar{K}\, dk\, dy \ .$$

The y and $\bar{K}$ integrals are trivially obtained and we have

$$V(\hat{q}) = H^{(0)}(\hat{q}) = \int\int\int \exp\left[ik\left[\frac{\alpha+\alpha'}{2} - \hat{q}\right]\right] \frac{\langle \alpha | H | \alpha' \rangle}{\left[\Lambda\left[\frac{k}{2}\right]\Lambda\left[-\frac{k}{2}\right]\right]^{1/2}} d\alpha\, d\alpha'\, dk \ . \tag{4.3}$$

The dependence of the potential on the spectrum results from the need to "unfold" the finite spread of the collective dynamical variables in the wave packets used to set up the energy kernel. In the present procedure it is thus easy to see that, when the overlap is narrow, the collective potential is well described by the diagonal part of the GCM energy kernel if we neglect the fluctuation energy which always exists in wave packet formalisms. Owing to the expected relationship between the overlap width and the number of particles participating in the motion, narrow overlaps will tend to occur in connection with collective modes in heavier nuclei; on the other hand, in light nuclei important corrections may arise from the dependence on the overlap spectrum. Let us consider now two particular cases.

A. Quadratic approximation with Gaussian overlap kernel

This approximation has been used since its appearance in the work by Griffin[2] as a test ground of nuclear collective motion theories. The quadratic approximation reads

$$\langle \alpha | H | \alpha' \rangle = N(\alpha,\alpha') \left[E_0 + \frac{C_1}{2}(\alpha - \alpha')^2 + \frac{C_2}{2}\left[\frac{\alpha+\alpha'}{2}\right]^2 \right] , \tag{4.4}$$

with

$$N(\alpha,\alpha') = \exp[-(\alpha-\alpha')^2/b^2] \ .$$

The introduction of a complex generator coordinate in this approximation permitted the treatment of low amplitude oscillations in a nuclear system, leading to random-phase approximation (RPA)-like equations.[16] It has been recently shown, however, that their result is in quantitative disagreement with the exact solution.[17] Here, we are dealing with a real generator coordinate only and consequently we are treating the nuclear vibration problem in a more restricted way.

Using now (4.3) it is trivial to get the collective potential

$$V(\hat{q}) = E_0 + \left[\frac{C_2}{16} - \frac{C_1}{4}\right] b^2 + \frac{C_2}{2}\hat{q}^2 \ .$$

The contribution coming from the spectrum, $[(C_2/16) - (C_1/4)]b^2$, appears explicitly here and corresponds to the fluctuation energy. In this simple case it reduces to a constant and is therefore trivial. To complete the description of the system we must calculate the mass parameter. It can be obtained by the use of (4.4), (4.2), and (3.5). After a trivial calculation we find

$$\frac{1}{2M(\hat{q})} = -\frac{C_1 b^4}{8\hbar^2} \ ,$$

which is independent of $\hat{q}$.

The b dependence of $M(\hat{q})$ might seem peculiar. However, E_0, C_1, and C_2 may be rewritten as [2]

$$E_0 = V_0 + \frac{\hbar^2}{\mathcal{M} b^2} \ ,$$

$$C_1 = \frac{4\hbar^2}{\mathcal{M} b^4} \ ,$$

$$C_2 = \mathcal{M}\Omega^2 \ .$$

These expressions are suggested by the form of $\langle\alpha|H|\alpha'\rangle$, when H is a harmonic oscillator Hamiltonian, and the states $|\alpha\rangle$ are Gaussians of parameter b centered on α. In terms of the new expansion parameters V_0 and Ω we find

$$M(\hat{q}) = \mathcal{M}$$

and

$$V(\hat{q}) = V_0 - \frac{\mathcal{M}\Omega^2 b^2}{16} + \tfrac{1}{2}\mathcal{M}\Omega^2\hat{q}^2 \ .$$

B. Isoscalar monopole vibrations

Many authors have discussed this particular mode of vibration using the GCM in cases where $A = 4n$.[18,19,12] In what follows we will briefly summarize the GCM results, and then we will apply our formalism to extract the collective potential and mass parameter.

Let us take the harmonic oscillator determinantal wave functions as the generating functions $|\vec{r};\beta\rangle$, and the inverse of the harmonic oscillator parameter as the generator coordinate β. This particular choice for the generating function, although easy to handle, exhibits an undesirable feature; the center of mass wave function depends on the generator coordinate, giving therefore an energy which does not separate into intrinsic and center of mass parts. However, it is possible to circumvent this problem, the procedure being described in the Appendix.

The interaction to be used is that of Skyrme,[20] spin-orbit, and Coulomb effects being neglected for simplicity. For light spherical nuclei ($A = 4n$) the GCM overlap kernel is[19]

$$N(\beta,\beta') = \left[\frac{2\beta\beta'}{\beta^2+\beta'2}\right]^T ,$$

where T is an integer constant which depends on A ($T = 6$, 36, and 120 for ^{4}He, ^{16}O, and ^{40}Ca, respectively). With a new generator coordinate introduced through $\beta = \beta_0 e^{\alpha}$,[18] the overlap kernel becomes translationally invariant

$$N(\alpha,\alpha') = \mathrm{sech}^T(\alpha - \alpha') \ . \tag{4.7}$$

This change of label does not affect the collective subspace; therefore the dynamical content of the method is preserved. The energy kernel, calculated in Ref. 19, is now written as

$$\begin{aligned} H(\alpha,\alpha') &= N(\alpha,\alpha')[C_1\,\mathrm{sech}(\alpha-\alpha')e^{\alpha+\alpha'} + C_2\cosh^{3/2}(\alpha-\alpha')e^{(3/2)(\alpha+\alpha')} \\ &\quad + C_3\cosh^{5/2}(\alpha-\alpha')e^{(5/2)(\alpha+\alpha')} + C_4\cosh^3(\alpha-\alpha')e^{3(\alpha+\alpha')}] \\ &= N(\alpha,\alpha')h(\alpha,\alpha') \ . \end{aligned} \tag{4.8}$$

Again the constants C_i's depend on A, and on the force parameters. All lengths are measured in units of β_0^{-1}.

A Fourier transformation diagonalizes the overlap kernel and the spectrum in this case is

$$\Lambda(K) = \frac{\pi K}{\Gamma(T)\sinh\left[\frac{K\pi}{2}\right]}\prod_{s=1}^{T/2-1}(4s^2+K^2) \ .$$

Unfortunately, this spectrum is not easy to handle, even though it displays no null space, and it has zero as limit point as $K \to \pm\infty$. However, we find that a Gaussian spectrum

$$\Lambda(K) = \left[\frac{2\pi}{T}\right]^{1/2}\exp\left[\frac{K^2}{2T}\right] ,$$

is a good approximation to the exact one, if we are treating heavy nuclei (^{16}O, ^{40}Ca). The corresponding Gaussian overlap kernel,

$$N(\alpha-\alpha') = \exp\left[-\frac{T}{2}(\alpha-\alpha')^2\right] ,$$

is, in turn, a good approximation to the exact one.[18]

The collective potential is now given by expression (4.3). Nevertheless, before performing that integration in (4.3), we will make some approximations in order to put it in such a form as to fully exploit the advantages of the Weyl transformation.

First we expand the reduced kernel $H(\alpha,\alpha')\,|\,N(\alpha,\alpha')$ in a power series in $\eta = \alpha - \alpha'$ and $\gamma = (\alpha+\alpha')/2$. Here we will adopt the notation

$$C_{nm} = \frac{1}{n!m!}\frac{\partial^{n+m}}{\partial\eta^n\partial\gamma^m}[H(\gamma,\eta)/N(\eta)]_{\substack{\eta=0\\ \gamma=\gamma 0}} ,$$

where γ_0 is the minimum occurring in the diagonal part of the energy kernel. At this stage we can fix the parameter β_0 defining the scale of lengths. We will choose β_0 such that γ_0 is equal to zero; i.e., the minimum of the diagonal part of the energy kernel occurs at that value of γ which corresponds to the oscillator parameter β_0^{-1}, which gives the variational rms radius.

With this expansion we can now integrate (4.3); the general term contributing to the potential is

$$G(\hat{q}) = \frac{C_{nm}}{2\pi} \int_{-\infty}^{+\infty} \exp\left[-\frac{T}{2}\eta^2\right] \eta^n d\eta \times \int_{-\infty}^{+\infty} \frac{\exp[ik(\gamma - \hat{q})]}{\Lambda(k/2)} \times \gamma^m dk\, d\gamma \ . \quad (4.9)$$

If we retain terms up to fourth order in the expansion of the reduced kernel we get, after a tedious but straightforward calculation,

$$V(\hat{q}) \simeq C_{00} + \frac{C_{20}}{T} - \frac{C_{02}}{4T} + \frac{1}{T^2}\left[3C_{40} - \frac{C_{22}}{4} + \tfrac{3}{16}C_{04}\right] + \frac{1}{T}(C_{21} - \tfrac{3}{4}C_{03})\hat{q} + \left[C_{02} + \frac{1}{T}(C_{22} - \tfrac{3}{2}C_{04})\right]\hat{q}^2 + C_{03}\hat{q}^3 + C_{04}\hat{q}^4 \ . \quad (4.10)$$

The expansion coefficients depend on the Skyrme parameters in addition to T. Evaluating these coefficients for ^{16}O and ^{40}Ca, we find that is sufficient to retain terms up to second order, if we are interested in the low lying vibrational states. This truncation can be justified by calculating the ratio $C_{03}q^3/C_{02}q^2$ near the minimum of the expression (4.10). The values are of the order of 0.25 for ^{16}O in contrast to the value 0.5 for ^{4}He. Thus the collective potential for the heavier nuclei is

$$V(\hat{q}) \simeq C_{00} + \frac{C_{20}}{T} - \frac{C_{20}}{4T} + C_{02}\hat{q}^2 \ . \quad (4.11)$$

The full expression (4.10) is needed for ^{4}He, however.

The linear term in (4.10) comes from the third order terms in the expansion of the reduced kernel. It causes a shifting of the minimum of the collective potential away from the minimum of the GCM energy kernel. Obviously, this implies a nuclear radius different from that calculated by the variational method, i.e., using the minimum β_0. It is interesting to note that those third order terms are associated to the asymmetry of the GCM energy kernel (C_{03}) and to the coupling of the diagonal terms and off-diagonal terms (C_{21}). In fact, we see this is an important effect only for light nuclei because the ratio

$$\frac{(C_{21} - \tfrac{3}{4}C_{03})T^{-1}}{C_{02} + (C_{22} - \tfrac{3}{2}C_{04})T^{-1}}$$

is relatively important when T is small. When we calculate the minimum of expression (4.11) for ^{4}He, using the Skyrme III interaction, we get $\beta^{-1} = 1.57$ fm. On the other hand, the use of (4.10) gives $\beta^{-1} = 1.30$ fm (with the same interaction). The calculation for ^{16}O and ^{40}Ca using (4.11) gives essentially the same results as those obtained from a direct treatment of the Griffin-Wheeler equation.[19] This is consistent with the validity of the quadratic approximation in these cases.

The mass parameters can be calculated in exactly the same way by the use of (3.5). Here, again, the dominant term is $-C_{20}/T^2$ coming from the quadratic approximation. A kinetic energy term comes from (3.3)

$$-\frac{C_{20}}{T^2}\hat{p}^2 = \text{kinetic energy} \ . \quad (4.12)$$

If we want a new momentum operator in proper units, we must introduce the parameter $(\beta_0^{-1}/\hbar c)^2$. In this case we see that the corresponding mass parameter comes out as

$$Mc^2 = \frac{-\hbar^2 T^2 \beta_0^2}{2C_{20}} \ . \quad (4.13)$$

This expression can be calculated in each specific case. In particular for ^{16}O we have

$$\frac{M}{m} = 42.6 \ ,$$

where m is the mass of the nucleon. However, this result is not invariant under canonical scaling of $\hat{p}$ and $\hat{q}$. In particular, if we had chosen β_0^{-1} to be the variational rms radius we would have obtained

instead

$$\frac{M}{m} = 16.8 \ ,$$

in close agreement with Giraud and Grammaticos.[12]

Another important feature of these nuclear systems can be studied now, once we have an analytical expression, although approximated, for the collective potential, namely the nuclear incompressibility modulus. This modulus is defined as

$$K = \frac{1}{A}\frac{d^2}{dq^2}V(q)\,|_{q=q_0} \ . \tag{4.14}$$

We expect the value of K to approach the value given by Flocard and Vautherin[19] as we go to heavier nuclei, i.e., both values tend to coincide when the quadratic approximation is sufficient to describe the monopole vibration. The incompressibility for ^{16}O is $K = 227.5$ MeV (interaction *S*III) using (4.14), which is greater than $K = 200.5$ MeV calculated with the diagonal part of the GCM energy kernel. Although this high incompressibility modulus can be partially associated to the Skyrme interaction, as already suggested in other work,[19] it is important to note that the difference between our result and that of Flocard and Vautherin[19] arises because the collective potential is not the diagonal part of the GCM energy kernel.

V. CONCLUSIONS

We have shown in detail how a procedure developed earlier for constructing a well defined subspace of the full many-body Hilbert space, on the basis of the GCM, can be exploited to give an explicit construction of the collective Hamiltonian, expressed in terms of collective dynamical variables, defined in that subspace. We started from the energy kernel (2.6) and from there proceeded to obtain the Weyl transform of the collective Hamiltonian.

In order to exploit the advantages of the Weyl transformation, and consequently to get the collective Hamiltonian as much as possible in an explicit form, we made a quasilocal expansion of the projected energy kernel (2.6). This led to a collective Hamiltonian written as a series in the collective variables. That expansion, which is not necessarily encompassed in the Weyl formalism, does not change, however, the general character of the procedure, but gives, in fact, an approximated but effective way of treating collective motions. The convergence properties of the series are affected by the features of the two GCM kernels. The kinematics of the GCM manifests itself through the width of the overlap kernel; narrow overlaps may give rise to rapidly convergent series for the collective Hamiltonian, although this is not meant to imply a "kinematic" criterion of collectivity since the convergence of the expansion can not be judged without reference to the GCM energy kernel.

The feasibility of the whole procedure was shown in two simple illustrative examples, namely the Gaussian overlap approximation (GOA) and monopole vibrations of light spherical nuclei. This latter example is nontrivial in the sense that the collective Hamiltonian is given in the form of an infinite series in powers of $\hat{q}$ and $\hat{p}$. The point emphasized in those two examples was the corrections to the simple variational treatment of the diagonal part of the energy kernel. In this connection it is interesting to note that the spectrum of the overlap kernel $\Lambda(K)$ plays an important role. Fluctuation energy corrections and a shifting of the equilibrium point characterizes the corrections in the monopole vibration. In this particular mode of vibration the incompressibility modulus can be compared with previous results[19]; our results show some discrepancies, exhibiting a higher degree of incompressibility than that obtained with the variational method using the same interaction; part of this effect is due to the particular interaction used[19]; however, our result is not conclusive since it is necessary to retain terms to higher order in our series in order to compare the two results.

Finally, it is important to stress that if we want to get analytical solutions for the collective Hamiltonians we must first of all be able to analytically diagonalize the overlap kernel. In many cases, however, this condition is not fulfilled; this introduces a new difficulty in the method. An alternative approach, which may eventually constitute the only way of treating that difficulty, is a computational one, in which one performs numerically the different stages of the whole scheme described here. Thus we get the collective potential and inertia parameter numerically. In this connection ^{8}Be has been treated by this computational scheme and the results will be presented in a forthcoming publication.

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APPENDIX

For the sake of simplicity we will only discuss the effect of the choice of the generating function $|\vec{r};\beta\rangle$

for the case of ^{4}He. The particular choice we have adopted is

$$|\vec{r};\beta\rangle \equiv |\beta\rangle = \mathcal{N}_0 \exp\left[\sum_{i=1}^{4} \frac{\vec{r}_i^{\,2}}{2\beta^2}\right] , \tag{A1}$$

where $\mathcal{N}_0$ is a normalization constant, can be rewritten as

$$|\beta\rangle = \mathcal{N}_0 \exp\left[-\frac{2\vec{R}^2}{\beta^2}\right] \exp\left[-\sum_{i=1}^{4} \frac{\vec{\rho i}^{\,2}}{2\beta^2}\right] , \tag{A2}$$

where we have made the coordinate transformation

$$\vec{\rho i} = \vec{r}_i - \vec{R} ,$$

$$\vec{R} = \tfrac{1}{4} \sum_{i=1}^{4} \vec{r}_i ,$$

with the additional condition

$$\sum_{i=1}^{4} \vec{\rho i} = 0 .$$

The remarkable feature of expression (A2) is that the center of mass contribution as well as the intrinsic one depend on the generator coordinate. Even though we have removed from the Hamiltonian effects of the center of mass motion, the β dependence of the center of mass wave function introduces undesirable spurious effects. This can, however, be avoided if we introduce a new nondeterminantal generating function

$$|\tilde{\beta}\rangle = \mathcal{N}_1 \exp\left[\sum_{i=1}^{4} \frac{\vec{r}_i^{\,2}}{2\beta_0^{\,2}}\right] \times \exp\left[-2\vec{R}^2 \left[\frac{\beta^2 - \beta_0^{\,2}}{\beta^2 \beta_0^{\,2}}\right]\right] ,$$

where β_0 is a constant.

The great advantage of this function is that it separates in the form

$$|\tilde{\beta}\rangle = \mathcal{N}_1 \exp\left[\frac{-2\vec{R}^2}{\beta_0^{\,2}}\right] \exp\left[-\sum_{i=1}^{4} \frac{\vec{\rho i}^{\,2}}{2\beta^2}\right] = |\rho(\beta_0)\phi(\beta)\rangle , \tag{A3}$$

where the center of mass contribution does not depend on the generator coordinate. In this form we can use the generator coordinate only for the intrinsic part, and by virtue of this separation, we can take into account the center of mass contributions without having to recourse to projection techniques.

Thus we can write

$$\langle\tilde{\beta}|H|\tilde{\beta}'\rangle = \langle\tilde{\beta}|H_{\text{int}}|\tilde{\beta}'\rangle + \langle\tilde{\beta}|H_{\text{c.m.}}|\tilde{\beta}'\rangle$$

and using (A3)

$$\langle\phi(\beta)|H_{\text{int}}|\phi(\beta')\rangle\langle\rho(\beta_0)|\rho(\beta_o)\rangle = \langle\phi(\beta)\rho(\beta_0)|H|\phi(\beta')\rho(\beta_0)\rangle - E_{\text{c.m.}}(\beta_0)\langle\phi(\beta)|\phi(\beta')\rangle . \tag{A4}$$

On the other hand, if we had used (A2),

$$\langle\phi(\beta)|H_{\text{int}}|\phi(\beta')\rangle\langle\rho(\beta)|\rho(\beta')\rangle = \langle\phi(\beta)\rho(\beta)|H|\phi(\beta')\rho(\beta')\rangle - \langle\rho(\beta)|H_{\text{c.m.}}|\rho(\beta')\rangle\langle\phi(\beta)|\phi(\beta')\rangle . \tag{A5}$$

From (A4) and (A5) we can now separate

$$\frac{\langle\phi(\beta)|H_{\text{int}}|\phi(\beta')\rangle}{\langle\phi(\beta)|\phi(\beta')\rangle} = h(\beta,\beta')\langle\rho(\beta_0)|\rho(\beta_0)\rangle - \langle\rho(\beta)|H_{\text{c.m.}}|\rho(\beta')\rangle \times \frac{\langle\rho(\beta_0)|\rho(\beta_0)\rangle}{\langle\rho(\beta)|\rho(\beta')\rangle} ,$$

where we have made use of

$$\langle\phi(\beta)\rho(\beta)|H|\phi(\beta')\rho(\beta')\rangle = \langle\phi(\beta)|\phi(\beta')\rangle\langle\rho(\beta)|\rho(\beta')\rangle h(\beta,\beta') . \tag{A6}$$

It is easy to calculate now the new GCM kernels for the intrinsic motion only, since we have all the expressions we need. Thus

$$\langle\phi(\beta)|\phi(\beta')\rangle = \left[\frac{2\beta\beta'}{\beta^2+\beta'^2}\right]^{9/2}$$

and

$$\langle\phi(\beta)|H_{\text{int}}|\phi(\beta')\rangle = \langle\phi(\beta)|\phi(\beta')\rangle \times \left[h(\beta,\beta') - \frac{3h^2}{2mA}\frac{4}{\beta^2+\beta'^2}\right] .$$

If we go to a new generator coordinate as before, $\beta = \beta_0 e^x$, we get finally

$$\langle \phi(x) | H_{\text{int}} | \phi(x') \rangle = \text{sech}^{9/2}(x - x')\tilde{h}(x,x') \ , \tag{A7}$$

where $\tilde{h}(x,x')$ is precisely the expression we have used in (4.8).

With this new generating function, the GCM energy kernel has the same structure as before, but here only the intrinsic contribution is taken into account. Furthermore, the new GCM overlap kernel corresponds to a system with one particle less than the original one; this gives a new value of $T\ (=\frac{9}{2})$, thus reflecting a larger width of this overlap with respect to the initial one. It is this feature of the new description that accounts for the redefinition of the collective parameters appearing in the collective Hamiltonian of the problem.

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