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THE KINEMATICS OF GENERATOR COORDINATES

by

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Abstract

The Generator Coordinate approach is used to construct a collective subspace of the full many-body Hilbert Space. The construction has a purely kinematical character, given the a priori (e.g., phenomenological) specification of a set of generator many-body states. It is based on the analysis of the properties of the overlaps of the generator states and on the use of the standard spaces of square integrable functions of quantum mechanics. Some well known misbehaviours of the Generator Coordinate weight functions are clearly identified as of kinematical origin. A standard representation in the collective phase space is introduced which eliminates them. It is also indicated how appropriate collective dynamical variables can be defined a posteriori. Hilbert-Schmidt overlap kernels and the Gaussian Overlap Approximation are treated as special examples.

I. Introduction

The study of collective phenomena in quantum many - body systems must deal, from the very start, with the difficult question of the choice of the relevant degrees of freedom. The study of a certain class of collective effects can in fact be contemplated in terms of the study of the many-body problem restricted to some "collective subspace" of the full many-body phase space. This subspace carries a limited number of dynamical variables of a collective nature.

In lukyier cases, such as when one is able to use self-consistent theories like the time dependent Hartree-Fock theory or some of its specializations like the Random Phase Approximation[1] the appropriate collective degrees of freedom are chosen by the (approximate) dynamical scheme itself. The dynamical specification of the relevant correlations for large amplitude, slow, collective nuclear modes characterizes also a self-consistent theory recently developed by Villars[2].

In most cases one has to rely on phenomenology for the choice of a collective phase space. The adequacy of some choice of collective phase space, however, is always basically a dynamical question, and, as such, it cannot be settled whithout explicit reference to the many-body Hamiltonian. In order that the restricted collective dynamics may be physically meaningful, one must have things so that the "collective subspace" is fairly closed with respect to the full many-body dynamics. The range of applicability of the fully dynamical approximations for the treatment of collective motion, such as the above mentioned ones, are of course also ultimately bound by this general criterion.

A general strategy for the phenomenological construction of a collective phase space was laid long ago by Hill, Wheeler and Griffin[3]. In the so called Generator Coordinate Method (GCM) there is a clear separation of two stages in the setting up of a scheme for collective motion.

The first stage involves the selection of a collective phase space, with no necessary reference to any particular collective dynamical variables. This proceeds on purely heuristic grounds. Consequentely, there is no built in guarantee that it be physically meaningful, as there are no built in devices to check its stability with respect to the full many-body dynamics. In order to offset this deficiency, physical criteria can be strongly emphasised through a considerable flexibility that one has in the selection of the collective phase-space.

The second stage consists of the establishment of a dynamical structure within the heuristically generated collective phase space. This is acomplished through the restriction of the many-body dynamics to the collective phase space, in terms of a physically motivated kinematics, which often leads one to consider mathematically awkward objects[4,5,7].

The point of view that the GCM can be used to set up a complete quantum mechanical scheme in some suitable collective phase space was explored explicitely by Brink and Weiguny in 1968[4] for the special case of the so called Gaussian Overlap Approximation[3]. It was latter suggested by C.W.Wong[5] that the GCM can be, in general, identified with the restriction of the many-body quantum mechanics to a subspace of the many-body Hilbert space through the consideration of biorthogonal representations. These considerations were

elaborated latter by Lathouwers[8], who recently gave also an approach based on a representation involving eigenfunctions of the suitably trimmed overlap kernel[7].

The implementation of these points of view involves, however, the explicit or implicit consideration of highly singular objects as representatives of rather ordinary many-body state vectors, if only to give some substance to the idea of a subspace selected from the many body Hilbert space[7].

This is due ultimately to undesirable mathematical properties of the physically motivated representations adopted in the GCM. In a qualitative way, the singularities appear as a result of the attempt to expand certain state vectors in terms of a complete, linearly independent set that includes vectors having arbitrarily small norm[9]. In this sense, these are purely kinematical singularities, that can be eliminated by an appropriate renormalization of the basis, without any recourse to dynamical arguments and working in terms of the usual square integrable functions of quantum mechanics.

In this paper we extend and improve the results of ref. [9], where the above program was carried through under suitable restrictive assumptions. We discuss, within a kinematical context, how the mathematical awkwardness of the GCM representations can be systematically avoided by working in terms of an appropriate, collective representation. This representation will, in particular, contain no kinematically generated misbehaviors, and leads to the definition of collective dynamical variables appropriate to the heuristically selected phase-space.

We begin by reviewing, in section II, the basic ingredients involved in the construction of the GCM phase space. Special care is taken in distinguishing between those ingredients having direct consequences on the nature of the resulting phase space and those having just an instumental character such as the labeling of the generator states. In section III we discuss in detail the shortcomings of the GCM phase spaces and establish a scheme in order to overcome then. The discussion is based on the properties of the overlap kernel constructed from the labeled generator states. We give next, in section IV, a discussion of the collective dynamics which results when we apply the ideas of section III to the removal of kinematic pathologies from the Griffin, Hill, Wheeler (GHW) equation, and consider some special cases and examples in section V. Finally some concluding remarks are given in section VI.

II - The many-body phase-space of the GCM

The method of Generator Coordinates is based on the consideration of many-body states that can be constructed as general linear superpositions of a pre-selected family of suitably parametrized many-body state vectors $|\alpha\rangle$. This is done by writing the general Generator Coordinate ansatz as

$$|f\rangle = \int |\alpha\rangle f(\alpha)\, d\alpha \, . \qquad \text{(II.1)}$$

We give in this section a systematized version of this construction with special emphasis on those aspects that are particularly relevant for the discussion of the following

sections. With this purpose in mind, it is convenient to distinguish three main ingredients involved in the setting up of eq. (II.1), namely, the selection of many-body states, the particular parametrization adopted for them (i.e; the adopted correspondence between states and labels α) and the class of functions $f(\alpha)$ that can be meaningfully admited.

The selection of many-body states is made essentially on the basis of physical arguments relating to the particular problem under consideration. This is certainly the most informal but nevertheless the most critical step in the whole method[3], as it will determine in a decisive way the "working space" selected for the purpose of truncating the full many-body problem. For the purpose of the following discussion we will simply assume that a suitable, in general non discrete family $\mathfrak{J}$ of normalized many-body states has been selected for its physical relevance. These states are called the generator states and will be generally denoted by ket symbols, $|\;\rangle$. It is often convenient to express the generator states in terms of a specific representation of the many-body Hilbert space $\mathcal{H}$. In this case, one speaks of generator functions $\langle\xi|\;\rangle$ where ξ denotes the particular representation which is adopted.

The generator states (or the generator functions) are handled by means of a parametrization, which puts them in a one-to-one correspondence with the points α of a label space denoted as $\mathbb{E}$. The choice of $\mathbb{E}$ and the establishment of a specific labeling strategy is clearly a matter of convenience and is in no way dependent on the specification of any collective variables for the problem at hand. The "collective" character itself eventually stems solely from the particular nature of the selected generator states. Actually we will be able to define dynamical variables to suit the chosen family of generator states on the basis of an "a posteriori " analysis of the characteristics of this family.

For definiteness, we will mostly refer to the standard case of one continuous, real generator coordinate as a prototype. The extention to the case of n real continuous generator coordinates involves nothing but an extention of the notation, and other situations can also be easily formulated as extentions of this case. Here $\mathbb{E}$ is some suitable (and possibly infinite) real interval and $\mathfrak{F}$, accordinggly, is a continuous family of states. We understand this in the sense that, for each vector $|\,\rangle$ of $\mathfrak{F}$, one can always find another vector $|'\rangle$, also of $\mathfrak{F}$, such that

$$\| \,|\,\rangle - |'\rangle \| < \varepsilon$$

for any given positive ε . As we shall see it is convenient that the labeling of the generator states be "adapted" to the continuity of $\mathfrak{F}$ in the sense that, if $\{\alpha_n\}$, is a sequence of labels converging to α in $\mathbb{E}$, then

$$\langle\alpha'|\left[|\alpha_n\rangle - |\alpha\rangle\right] \longrightarrow 0 \qquad \text{(II.2)}$$

for any $|\alpha'\rangle$ in $\mathfrak{F}$ (i.e , the sequence $\{|\alpha_n\rangle\}$ is weakly convergent to $|\alpha\rangle$ in $\mathfrak{F}$)[6]. These conditions are in fact sufficient to interpret eq. (II.1) as a Riemann integral for the special class of infinitely differentiable weight functions $f(\alpha)$ with compact support in $\mathbb{E}$. We can write

the Riemann sum corresponding to a given partition of the support of $f(\alpha)$

$$|f_N\rangle = \sum_{i=1}^{N} |\alpha_i\rangle f(\alpha_i)(\alpha_i - \alpha_{i-1})$$

and easily show that refinements of the partition such that $\max(\alpha_i - \alpha_{i-1}) \rightarrow 0$ as $N \rightarrow \infty$ generate a Cauchy sequence of many-body vectors in $\mathfrak{H}$, $\{|f_N\rangle\}$ (see Appendix 1). The vector $|f\rangle$ defined by eq. (II.1) is in this case the limit, in $\mathfrak{H}$, of this sequence.

This now gives us enough grounds to tackle the third ingredient for eq. (II.1), namely the class of allowable weight functions $f(\alpha)$. We would like to identify this class with the entire Hilbert space of square integrable functions on $\mathbb{E}$, $L^2(\mathbb{E})$. The preceding argument shows that smooth functions of compact support in $\mathbb{E}$, which are dense in $L^2(\mathbb{E})$, belong to it. We can thus describe the GHW ansatz (II.1) as a linear transform from $L^2(\mathbb{E})$ to the many-body Hilbert space $\mathfrak{H}$, which is defined in a dense subset of $L^2(\mathbb{E})$, and in order to be able to extend it uniquely to the full space, we have to require that it be a bounded tranform[10]. This will make it also a continuous transform, so that the extention of eq. (II.1) to an arbitrary function $f(\alpha)$ of $L^2(\mathbb{E})$ can be defined in terms of a sequence of smooth functions of compact support, $\{f_n(\alpha)\}$, converging to $f(\alpha)$, as

$$|f\rangle = \lim_{n\to\infty} \int |\alpha\rangle f_n(\alpha)\,d\alpha \equiv \int |\alpha\rangle f(\alpha)\,d\alpha \qquad \text{(II.3)}$$

The inner product (in $\mathcal{H}$) of two such many-body state vectors is then

$$\langle f_1 | f_2 \rangle = \int d\alpha' \int d\alpha\, f_1^*(\alpha') \langle \alpha' | \alpha \rangle f_2(\alpha) . \qquad \text{(II.3a)}$$

This equation shows that metric properties of the many-body vectors generated by the GHW ansatz are translated to the language of weight functions by means of the two-point function on $\mathbb{E}$

$$N(\alpha', \alpha) = \langle \alpha' | \alpha \rangle . \qquad \text{(II.4)}$$

Also, the right hand side of eq. (II.3a) defines a continouous linear functional on $L^2(\mathbb{E})$. It follows therefore from the Riesz lemma that there is a unique function $g_2(\alpha)$ of $L^2(\mathbb{E})$ such that

$$\int d\alpha' \int d\alpha\, f_1^*(\alpha') N(\alpha', \alpha) f_2(\alpha) = \int d\alpha'\, f_1^*(\alpha') g_2(\alpha')$$

for all $f_1(\alpha')$. This applies of course to any function $f_2(\alpha)$, so that

$$g(\alpha') = \int d\alpha\, N(\alpha', \alpha) f(\alpha) = (\hat{N} f)(\alpha') \qquad \text{(II.5)}$$

characterizes a bounded linear operator $\hat{N}$ in $L^2(\mathbb{E})$. It follows moreover from the properties of the inner product involved in eq. (II.4) that $\hat{N}$ is also a hermitean (and hence self-adjoint), positive operator.

Conversely, if $\hat{N}$, defined by eq. (II.5), is a

bounded, self-adjoint operator in $L^2(\mathbb{E})$, the GHW ansatz, eq. (II.1), can be extended via eqs. (II.3a) and (II.3) to the full space $L^2(\mathbb{E})$. However, the boundedness of $\hat{N}$ is not guaranteed "a priori" for any set of labeled generator states, and we are thus left with the question whether it can be achieved. We note, in this connection, that the kernel (II.4) depends in an essential way on the particular labeling procedure adopted for the generator states. A change of labels that preserves the continuity condition (II.2) is induced by a continuous monotonic function $\beta = m(\alpha)$, from $\mathbb{E}$ to the alternate label space $\tilde{\mathbb{E}} = m(\mathbb{E})$, having an inverse $\alpha = m^{-1}(\beta)$ with α in $\mathbb{E}$ and β in $\tilde{\mathbb{E}}$. We may also without loss of generality assume that

$$\frac{dm(\alpha)}{d\alpha} > 0 , \qquad \text{all } \alpha \text{ in } \mathbb{E} .$$

We can then consider the relabeling

$$|\alpha\rangle \longrightarrow |\widetilde{m(\alpha)}\rangle = |\tilde{\beta}\rangle$$

where the tilde indicates that the same vectors are identified by the new labels, and construct the corresponding overlap kernel

$$\tilde{N}(\beta', \beta) = \langle \tilde{\beta}' | \tilde{\beta} \rangle = N\left(m^{-1}(\beta'), m^{-1}(\beta)\right)$$

which occurs if we use the general ansatz (II.1) in terms of the new labels, i.e.

$$|\tilde{f}\rangle = \int_{\tilde{\mathbb{E}}} d\beta\, |\tilde{\beta}\rangle \tilde{f}(\beta) \qquad \text{(II.6)}$$

It should be stressed that the passage from eq. (II.1) to eq. (II.6) differs from a mere change of dummy variables (for $\tilde{f}(\beta) = f(m^{-1}(\beta))$) by a change in integration measure, the new label β being directly taken as the integration variable in (II.6). Corresponding to eq.(II.3a) we get now

$$\langle \tilde{f}_1 | \tilde{f}_2 \rangle = \int d\beta' \int d\beta \, \tilde{f}_1^*(\beta') \tilde{N}(\beta',\beta) \tilde{f}_2(\beta) < \infty$$

which, now changing variables to the original labels α, becomes

$$\langle \tilde{f}_1 | \tilde{f}_2 \rangle = \int d\alpha' \int d\alpha \left(\tilde{f}_1^*(m(\alpha')) \sqrt{\frac{dm(\alpha')}{d\alpha'}} \right) \left[\sqrt{\frac{dm(\alpha')}{d\alpha'}} N(\alpha',\alpha) \sqrt{\frac{dm(\alpha)}{d\alpha}} \right] \left(f_2(m(\alpha)) \sqrt{\frac{dm(\alpha)}{d\alpha}} \right). \tag{II.7}$$

When the $\tilde{f}_i(\beta)$ are in $L^2(m(\mathbb{E}))$, the first and last brackets of (II.7) are in $L^2(\mathbb{E})$. This equation thus shows that the boundedness of $\tilde{N}(\beta',\beta)$ in $L^2(m(\mathbb{E}))$ is equivalent to the boundedness in the original $L^2(\mathbb{E})$ of the modified operator

$$N_m(\alpha',\alpha) = \sqrt{\frac{dm(\alpha')}{d\alpha'}} \, N(\alpha',\alpha) \sqrt{\frac{dm(\alpha)}{d\alpha}} \, . \tag{II.8}$$

Furthermore, it can be easily seen that some function $m(\alpha)$ can always be found that makes (II.8) a bounded operator. In fact, we have

$$\int d\alpha' \int d\alpha \, | N_m(\alpha',\alpha)|^2 = \int_{\tilde{\mathbb{E}}} d\beta' \int_{\tilde{\mathbb{E}}} d\beta \, | \tilde{N}(\beta',\beta)|^2$$

and, from the assumed normalization of the generator states,

$$| \tilde{N}(\beta',\beta)|^2 \leq 1 \, .$$

Therefore, choosing the new label space $\tilde{\mathbb{E}}$ to have a finite measure we guarantee that $\tilde{N}(\beta',\beta)$ is a kernel of the Hilbert-Schmidt type (actually, it is trace class) in $L^2(\tilde{\mathbb{E}})$.

As a result of this discusion we see that, by means of proper choice of labels, we can make the overlap kernel of the GCM a Hilbert-Schmidt kernel in a Hilbert space of square integrable weight functions. A complete treatment of this type of kernel has been given in ref. [9]. We will also show in section III (see also Appendix 2) that there is no loss of generality in restricting the labeling strategy, as the collective subspace to be constructed from a given set of generator states is stable against acceptable (in the sense discussed above) changes of labels. This actually makes the discussion of ref. [9] completely general. In pratice, however, it may be both natural and, above all, convenient to consider overlap kernels which, although bounded, are not of Hilbert-Schmidt type. Some illustrative examples of this can be found in section V. We will thus make only the weaker assumption of having bounded overlap kernels in the formal development of sections III and IV.

We will show in the following sections that the mathematical difficulties of the GCM stem from the fact that, in general, the mapping from $L^2(\mathbb{E})$ to $\mathcal{H}$ given by the GHW ansatz (II.1) does not have a bounded inverse. An immediate problem is, of course, the null space of $\hat{N}$, which altogether excludes the existence of the inverse mapping. Functions in the null space of $\hat{N}$ are, however, associated with the null vector of $\mathcal{H}$ (as can be seen from eq. (II.3a)), and express relations of linear dependence among the generator states. There is no loss of generality, therefore, involved in projecting out the null space of $\hat{N}$ when using eq. (II.1), so that an inverse mapping can actually be defined. The fact that it will not in general be a bounded operator means that Cauchy sequences of vectors $|f\rangle$ defined through eq. (II.1) can be associated with non-convergent sequences of functions $f(\alpha)$. This implies then that the set of many-body state vectors generated by means the GHW ansatz will not be complete, in general. We will refer to this set as the GHW phase space[9].

Our approach to deal with this situation will consist in trying to define an alternate mapping, from the GHW space to a L^2 space, which is isometric. This can then be extended uniquely to a closed subspace of the many-body Hilbert space, which can serve as a collective phase space.

III - Straightening up the Kinematics

In the preceding section we showed that, by a proper labeling of the generator states, the basic GHW ansatz, eq. (II.1), can be defined for the class of square integrable functions on the label space $\mathbb{E}$. We showed, at the same time, that the overlap kernel $N(\alpha',\alpha)$, eq. (II.4), can be generally assumed to define a bounded positive (and hence self-adjoint) operator on this weight function space. Here we proceed to construct a complete subspace of the many-body Hilbert space on the basis of these properties. This subspace is actually the completion of the GHW phase space introduced above and forms the proper kinematical substrate for the establishment of a dynamical scheme based on the chosen family of generator states.

The basic tool for this construction the "diagonalization" of the overlap operator $\hat{N}$. This can be done, in an

abstract form, using the spectral theorem of functional calculus (See Appendrix 2). The argument can also be cast in the perhaps more familiar language of Dirac bra and ket vectors, which we adopt, for convenience, in this section.

We begin, therefore, by considering a space of ket vectors, written with rounded brackets, $|\,)$, which are associated to the elements of the function space $L^2(\mathbb{E})$ by means of a suitable representation α defined by

$$1 = \int |\alpha)\,d\alpha\,(\alpha| \qquad , \qquad (\alpha|\alpha') = \delta(\alpha-\alpha')$$

as

$$f(\alpha) = (\alpha|f).$$

The overlap function, eq. (II.4), corresponds thus to a bounded, self-adjoint operator $\hat{N}$ in this space, for which we consider the eigenvalue problem

$$\hat{N}\,|k) = \Lambda(k)\,|k) \tag{III.1}$$

In case $\hat{N}$ has a continuous spectrum, the kets $|k)$ are improper eigenvectors which we assume to be normalized as

$$(k|k') = \delta(k-k').$$

We also assume completeness of the set of eigenvectors of $\hat{N}$ in the sense that a resolution of unity exists in the form

$$\int |k)\,d\mu(k)\,(k| = 1.$$

The measure $\mu(k)$ will include in general a discrete part corresponding to the discrete spectrum of $\hat{N}$, in addition to a continuous part (usually a Lebesgue measure) when there is also a continuous spectrum.

The existence of such a resolution of unity amounts to the fact, supported by the content of the spectral theorem, that the brackets $(k|\alpha)$ carry a unitary transformation of the function space $L^2(\mathbb{E})$ which reduces the operator $\hat{N}$ to diagonal (or to multiplication operator) form. Thus, corresponding to each function $f(\alpha)$ we can consider

$$\varphi(k) = \int (k|\alpha) f(\alpha) d\alpha = \int (k|\alpha)(\alpha|f) d\alpha = (k|f) . \quad \text{(III.2)}$$

which is, from this point of view, just another representation of the ket $|f)$. The overlap of two GHW state vectors, eq. (II.3a), can also be cast in the form

$$\langle f_1 | \cdot f_2 \rangle = \int d\mu(k)(f_1|k)\Lambda(k)(k|f_2) = (f_1|\hat{N}|f_2) \quad \text{(III.3)}$$

in which use was made of the relation

$$(k|\hat{N}|k') = \Lambda(k)\, \delta(k-k')$$

which follows directly from eq. (III.1).

III.1 - Removal of the null space of $\hat{N}$

The first point to be made in connection with eq. (III.3) is that kets $|f_0)$ lying in the null space of $\hat{N}$, i.e., satisfying

$$(k|\hat{N}|f_0) = \Lambda(k)(k|f_0) = 0 \quad \text{(III.4)}$$

for all k, give rise, by means of the GHW ansatz, eq. (II.1), to many-body vectors of zero norm. They correspond thus to relations of linear dependence among the generator states which allow us to associate many different weight functions to the same GHW state vector. This undesirable feature can however be easily removed by considering the projection operator

$$\chi_{\hat{N}} = \int d\mu(k)\, |k)\, \chi_\Lambda(k) (k| \quad \text{(III.5)}$$

where the function $\chi_\Lambda(k)$ is defined as

$$\chi_\Lambda(k) \doteq \begin{cases} 0 & \text{if } \Lambda(k) = 0 \\ 1 & \text{if } \Lambda(k) \neq 0 \end{cases} \quad \text{(III.6)}$$

and allowing only for kets $|f)$ lying in the subspace associated with it. In other words, this amounts to the exclusion, from any weight function $f(\alpha)$, of components $f_0(\alpha)$ in the null space of the overlap kernel $N(\alpha',\alpha)$. In fact

$$\int (k|\chi_{\hat{N}}|\alpha') f_0(\alpha') d\alpha' = \int d\mu(k)(\alpha|k)\chi_\Lambda(k)(k|f_0) = 0$$

in view of eqs. (III.4) and (III.6). The subspace of $L^2(\mathbb{E})$ associated with the projection operator $\chi_{\hat{N}}$ will be refered to as the weight function space $\mathcal{L}_f$.

III.2 - The "collective" many-body subspace

We proceed now to the construction of the complete subspace of the many-body Hilbert space $\mathfrak{H}$ which naturally extends the GHW phase-space. For this purpose we note first that, if $|f\rangle$ is in the GHW phase-space, i.e., if it is of the form

$$|f\rangle = \int d\alpha\, |\alpha\rangle (\alpha|f)$$

with $(\alpha|f)$ in the weight-function space $\mathcal{L}_f$ (note that the null space of $\hat{N}$ has been projected out), then

$$\langle\alpha|f\rangle = (\alpha|\hat{N}|f)$$

which is also in $\mathcal{L}_f$. We can then use this fact to define the ket $|\bar{f})$ (or the function $\varphi_{\bar{f}}(k) = (k|\bar{f})$) by

$$\Lambda^{1/2}(k)(k|\bar{f}) = \int d\alpha\,(k|\alpha)\langle\alpha|f\rangle = \Lambda(k)\,\varphi(k) \qquad \text{(III.7)}$$

A straightforward calculation shows now that

$$(\bar{f}|\bar{f}) = \langle f|f\rangle$$

i.e. the mapping v which associates to each GHW state vector $|f\rangle$ the ket $|\bar{f})$ (or the function $\varphi_{\bar{f}}(k)$)

$$|\bar{f}) = v|f\rangle \qquad \text{(III.8)}$$

is isometric. It can be written formally as

$$v = \int d\mu(k) \int d\alpha\; \frac{|k)(k|\alpha)\,\langle\alpha|}{\Lambda^{1/2}(k)} \qquad \text{(III.9)}$$

and depends explicitely on the overlap properties of the generator states through $\Lambda(k)$. Note that this expression is meant in the sense that $v|f\rangle$ is calculated by writing $\langle\alpha|f\rangle$ in the integrand for the integral over α .

The isometric mapping v has been defined, in eq.(III.7), for all vectors $|f\rangle$ of the GHW phase-space. We can now show that the image, in $\mathcal{L}_f$, of this phase-space is dense, although in general not complete. This will allow us to uniquely extend v to the completion of the GHW phase-space, and to use $\mathcal{L}_f$ as a convenient representation of the complete phase-space. But the proof is also instructive in that it reveals in a clear way the relationship between weight functions and many-body vectors in terms of the properties of the overlap operator $\hat{N}$.

Our aim is therefore to show that we are able to approximate any function

$$\varphi(k) = (k|f)$$

such that

$$\chi_{\hat{N}}|f) = |f)$$

by a Cauchy sequence of functions $\varphi_n(k)$ that are v-images of GHW state-vectors. For this purpose, let

$$\varphi_n(k) = \begin{cases} \varphi(k) & \text{if } \Lambda(k) > \frac{1}{n} \\ 0 & \text{if } \Lambda(k) < \frac{1}{n} \end{cases}$$

The explicit removal of the null space of $\hat{N}$ now guarantees that

$$\lim_{n\to\infty} \|\varphi_n - \varphi\| = 0 \qquad \text{(III.10)}$$

since $\Lambda(k)$ is almost everwhere different from zero in the weight function space. On the other hand, the $\varphi_n(k)$ allow us to set up the weight functions

$$(\alpha|f_n) = \int d\mu(k)\, \frac{(\alpha|k)}{\Lambda^{1/2}(k)}\, \varphi_n(k)\,. \qquad \text{(III.11)}$$

If $|f_n\rangle$ denotes the GHW state vector generated from the weight function $(\alpha|f_n)$, it is easy to check that

$$\varphi_n(k) = (k|v|f_n\rangle$$

which proves the desired result.

We are therefore allowed to consider the unique extention V of the isometric mapping v from the many-body Hilbert space $\mathcal{H}$ to the entire closed space $\mathcal{L}_f$. V is a partial isometry, the initial space of which we call the "collective" many-body subspace. It is the subspace of $\mathcal{H}$ associated with the projection operator

$$\mathcal{P} = V^+ V. \tag{III.12}$$

The fact that the final space of V is the entire $\mathcal{L}_f$ can, on the other hand, be expressed by

$$\chi_{\hat{N}} = V V^+ .$$

The relationship between vectors in the collective subspace and weight functions can also be established from eq. (III.11). We see there that going from vectors in the collective subspace (or from the corresponding functions $\varphi(k)$) to the appropriate weight functions for the GHW ansatz, eq. (II.1), involves the use of the operator $\hat{N}^{-1/2}$ (or $\Lambda^{-1/2}(k)$). This is, in general, an unbounded operator in $\mathcal{L}_f$. Its natural domain is the V-image of the GHW phase-space. It was shown to be dense in $\mathcal{L}_f$ and, correspondingly, the GHW phase-space is dense in the collective subspace. We are thus able to approximate arbitrary vectors in the collective subspace by sequences of GHW state vectors, but the corresponding sequences of weight functions will not, in general, converge.

An additional point to be made concerns the role played by the specific labeling adopted for the generator states in the resulting collective subspace projector $\mathcal{P}$. We are able to show (see Appendix 3) that, provided the general conditions regarding the bounded character of the overlap operator are met, the collective subspace is actually independent of the particular labelling procedure.

Formaly, we show that, from the fact that

$$P|c\rangle = |c\rangle$$

it follows also that

$$P'|c\rangle = |c\rangle$$

where P' is the collective subspace projector obtained by following the construction of P with modified labels. The generator states themselves are of course contained in the collective phase space, even if they do not have square integrable weight functions, in general. Their collective wave-functions, on the other hand, are given as

$$(k|V|\alpha\rangle = \Lambda^{1/2}(k)(k|\alpha) .$$

They are normalized to one for every α . These facts are consistent with the intuitive "intrinsic" description of the collective subspace as the smallest subspace of the many-body Hilbert space that contains the generator states as a subset.

IV - Quantum Mechanics in the Collective Subspace

We have shown in the preceding section that a set of generator states can be associated with a projection operator P which selects a subspace of the many-body Hilbert space $\mathcal{H}$.

This subspace constitutes the completion of the set of many-body state vectors that can be written in terms of the generator states by using the GHW ansatz with square integrable weight functions. The operator P allows us then to project the many-body dynamics, contained in the many-body, time dependent Schrodinger equation, onto the collective subspace. This means that we consider the restricted problem

$$PHP|\Psi\rangle = i\hbar\frac{\partial|\Psi\rangle}{\partial t} \qquad \text{(IV.1)}$$

with $P|\Psi\rangle = |\Psi\rangle$. This is now a conventional quantum mechanical problem. The spectrum of the restricted hamiltonian, PHP, may include, in general, both a discrete part and a continuum, which correspond to bound states and to scattering states respectively. The latter, as is usual, do not properly belong to the collective subspace as they do not have a finite norm. Scattering situations can however be treated in terms of vectors of finite norm e.g. by using wave-packets in a time-dependent description.

The form eq. (III.12) of the projection P, on the other hand, allows us to use the isomorphism of $\mathcal{L}_f$ and the collective subspace and consider a representation of eq. (IV.1) in terms of the function space $\mathcal{L}_f$. The corresponding dynamical equation now reads

$$\int d\mu(k')\,(k|VHV^{+}|k')\,\varphi(k',t) = i\hbar\frac{\partial\varphi(k,t)}{\partial t} . \qquad \text{(IV.2)}$$

It is also easy to write the formal expression for the restricted hamiltonian in this representation with the help of eq. (III.9):

$$(k|VHV^{+}|k') = \int d\alpha \int d\alpha' \, \frac{(k|\alpha)}{\Lambda^{1/2}(k)} \langle\alpha|H|\alpha'\rangle \frac{(\alpha'|k')}{\Lambda^{1/2}(k')} \qquad \text{(IV.3)}$$

If eq.(IV.2) is formally reexpressed in terms of GHW weight-functions, related to the collective wave functions φ by means of eq. (III.11), we obtain the familiar form of the (time-dependent) GHW equation.

The collective hamiltonian written as in eq.(IV.3) has been frequently used in the literature, chiefly in connection with the numerical treatment of the GCM. It involves three possibly unbounded ingredients, namely the two $\Lambda^{-1/2}$ factors and the GHW energy kernel $\langle\alpha|H|\alpha'\rangle$. The unbounded character of the former, however, stems from purely kinematical sources, while that of the energy kernel is related to the dynamics of the many-body problem. The kinematical divergences are related to the properties of the generator states, and are in fact cancelled by the behavior of the energy kernel in actual evaluations of eq. (IV.3). This is shown expicitely for the examples treated in the following section. When going from eq. (IV.2) to the GHW equation, however, one considers weight functions which are formal $\Lambda^{1/2}$ transforms of the collective wave functions φ . Unlike the energy kernel, the latter are however not smoothed by dependence on the generator states and this predisposes weight functions to "violent behavior".

The above discussion was carried through in the specific representation of the collective subspace in which the overlap operator is represented as a multiplication operator. This is, of course, convenient for sorting out any kinematical oddities inherent to the generator coordinate representation, but other representations may be preferable or more convenient from a physical point of view. We therefore conclude this section with some comments on this point.

The representation used in eq.(IV.2) can be characterized in terms of the operator $\mathscr{k}$ defined in $\mathcal{L}_f$ as

$$(\kappa|\mathscr{k}|\alpha) = \kappa(\kappa|\alpha) . \qquad \text{(IV.4)}$$

Note that the bracket $(\kappa|\alpha)$ stands for the unitary transformation of the original weight function space that diagonalizes the overlap kernel. The point in defining this operator is that it can be translated to the many-body language by means of the isometry V:

$$K = V^{+}\mathscr{k}V = \int d\kappa \int d\alpha \int d\alpha' \, |\alpha\rangle(\alpha|\kappa)\frac{\kappa}{\Lambda(\kappa)}(\kappa|\alpha')\langle\alpha'| .$$

K is thus a "natural" collective variable associated with the representation κ , given as an operator in the many-body Hilbert space $\mathcal{H}$. It is clear moreover that a transformation theory can be established in the collective subspace based on unitary transformations of the collective wavefunction space $\mathcal{L}_f$.

We may also give an "a posteriori" formal criterion for the adequacy of the collective subspace constructed from a given set of generator states, along the lines discussed in the Introduction. In fact, the condition for the collective space to be dynamically invariant can be simply expressed as

$$[P, H] = 0 .$$

It is perhaps worth noting that this condition allows in general for the breaking of symmetries of H under projection onto the

collective subspace. In order to guarantee further that a set of symmetries of H, $\{S_i\}$, is preserved in the reduced collective problem we have to ensure further that

$$[P, S_i] = 0$$

i.e., that the projection be well adapted to the cleavage of the many-body Hilbert space determined by the symmetry operators.

V - Special cases and examples

In this section we show that the scheme developed in the preceding sections can be actualy implemented in cases of physical interest. We begin by reviewing the results already given in ref. [9] with some appropriate changes in language and emphasis. We then go on to the treatment of the standard Gaussian Overlap Approximation[3], which involves an overlap kernel which is not of Hilbert-Schmidt type and that may be shown to have a purely continuous spectrum. We discuss this case in terms of improper eigenfunctions and also in terms of a relabeling of the generator states that effectively reduces the overlap kernel to one of the Hilbert-Schmidt type. A comparison of the two approaches exhibits the invariance of the collective phase space explicity. The same comparison also illustrates the possible gains, in terms of simplicity, of working directly in terms of the continuous representation.

V.1 - Hilbert-Schmidt overlap kernels

The general tratment of the preceding sections finds a particularly simple realization when the overlap kernel is of the Hilbert-Schmidt type in $L^2(\mathbb{E})$. Although a discussion of this case was given earlier [9], we repeat its essential points here in a somewhat modified form which is better suited for the purpose of illustration of the general procedure. It is also worth stressing that, in view of the reducibility of any given case to the present one by a suitable change of labels, and of the independence of the constructed collective subspace of the adopted labeling procedure, this discussion is actually of general validity.

The major simplifying factor for the treatment of overlap kernels of the Hilbert-Schmidt type is the content of the Hilbert-Schmidt theorem[10]. It can be expressed by saying that in this case the unitary mapping $(k|\alpha)$ can be implemented in terms of a complete, orthonormal set of eigenfunctions $u_i(\alpha)$, i.e.

$$\int N(\alpha,\alpha')\, u_i(\alpha')\, d\alpha' = \lambda_i u_i(\alpha) \qquad (V.1)$$

with

$$\int u_i^*(\alpha)\, u_j(\alpha)\, d\alpha = \delta_{ij} \; .$$

The spectrum is discrete, and the only possible limit point is at $\lambda=0$. The label i of $u_i(\alpha)$ plays the role of the new variable k. The complete set of eigenfunctions $u_i(\alpha)$ can in fact be used to define a unitary mapping of $L^2(\mathbb{E})$ onto the space of square summable complex number sequences $\ell^2(\mathbb{Z})$. This mapping is given by

$$f(\alpha) \longrightarrow \{f_i\} \; ; \quad f_i = \int d\alpha\, u_i^*(\alpha) f(\alpha) \qquad (V.2)$$

i.e., the sequence $\{f_i\}$ is the set of components of the function f in the orthonormal set $\{u_i\}$.

The projector $\chi_{\hat{N}}$ that eliminates the null space of the overlap kernel can be immediarely written as

$$\chi_{\hat{N}} = \sum_{\substack{i \\ \lambda_i \neq 0}}{}' u_i(\alpha)\, u_i^*(\alpha') \qquad (V.3)$$

The restriction of N to the subspace associated with $\chi_{\hat{N}}$ does not have a null space, even though it may still have arbitrarily small eigenvalues.

It is also easy to identify the isometric mapping defined by eqs. (III.7) and (III.8) in this case. Eq.(III.7) can be cast as

$$\bar{f}_i = \sqrt{\lambda_i}\, f_i \qquad (V.4)$$

so that the many-body vector generated by $f(\alpha)$ is isometrically associated with the sequence $\{\bar{f}_i\}$. The removal of the null space from $L^2(\mathbb{E})$ ammounts to the exclusion of all components f_i associated with zero eigenvalues. Whenever infinitely many eigenvalues are different from zero, however, we see that not every square-summable sequence $\{\bar{f}_i\}$ can be associated with square-integrable weight functions, on the account of the limit point at $\lambda=0$. They are associated, through the extended mapping V, to many-body vectors that cannot be generated by acceptable weight-functions through the GHW ansatz. These vectors can always be approximated, in the many-body Hilbert space, by sequences of "regular" many-body vectors, in the sense that they have acceptable weight-functions [9].

Since a Hilbert-Schmidt kernel has eigenfunctions belonging to $L^2(\mathbb{E})$, we can in this special case explicitely construct a set of orthonormal many-body vectors via the GHW ansatz as

$$|i\rangle = \frac{1}{\sqrt{\lambda_i}} \int |\alpha\rangle u_i(\alpha)\, d\alpha \,. \qquad \text{(V.5)}$$

These are the "natural states" considered by Lathouwers in Ref. [7].

It is easy to check that

$$\langle i | f \rangle = \bar{f}_i$$

so that the $\bar{f}_i$ are the amplitudes of vectors belonging to the collective space (which can in this case be defined as the subspace generated by the orthonormal set (V .5)) along the vectors $|i\rangle$.

We finaly consider the transcription of eq. (IV.3). We obtain

$$h(i,j) = \int d\alpha \int d\alpha' \; \frac{u_i^*(\alpha)}{\sqrt{\lambda_i}} \langle\alpha| H |\alpha'\rangle \frac{u_j(\alpha')}{\sqrt{\lambda_j}}$$

so that

$$h(i,j) = \langle i | H | j \rangle \qquad \text{(V.6)}$$

i.e., the collective Hamiltonian kernel is just the matrix representation of the many-body Hamiltonian in the orthonormal basis (V.5) of the collective subspace. We see thus that the vanishing of the λ_i actually compensates for the vanishing of the norm of the corresponding GHW integrals with the $u_i(\alpha)$.

V.2 - Translational invariant overlap kernels

A class of overlap kernels for which an explicit form for equation (III.1) can be immediatly found is the class of square integrable functions $N(\alpha-\alpha')$ of label differences only. In fact the unitary transformation U can be taken in this case as a Fourier transform

$$\int dk' \int d\alpha \int d\alpha' \; (k|\alpha) N(\alpha-\alpha') (\alpha'|k') \varphi(k') = \Lambda(k) \varphi(k)$$

where

$$(\alpha|k) = \frac{1}{\sqrt{2\pi}} e^{-ik\alpha}$$

and

$$\Lambda(k) = \int d\alpha \; e^{ik\alpha} N(\alpha) \,.$$

The plane waves $(\alpha|k)$ play in this case the role of improper eigenfunctions of $\hat{N}$. The positivity and boundedness of $\hat{N}$, on the other hand, guarantee that $\Lambda(k)$ is a positive, bounded function of k.

The standard case of the gaussian overlap

$$N(\alpha-\alpha') = e^{-\frac{(\alpha-\alpha')^2}{b^2}}$$

is included in this case. Here we have [11]

$$\Lambda(k) = b\sqrt{\pi}\; e^{-\frac{k^2 b^2}{4}}$$

which shows that the gaussian overlap kernel does not have a null space but its spectrum approaches zero as a limit point as $|k| \rightarrow \infty$.

The fact that gaussian overlaps can be handled in terms of Fourier transforms has been extensively exploited by Giraud, Hocquenghem and Lumbroso [13] who developed a "momentum space" treatment of the GHW equation for scattering problems. Here we just illustrate the use of eq. IV.8 in this case by taking as an example the standard quadratic expansion of the GHW energy kernel [2]

$$\langle\alpha|H|\alpha'\rangle \simeq N(\alpha-\alpha')\left[E_0+\frac{\hbar^2}{2M}\left(\frac{2}{b^2}-\frac{4(\alpha-\alpha')^2}{b^4}\right)+\frac{M\omega^2}{2}\left(\frac{\alpha+\alpha'}{2}\right)^2\right] \quad (V.8)$$

for which it is readily found, by means of a double Fourier transform

$$\int d\alpha\int d\alpha' \;(k|\alpha)\langle\alpha|H|\alpha'\rangle(\alpha'|k') = \Delta^{1/2}(k)\; h(k,k')\; \Delta^{1/2}(k')$$

that

$$h(k,k') = \left[E_0 - \frac{M\omega^2 b^2}{16}+\frac{\hbar^2k^2}{2M}\right]\delta(k-k') - \frac{M\omega^2}{2}\,\delta''(k-k') \quad (V.9)$$

The Schroedinger equation in the collective subspace is identical to

$$\frac{\hbar^2k^2}{2M}\varphi_n(k) - \frac{M\omega^2}{2}\frac{d^2\varphi_n(k)}{dk^2} = \left(E_n+\frac{M\omega^2b^2}{16}\right)\varphi_n(k) \quad (V.10)$$

This is just the momentum space version of a standard harmonic oscillator hamiltonian. Note again the cancellation of all dependence on the overlap kernel by the $\Delta^{-1/2}$ factors. In particular equation (V.10) is independent of the width of the overlap kernel, b, except for a trivial additive constant in the zero point energy.

So the solutions of (V.10) are

$$\varphi_n(k) = \phi_n\left(\sqrt{\frac{\hbar}{M\omega}}\,k\right) \quad (V.11)$$

$$E_n = E_0 - \frac{M\omega^2b^2}{16} + \left(n+\frac{1}{2}\right)\hbar\omega \quad (V.12)$$

where ϕ_n are harmonic oscillator wave functions. The normalized ground state amplitude is given by

$$\varphi_0(k) = \left(\frac{\hbar}{M\omega\pi}\right)^{1/4} e^{-\frac{\hbar}{2M\omega}k^2} \quad (V.13)$$

for any value of the oscillator parameter.

If, on the other hand, we try to reconstruct the GHW weight function which is associated with $\varphi_0(k)$ we find by means of equation (III.7) that

$$f_0(\alpha) = \frac{1}{2\pi}\left(\frac{4\hbar}{M\omega b^2}\right)^{1/4}\int_{-\infty}^{\infty} e^{-ik\alpha}\, e^{-\frac{k^2}{2}\left(\frac{\hbar}{M\omega}-\frac{b^2}{4}\right)}dk \quad (V.14)$$

which exists only as long as $\frac{\hbar}{M\omega} > \frac{b^2}{4}$.

This limitation[4] has the same origin as the "ultraviolet" catastrophe of ref.[13] namely it is a run off situation in an attempt to compensate for the lack of high k components in the family of generator states. We can also check that the many-body state vector which is associated with $\varphi_0(k)$ by means of the operator V (see eq.III.8) can in any case be arbitrarily approximated by state vectors possesing acceptable weight functions. It suffices in fact to consider the sequence of state vectors constructed as in eq. (II.1) with the weight functions

$$f_0^{(N)}(\alpha) = \frac{1}{2\pi}\left(\frac{4\hbar}{M\omega b^2}\right)^{1/4}\int_{-N}^{N} e^{-ik\alpha}\, e^{-\frac{k^2}{2}\left(\frac{\hbar}{M\omega}-\frac{b^2}{4}\right)}dk \quad (V.15)$$

where N is a positive integer.

It can be easily checked that these many-body vectors converge in the norm of the many-body Hilbert-space to the vector associated with the amplitude $\varphi_0(k)$. At the same time if $\frac{\hbar}{M\omega} < \frac{b^2}{4}$ the sequence of functions $f_0^{(N)}$ diverges in the weight function space $\mathcal{L}_f$.

We could also solve the case of the gaussian overlap by using an appropriate ralabelling of the generator states.

In the case of the gaussian overlap we use

$$\beta = \operatorname{erf}\left(\sqrt{r}\,\frac{\alpha}{b}\right) = \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{r}\frac{\alpha}{b}} e^{-t^2}\,dt \qquad \text{(V.16a)}$$

where r is a free parameter.

The new generator states are related to the old ones by the transformation

$$|\tilde{\beta}\rangle = |\,\widetilde{\operatorname{erf}\left(\sqrt{r}\,\tfrac{\alpha}{b}\right)}\rangle = |\alpha\rangle. \qquad \text{(V.16b)}$$

The GHW ansatz now becomes

$$|f\rangle = \int_{-1}^{1} |\tilde{\beta}\rangle\, \tilde{f}(\beta)\, d\beta. \qquad \text{(V.17)}$$

The kernel

$$\tilde{N}(\beta,\beta') = \langle\tilde{\beta}\,|\,\tilde{\beta}'\rangle$$

is a Hilbert-Schmidt kernel since

$$\int_{-1}^{1} d\beta \int_{-1}^{1} d\beta'\, |\tilde{N}(\beta,\beta')|^2 \leq 4$$

which is easily obtained if we use the inequality

$$|\langle\tilde{\beta}\,|\,\tilde{\beta}'\rangle|^2 \leq 1$$

which follows from the fact that the states $|\tilde{\beta}\rangle$ are normalized.

The eigenfunctions of the kernel satisfy the equation

$$\int_{-1}^{1} \tilde{N}(\beta,\beta')\, \tilde{g}_n(\beta')\, d\beta' = \lambda_n\, \tilde{g}_n(\beta) \qquad \text{(V.18)}$$

which by the change of variables (V.16a) reduces to

$$\int_{-\infty}^{\infty} \bar{N}(\alpha,\alpha')\, g_n(\alpha')\, d\alpha' = \lambda_n\, g_n(\alpha) \qquad \text{(V.19)}$$

where

$$\bar{N}(\alpha,\alpha') = \sqrt{\frac{d\beta(\alpha)}{d\alpha}}\, \langle\alpha\,|\,\alpha'\rangle \sqrt{\frac{d\beta(\alpha')}{d\alpha'}} =$$

$$= \frac{2}{\sqrt{\pi}}\, \frac{\sqrt{r}}{b}\, \exp -\frac{1}{4}\left[\frac{r(\alpha+\alpha')^2}{b^2} + \frac{(r+4)(\alpha-\alpha')^2}{b^2}\right] \qquad \text{(V.20)}$$

and

$$g_n(\alpha) = \sqrt{\frac{d\beta(\alpha)}{d\alpha}}\; \tilde{g}_n\left(\operatorname{erf}\left(\sqrt{r}\,\frac{\alpha}{b}\right)\right). \qquad \text{(V.21)}$$

Using a formula given by Mehler[12]

$$\exp -\frac{1}{4}\left[\frac{1-K}{1+K}(\alpha+\alpha')^2 + \frac{1-K}{1+K}(\alpha-\alpha')^2\right] = \sum_{n=0}^{\infty} \left[\pi(1-K^2)\right]^{1/2} K^n \phi_n(\alpha)\, \phi_n(\alpha') \qquad \text{(V.22)}$$

where K is a positive number smaller than one and ϕ_n an oscillator wave function, it can be shown that

$$\tilde{N}(\alpha,\alpha') = \frac{t^{1/2}}{b}\sum_{n=0}^{\infty}\frac{(t-r)^{n+1}}{(t+r)^{n}}\,\phi_n\!\left(t^{1/2}\frac{\alpha}{b}\right)\phi_n\!\left(t^{1/2}\frac{\alpha'}{b}\right) \qquad \text{(V.23)}$$

where t is given by

$$t^2 = r^2 + 4r .$$

Equations (V.19) and (V.23) show that

$$g_n(\alpha) = \left(\frac{t^{1/2}}{b}\right)^{1/2}\phi_n\!\left(t^{1/2}\frac{\alpha}{b}\right) \qquad \text{(V.24)}$$

and

$$\lambda_n = \frac{(t-r)^{n+1}}{(t+r)^{n}} . \qquad \text{(V.25)}$$

The $\tilde{g}_n(\beta)$ is given by equation (V.21).

The diagonalization of the hamiltonian in the collective subspace reduces to

$$\sum_{n,n'} h_{nn'}\varphi_{n'}^{(m)} = E_m \varphi_n^{(m)} \qquad \text{(V.26)}$$

where

$$h_{nn'} = \int_{-1}^{1}d\beta\int_{-1}^{1}d\beta'\,\frac{\tilde{g}_n^*(\beta)}{\sqrt{\lambda_n}}\langle\tilde{\beta}|H|\tilde{\beta}'\rangle\frac{\tilde{g}_{n'}(\beta')}{\sqrt{\lambda_{n'}}} . \qquad \text{(V.27)}$$

Using the quadratic expansion (V.8) it can be shown that

$$h_{nn'} = \varepsilon_0\delta_{nn'} + \frac{1}{2}B\left[\sqrt{(n'+1)(n'+2)}\,\delta_{n,n'+2} + \sqrt{(n'-1)n'}\,\delta_{n,n'-2}\right] + A n\delta_{nn'} \qquad \text{(V.28)}$$

where

$$\varepsilon_0 = E_0 - \frac{M\omega^2 b^2}{16} + \frac{A}{2}$$

$$A = \frac{\hbar\omega}{2}\left(\xi + \frac{1}{\xi}\right) \quad ; \quad B = \frac{\hbar\omega}{2}\left(\xi - \frac{1}{\xi}\right)$$

with

$$\xi = \frac{b^2}{4}\frac{t}{r}\frac{M\omega}{\hbar}$$

This is just the well known form of an oscillator hamiltonian expressed in terms of the number representation appropriate for an oscillator of a different frequency. We can, in fact, introduce the collective raising and lowering operators

$$c^+|n\rangle = \sqrt{n+1}\,|n+1\rangle \quad ; \quad c|n\rangle = \sqrt{n}\,|n-1\rangle$$

based on the discrete, orthonormal set of many-body states

$$|n\rangle = \frac{1}{\sqrt{\lambda_n}}\int_{-1}^{+1}\tilde{g}_n(\beta)\,|\tilde{\beta}\rangle\, d\beta .$$

The hamiltonian can then be written in operator form as

$$h = \varepsilon_0 + \frac{\hbar\omega}{2}\left(\xi+\frac{1}{\xi}\right)c^+c + \frac{\hbar\omega}{4}\left(\xi-\frac{1}{\xi}\right)(c^+c^+ + cc) \qquad \text{(V.29)}$$

Collective "position" and "momentum" variables Q and P can now be introduced as

$$P = \frac{i\hbar}{\sqrt{2}}\frac{2}{b}\sqrt{\frac{r}{t}}\,(c^+ - c) \quad ; \quad Q = \frac{1}{\sqrt{2}}\frac{b}{2}\sqrt{\frac{t}{r}}\,(c^+ + c) \qquad \text{(V.30)}$$

which allow h to be recast in the form

$$h = E_0 - \frac{M\omega^2 b^2}{16} + \frac{P^2}{2M} + \frac{1}{2} M\omega^2 Q^2 . \qquad (V.31)$$

This shows again that by means of a suitable cannonical transformation performed on the "number representation" given naturally by the discrete spectrum of the modified Hilbert-Schmidt overlap kernel we are able to reduce the collective hamiltonian h to that of an harmonic oscillator of frequency ω. All reference to parameters that characterise the Generator Coordinate representation has again disappeared (except for the trivial additive constant in the total energy, which comes from the explicit form of the energy kernel, eq. (V.8)). In this case, the cannonical transformation is essentially a change of scale given by

$$c^+ = e^{-i\ln\xi^{1/2} D}\, a^+\, e^{i\ln\xi^{1/2} D} \qquad (V.32)$$

where D is the dilatation operator

$$D = \frac{1}{2\hbar}(QP + PQ)$$

and a^+ is the creation operator for the oscillator hamiltonian (V.31),

$$a^+ = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{M\omega}{\hbar}}\, Q - \frac{i}{\sqrt{\hbar M\omega}}\, P\right].$$

The corresponding transformation for the discrete orthonormal set $|n\rangle$ is

$$|n\rangle = e^{-i\ln\xi^{1/2} D}\, |\varphi_n\rangle \qquad (V.33)$$

where the $|\varphi_n\rangle$ are eigenfunctions of the hamiltonian (V.31).

Remembing that ξ is given by

$$\xi = b'^2 \frac{M\omega}{\hbar}$$

where

$$b'^2 = \frac{b^2}{4}\frac{t}{r}$$

and since, by definition, the last factor of b'^2 is always larger than one, it is possible, for $\frac{4\hbar}{M\omega} > b^2$, to choose the free parameter r of the relabeling function in such a way that $\xi = 1$. THis gives

$$r_c = \frac{4}{\left(\frac{4}{b^2}\frac{\hbar}{M\omega}\right)^2 - 1} .$$

In this case the eigenfunctions of the relabeled overlap kernel produce states $|n\rangle$ with the right size parameter for the dynamical problem and h is diagonal in the number representation constructed from these eigenfunctions.

This interpretation also shows that what is involved in our adopted relabeling of the generator states are, from the point of view of the collective phase space, changes of scale of the orthonormal Hilbert-Schmidt discrete base. This is clearly a unitary transformation, in agreement with the general result of sec. III.2. We may even extend this family of unitary transformations to the special case r=0, which corresponds to the original gaussian overlap. The transformation is, in this limiting case,

$$U_{nk} = \frac{1}{\sqrt{\Lambda(k)\lambda_n}} \int_{-\infty}^{\infty} d\alpha \int_{-1}^{+1} d\beta\, (\tilde{n}|\beta)\langle\tilde{\beta}|\alpha\rangle(\alpha|k)$$

which, using the explicit form for the various brackets, can be reduced to

$$U_{nk} = (-i)^n \left[\sqrt{\frac{t}{r}}\,\frac{b}{2}\right]^{1/2} \phi_n\left(\sqrt{\frac{t}{r}}\,\frac{b}{2}\,k\right). \qquad (V.32)$$

The unitary character of this transformation is expressed by the usual orthonormality and completeness relations for the harmonic oscillator wavefunctions ϕ_n.

VI - Conclusions and Discussion

The approach described in the preceding sections has been aimed at establishing a clear and complete connection between the Generator Coordinate Method and a restriction of the quantum mechanics of a many-body system to a well defined subspace of the full many-body Hilbert space. We have shown that the selected subspace is determined solely by the adopted set of generator states. It is the smallest closed subspace of the many-body Hilbert space that contains the generator states.

This subspace, which we called the collective many-body subspace, can be unitarily represented in terms of a Hilbert space of square integrable wave functions of collective variables. The microscopic structure of these variables can be established, in terms of the generator states, via the unitary representation of the collective subspace.

The construction of the collective subspace itself is based on the Griffin-Hill-Wheeler ansatz, which consists in taking linear combinations of the generator states, with the consideration of standard square integrable weight functions only. The two most delicate points involved in this construction are i) the elimination of weight functions associated with the null many-body vector (which express therefore relations of linear dependence among the generator states) and ii) the completion, in the norm of the many-body Hilbert space, of the image of the space of square integrable weight functions by the Griffin-Hill-Wheeler ansatz. What we need, in this connection, is not just an abstract completion, which would be of little practical use, but an explicit construction of the collective subspace. This is what is afforded by its unitary representation in terms of collective wave functions. The proper treatment of point i) above is essential for this step.

From this point of view, the Generator Coordinate Method can be seen as a tool allowing us to set up a complete, reduced quantum scheme corresponding to heuristic restrictions imposed on the allowed degrees of freedom of the many-body system. This is in fact guaranteed by the existence of a standard, orthonormal representation of the collective subspace. In particular, special procedures are in principle not required for the treatment of scattering problems as opposed to the treatment of bound state problems, as scattering states are, as usual, associated with the continuous spectrum of the collective (i.e., projected) Hamiltonian. It is of course possible to try and reexpress any information in the Generator Coordinate representation, but we will in general obtain very singular objects, and whose singularities have no physical significance, as they are generated in the adopted kinematical scheme.

Closest in content to this work is the recent work by Lathouwers[7], which develops a scheme for Hilbert-Schmidt overlap kernels. It is interesting to note that the collective space is introduced in that work through the formal use of the Hill-Wheeler-Griffin ansatz with higly singular weight "objects", in a way that is reminiscent of situations which have been met in the quantum theory of coherence[14]. In the case of the Generator Coordinate Method, however, as opposed to that of quantum optics, no gain comes from the use of the non-orthogonal representation once the possibility of a collective orthonormal representation is realized. We may also add another remark of a more technical nature. It relates to the failure to properly dispose of the null space of the overlap kernel. This not only will give rise to difficulties in direct applications of the results of ref.[7] to such simple cases as the Lipkin model, [9], but also prompts misleading conclusions, such as the unqualified exclusion of biorthogonal states to the generator states from the many-body Hilbert space.

We finaly mention the important problem of the evaluation of the dynamical invariance of the collective phase space selected by a given set of generator states. The formal criterion given in section IV may be very hard to use, since changes in the commutator of the projection operator for the collective space, P, with the full many-body Hamiltonian H are not easily gauged from changes in the number or structure of the generator states. We feel that it is possble, however, to make some definite statements for families of generator states of particular form in the presence of symmetries (or quasi-symmetries, such as the "Galilean" quasi-invariance implied by the validity of adiabatic approximations). This is left for future work.

One of the authors (AFRTP) aknowledges long discussions with J.F.Perez, who also initiated him in the manipulation of the mathematical tools used in this work.

Appendix 1

Consider the Riemann sum for eq.(II.1)

$$|f_N\rangle = \sum_{i=1}^{N} |\alpha_i\rangle f(\alpha_i)(\alpha_i - \alpha_{i-1})$$

with $\max|\alpha_i-\alpha_{i-1}| = \Delta\alpha_{max}$, and the refinement of this partition of the label space obtained by adding p-1 extra points $\alpha_{i,j}$ to each interval such that $\alpha_{i,0} = \alpha_{i-1}$ and $\alpha_{i,p} = \alpha_i$. The corresponding sum is

$$|f_{N,p}\rangle = \sum_{i=1}^{N}\sum_{j=1}^{p} |\alpha_{i,j}\rangle f(\alpha_{i,j})(\alpha_{i,j} - \alpha_{i,j-1}) .$$

The norm of the difference of these two vectors is

$$\| |f_N\rangle - |f_{N,p}\rangle \|^2 =$$

$$= \sum_{i,\ell}\sum_{j,m=1}^{p} \Big\{ \Big[f^*(\alpha_\ell) f(\alpha_i)\langle\alpha_\ell|\alpha_i\rangle + f^*(\alpha_{\ell,m}) f(\alpha_{i,j})\langle\alpha_{\ell,m}|\alpha_{i,j}\rangle -$$

$$- f^*(\alpha_\ell) f(\alpha_{i,j})\langle\alpha_\ell|\alpha_{i,j}\rangle - f(\alpha_i) f^*(\alpha_{\ell,m})\langle\alpha_{\ell,m}|\alpha_i\rangle \Big] \times$$

$$\times (\alpha_{i,j} - \alpha_{i,j-1})(\alpha_{\ell,m} - \alpha_{\ell,m-1}) \Big\} .$$

From the weak continuity of the labelling it follows that, provided $\Delta\alpha_{max}$ is made sufficiently small, we can make

$$|\langle\alpha_\ell|\alpha_i\rangle - \langle\alpha_\ell|\alpha_{i,j}\rangle| < \varepsilon$$

for given ℓ and i, and for all j. This in turn implies that, for continuous weight functions f with compact support (which will give a finite number of contributions to the Riemann sum for finite $\Delta\alpha_{max}$), the norm of $|f_{\nu,p}\rangle$ will be arbitrarily close to that of $|f_N\rangle$ for any p, provided N is sufficiently large. The sequence of refinements of the type considered is therefore a Cauchy sequence in the many-body Hilbert space $\mathcal{H}$ and has thus a limit in this space. It is also easy to check that this limit is independent of the particular partitioning procedure which is adopted, as long as the stated requirements concerning $\Delta\alpha_{max}$ are met.

Appendix 2

The spectral theorem for bounded positive operators such as $\hat{N}$ asserts[11] that a unitary mapping U from $L^2(\mathbb{E})$ to a finite measure space $L^2(M,\mu)$ can be found such that

$$(U\hat{N}U^{-1}\varphi)(k) = \Lambda(k)\,\varphi(k)$$

for any $\varphi(k)$ in $L^2(M,\mu)$, where $\Lambda(k)$ is a bounded, non-negative function on M. We indicate by k a general point of M.

Before trying to invert the operator $\hat{N}$ we must dispose of its null space. This can be done by defining the operator m_Λ in $L^2(M,\mu)$ as

$$(m_\Lambda\varphi)(k) = \chi_\Lambda(k)\,\varphi(k)$$

where $\chi_\Lambda(k)$ is the characteristic function defined as in eq. (III.6). The operator

$$\chi_{\hat{N}} = U^{-1}m_\Lambda U$$

is then a projection operator in $L^2(\mathbb{E})$ which anihilates the null space of $\hat{N}$. We may thus restrict ourselves to the sub-space

$$\mathcal{L}_f = \chi_{\hat{N}}\,L^2(\mathbb{E})$$

or, in an equivalent way, to its unitary transform

$$U\mathcal{L}_f \subset L^2(M,\mu)$$

where the restriction of $\hat{N}$ becomes a positive multiplication operator differing from zero almost everywhere.

An isometry v from the GHW phase space to $U\mathcal{L}_f$ can be constructed as in eq. (III.7):

$$v|f\rangle = \varphi_f(k)$$

with

$$\Lambda^{1/2}(k)\,\varphi_f(k) = (U\langle\alpha|f\rangle)(k),$$

the function $\langle\alpha|f\rangle$ being in $\mathcal{L}_f$. It is in fact straight-forward to show that

$$\|\varphi_f\|^2 = \int d\mu\,\varphi_f^*(k)\,\varphi_f(k) = \int d\mu\,(Uf)^*(k)\,\Lambda(k)\,(Uf)(k) =$$
$$= \langle f|f\rangle .$$

As in section III.2, we can easily show that the set $\{\varphi_f(k)\}$, when $|f\rangle$ spans the GHW phase space, is dense in $U\mathcal{L}_f$. This allows us finally to uniquely extend v to the complete sub-space $U\mathcal{L}_f$. Let V be this extention. It is the partial isometry from the many-body Hilbert space $\mathcal{H}$ to $U\mathcal{L}_f$, which defines the projector P by means of eq.(III.12).

Appendix 3

In order to show the stability of the collective space associated with the Griffin-Hill-Wheeler procedure we construct a sequence of many-body vectors in terms of relabel-ed generator states that converges to some pre-assigred vector in the original collective space. To this effect we note first that, if $|C\rangle$ is any such vector, it can always be characterized as the limit of a sequence of vectors $|C_n\rangle$ belonging to the (in general not complete) GHW phase space, i.e.:

$$|C\rangle = \lim_{n\to\infty} |C_n\rangle$$

$$|C_n\rangle = \int |\alpha\rangle f_n(\alpha)\, d\alpha \ , \quad \int |f_n(\alpha)|^2 d\alpha < \infty \quad \forall\, n .$$

We consider now a change in labelling given by some continuous monotonic frunction $\beta = m(\alpha)$ having an inverse $\alpha = m^{-1}(\beta)$. We have then that

$$|C_n\rangle = \int |\widetilde{m(\alpha)}\rangle f_n(\alpha)\, d\alpha = \int |\tilde{\beta}\rangle f_n(m^{-1}(\beta))\, \frac{d\alpha}{d\beta}\, d\beta \equiv$$

$$\equiv \int |\tilde{\beta}\rangle g_n(\beta)\, d\beta$$

with

$$\int |g_n(\beta)|^2 d\beta = \int |f_n(\alpha)|^2 \left(\frac{dm}{d\alpha}\right)^{-1} d\alpha .$$

We have to distinguish between two different situations. In the first we have

$$\inf \left|\frac{dm}{d\alpha}\right| = \bar{\alpha} > 0 .$$

Then the $g_n(\beta)$ are square integrable functions and the sequence $|C_n\rangle$ belongs to the GHW phase space of the relabeled generator states, thus proving the desired result that $|C\rangle$ is in the corresponding collective space. In the second situation, on the other hand, we have

$$\inf \left|\frac{dm}{d\alpha}\right| = 0 ;$$

since $m(\alpha)$ has an inverse, this can happen only when the derivative $dm/d\alpha$ has zero as a limit point. By isolating this limit point with a set of nested intervals Δ_N such that for $N\to\infty$ we recover the full α-space we can construct the sequence of square-integrable functions in β-space

$$g_n^{(N)}(\beta) = \begin{cases} 0, & \text{if } m^{-1}(\beta) \text{ is in } \Delta_N \\ f_n(m^{-1}(\beta))\, \dfrac{dm^{-1}(\beta)}{d\beta} & \text{otherwise} . \end{cases}$$

The GHW vectors

$$|C_n^{(N)}\rangle = \int |\beta\rangle g_n^{(N)}(\beta)\, d\beta$$

will then converge to $|C_n\rangle$ as $N\to\infty$, and we have replaced the original sequence by the double sequence $\{|C_n^{(N)}\rangle\}$ of vectors belonging to the new GHW phase space. From this it is easy to extract a subsequence that converges to $|C\rangle$. In fact, write

$$\| |C\rangle - |C_n^{(N)}\rangle \| = \| |C\rangle - |C_n^{(N)}\rangle + |C_n\rangle - |C_n\rangle \| \leqslant$$

$$\leqslant \| |C\rangle - |C_n\rangle \| + \| |C_n\rangle - |C_n^{(N)}\rangle \| .$$

By an appropriate choice of n, say $n(\nu)$, the first term can be made smaller than $1/2\nu$; we can then choose a sufficiently large N, say $N(\nu)$, so that the same is true for the second term. Thus

$$\| |C\rangle - |C_{n(\nu)}^{(N(\nu))}\rangle \| < \frac{1}{\nu}$$

and the sequence of GHW vectors $|C_{n(\nu)}^{(N(\nu))}\rangle$ converges to $|C\rangle$ which proves the desired result.

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