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THE METHOD OF MOMENTS AND NESTED HILBERT SPACES IN QUANTUM MECHANICS *

E. Adeniyi Bangudu **
International Centre for Theoretical Physics, Trieste, Italy.

ABSTRACT

It is shown how the structures of a nested Hilbert space H_I, associated with a given Hilbert space H_0, may be used to simplify our understanding of the effects of parameters, whose values have to be chosen rather than determined variationally, in the method of moments. The result, as applied to non-relativistic quartic oscillator and helium atom, is to associate the parameters with sequences of Hilbert spaces, while the error of the method of moments relative to the variational method corresponds to a nesting operator of the nested Hilbert space. Difficulties hindering similar interpretations in terms of rigged Hilbert space structures are highlighted.

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** Permanent address: Department of Mathematics, University of Ilorin, P.M.B. 1515, Ilorin, Kwara State, Nigeria.

I. INTRODUCTION

A number of variants of the Rayleigh-Ritz variational method, particularly those employing non-symmetric matrices in the set of algebraic equations, the solutions of which are expected to be good approximations to the eigenvalues and eigenfunctions of the Schrödinger equations of quantum systems, are here described as the method of moments. A prominent and undesirable feature of this method is its non-monotonic convergence to the appropriate eigenvalues with increase in the number of basis functions, in terms of which the approximate eigenfunctions are normally expanded. Since the method is supposed to be an alternative to the Rayleigh-Ritz variational method, optimum values for the parameters invariably contained in the basis functions can no longer be determined by the energy extremum criterion, and remain largely but judiciously chosen; yet their values affect convergence. Although convergence, under different values of these parameters, is interpreted as an indication of the stability of the method, the aim of this paper, in re-investigating the actual applications of the method, is to remove this element of arbitrariness in the values assignable to the parameters.

The method of moments, in its most general form, depends on the availability of basis vectors that span two different subspaces (the co-ordinate and projective subspaces) of the same Hilbert space of the problem being solved. The rigged and nested Hilbert spaces are each defined from families of Hilbert spaces; hence the novel idea of using them to attempt the resolution of the doubt as to whether or not the basis vectors employed in the examples (the quartic oscillator and helium atom) actually satisfy this requirement. In this approach, a well-defined correspondence between the parameters and Hilbert spaces of a nested Hilbert space is established, under the standard realization of a Hilbert space as a space of functions. The nesting operators are also shown to be more effective and easily realizable indicators of the relative error between the method of moments and the variational method. Some unresolved difficulties are encountered with rigged Hilbert space.

Sec.II reviews the different forms of the method of moments and gives details of its application to the quartic oscillator and helium atom problems as examples. Sec.III contains the relevant aspects of the construction of a nested Hilbert space, particularly that associated with a given Hilbert space, and thus provides the necessary structure in terms of which the method of moments is analysed in Sec.IV. The difficulties to be resolved before a rigged Hilbert space can be similarly applied to the method of moments is summarized in Sec.V.

II. THE METHOD OF MOMENTS

There are a number of approaches to the derivation of linear algebraic equations for the solution of the Schrödinger equation

$$\underset{\sim}{H} \Psi = \mathcal{E} \Psi \qquad (1)$$

of a quantum-mechanical system. Each starts with some arbitrary set of complete basis vectors

$$\{\phi_i\} \quad , \quad (i = 0,1,2,\ldots) \qquad (2)$$

in the Hilbert space H_0 of the Hamiltonian operator $\underset{\sim}{H}$ of the system and assumes the expansion of each state vector Ψ as linear combination of the set (2) in the form

$$\Psi = \sum_{i=0}^{\infty} \alpha_i \phi_i \quad . \qquad (3)$$

The simplest approach is to use (3) in (1) and take the scalar product, in the Hilbert space H_0, with each of the basis vectors. This leads to the set of algebraic equations

$$\sum_{i,j=0}^{\infty} (H_{ji} - \mathcal{E} M_{ji}) \alpha_i = 0 \quad , \qquad (4)$$

where

$$H_{ji} = (\phi_j, \underset{\sim}{H} \phi_i) \quad , \qquad (5)$$

$$M_{ji} = (\phi_j, \phi_i) \qquad (6)$$

$$(i,j = 0,1,2,\ldots) \quad .$$

The various state energies, $\mathcal{E}_k$, $(k = 0,1,2,\ldots)$ are obtained as roots of the determinant equation

$$\| H_{ji} - \mathcal{E} M_{ji} \| = 0 \qquad (7)$$

that give a non-trivial solution of (4) for the initially unknown expansion coefficients α_i, and the corresponding state vectors, Ψ_k .

The hypervirial relations are introduced by Hirschfelder (1960) [1], and shown to be sufficient for the determination of the state vectors. (An operator $\underset{\sim}{W}$ is described as hypervirial if it does not commute with the Hamiltonian $\underset{\sim}{H}$ but satisfies the relation

$$(\Psi \, , [\underset{\sim}{H}, \underset{\sim}{W}] \Psi) = 0 \quad . \qquad (8).)$$

In particular, if the ground state vector Ψ_0 and energy $\mathcal{E}_0$ are assumed to be known, Coulson (1965) [2] suggested the expansion of excited state vectors as in (3) and the use of a sequence $\{\underset{\sim}{W}_j\}$ $(j = 0,1,2,\ldots)$ of linearly independent hypervirial operators to give the set of algebraic equations, (4), with $\mathcal{E}$ replaced by $(\mathcal{E}_0 - \mathcal{E})$ and the H_{ji} , M_{ji} now defined as

$$H_{ji} = (\Psi_0, [\underset{\sim}{H}, \underset{\sim}{W}_j] \phi_i) \quad , \qquad (5a)$$

$$M_{ji} = (\Psi_0, \underset{\sim}{W}_j \phi_i) \qquad (6a)$$

are no longer symmetric matrices. Schwartz's (1967) [3] proposal uses only one operator $\underset{\sim}{W}$, with no assumption on any state vector nor energy, but with H_{ji}, M_{ji} defined as

$$H_{ji} = (\phi_j, \underset{\sim}{W} \underset{\sim}{H} \phi_i) \quad , \qquad (5b)$$

$$M_{ji} = (\phi_j, \underset{\sim}{W} \phi_i) \quad , \qquad (6b)$$

where H_{ji} is non-symmetric for a non-trivial choice of $\underset{\sim}{W}$. This approach is the first under the name, "method of moments".

The trans-correlated polydetor approximation of Boys (1969) [4], Boys and Handy (1969) [5] transforms $\underset{\sim}{H}$ to the form

$$\underset{\sim}{H}_{tc} = \underset{\sim}{S}^{-1} \underset{\sim}{H} \underset{\sim}{S} \quad , \qquad (9)$$

where $\underset{\sim}{S} = \exp(\underset{\sim}{L})$ and $\underset{\sim}{L}$ is a real function of the quantum system's co-ordinates acting as operators, so that M_{ji} remains as in (6) but H_{ji} becomes

$$H_{ji} = (\phi_j, \underset{\sim}{H}_{tc} \phi_j) \qquad (5c)$$

and is generally non-symmetric.

The Galerkin-Petrov approach (Bangudu, Jankowski and Dion (1973))[6] uses elements of a second set of basis vectors $\{\chi_j\}$ $(j = 0,1,2,\ldots)$ of the same Hilbert space H_0 to define the non-symmetric H_{ji} and symmetric M_{ji} in the form

$$H_{ji} = (\chi_j, \underset{\sim}{H}\,\phi_i) \qquad (5d)$$

$$M_{ji} = (\chi_j, \phi_i) \quad . \qquad (6d)$$

The different approaches are easily seen to be equivalent either to the use of symmetric matrices or to the case in which the matrices are not symmetric. In application, one chooses $\{\phi_i\}$ $(i = 0,1,\ldots,N-1)$ as the basis of a finite (N) dimensional subspace F_N (called the co-ordinate space) and, for the second case, another set $\{\chi_i\}$ $(i = 0,1,\ldots,N-1)$ as the basis of a different subspace G_N (called the projective space) of the same Hilbert space H_0. The remaining procedure of determining approximate solutions to (1) by solving (4) is theoretically similar to the Galerkin method or Galerking-type method involving two subspaces [7] (for the second case) of finding approximations to the weak solution of boundary value problems. In practise, however, the solution of (7) for the approximate energy values, which are of more significance in quantum mechanics than approximate state vectors, is usually sufficient to indicate the effectiveness of either case.

The general form of the method of moments has received better attention since it appears to be the closest alternative to the variational method which cannot be accurately performed (because of the difficult integrals involved), particularly when trial basis vectors $\{\phi_i\}$ include correlation factors. In such cases the $\{\chi_i\}$ set of basis vectors are to be selected to lead to more manageable integrals for the matrix elements. Application of the method to simple systems has provided fairly good results for the ground and the lower excited state energy values [5,6,8]. The convergence of the energy values to the "exact" values with increase in N (the dimension of the subspaces) depends expectedly on the choice of the basis sets $\{\phi_i\}$, $\{\chi_i\}$ and it is always non-monotonic; unlike those of the variational method that are always upper bounds to the "exact" values.

Jankowski (1976) [9] proved a theorem that if the basis sets $\{\phi_i\},\{\chi_i\}$ are orthonormal in their respective subspaces F_N, G_N and are such that

$$\left.\begin{aligned} &(\chi_j, \phi_i) = M_i\,\delta_{ij} \\ \text{where}\quad &0 < M_i \leq 1, \quad (i,j = 0,1,\ldots,N-1) \end{aligned}\right\} \qquad (10)$$

then the maximization of any one of the suggested functions of the M_i's (such as their sum, the sum of their squares or their products) should lead to more reliable results. The illustrative computations confirm this [9,10]; but apart from the non-monotonic convergence, there still remains another unsatisfactory aspect of the method of moments. Parameters, usually scale factors [5,6,8], are employed in the choice of the basis sets $\{\phi_i\}$ or $\{\chi_i\}$ (or what corresponds to the latter), and although their values affect convergence there is as yet no way of determining optimum values for them. Instead, the fact that different, though judicious, choices of values for the parameters lead to convergence (at differing rates) is interpreted as an indication of the stability of the method. There is thus an obvious need to remove this element of arbitrariness from this method to make it more acceptable.

2.1 Examples

a) The quartic oscillator [6]

Here the set $\{\phi_i\}$ $(i = 0,1,2,\ldots)$ of Hermite functions, which are eigenfunctions of the harmonic oscillator, is chosen as one of the realizations of orthonormal basis for H_0. They are defined on the real line by

$$\left.\begin{aligned} \phi_i(x) &= \pi^{-1/4}(2^i i!)^{-1/2} e^{-x^2/2} h_i(x) , \\ \text{where}\quad h_i(x) &= (-1)^i e^{x^2} \frac{d^i}{dx^i} e^{-x^2} . \end{aligned}\right\} \qquad (11)$$

The orthonormal projective basis set $\{\chi_i\}$ for the same H_0 is obtained by scaling; i.e.

$$\begin{aligned} \chi_i(x) &= (1+b)^{1/2} \phi_i[(1+b)x] \\ &= \pi^{1/4}\left(\frac{1+b}{2^i i!}\right)^{1/2} \exp[-\tfrac{1}{2}(1+b)^2x^2]\; h_i[(1+b)x] , \end{aligned} \qquad (12)$$

where $(1 + b)$ is the scale factor with b taking any real value greater than -1. The Hamiltonian of the system, in reduced units, is

$$\underset{\sim}{H} = -\frac{d^2}{dx^2} + x^4 \qquad (13)$$

and completes the requirements for the method of moments, which is expected to produce its best results for optimum value of b, since the M_i numbers of (10) are now the overlap integrals, $M_i = (\chi_i, \phi_i)$.

The $\chi_i(x)$'s are related to the $\phi_i(x)$'s through

$$\left.\begin{aligned} \chi_j(x) &= \sum_{i=0}^{j} \alpha_{ji}\, x^{j-i} \exp[-\tfrac{1}{2}(2b+b^2)x^2]\, \phi_i(x), \\ \text{where} \quad \alpha_{ji} &= \left(\frac{(1+b)2^i i!}{2^j j!}\right)^{1/2} \frac{j!\,(2b)^{j-i}}{i!\,(j-i)!} \end{aligned}\right\} \qquad (14)$$

This simplifies computation but raises the question of the suitability of expressing the solution of (1), with $\underset{\sim}{H}$ given by (13), as a linear combination of (11) or even (12) when (11) and (12) are not so related, as expected of complete orthonormal systems for H_0. It is easily verified, however, that (14) reduces to two simpler relations:

i) the relation

$$\chi_i^{\prime}(x) = \exp[-\tfrac{1}{2}(2b+b^2)x^2]\, \phi_i(x) \qquad (15)$$

which produces independent functions in H_0, and

ii) the application of Gram-Schmidt orthogonalization on the $\chi_i^{\prime}(x)$'s $(i = 0,1,2,...)$ results in the orthonormal set (12).

Yet, in the light of nested Hilbert space associated to an orthonormal basis of a given Hilbert space, it is Eq.(15) that raises the question

Do the sets $\{\phi_i\}$ and $\{\chi_i\}$ span the same Hilbert space H_0 as required by all the analysis of the method of moments? (Q)

b) The helium atom

In Hylleraas variables ($s = r_1 + r_2$, $t = r_1 - r_2$, $u = r_{12}$, where $0 \leq t \leq u \leq s \leq \infty$) there are many possible choices of basis sets but typical sets, which produce good results [10], are "correlation factor basis" as the co-ordinate basis set $\{\phi_i\}$, realized in three-dimensional space as

$$\phi_i(s,t,u) = e^{-\alpha s}\, s^{\ell}\, t^{2n}\, (1 + \beta u) \qquad (16)$$

and "configuration interaction basis" as the projective basis set $\{\chi_i\}$ given by

$$\chi_i(s,t) = e^{-\alpha s}\, s^{\ell}\, t^{2n} \qquad (17)$$

Note: α, β are parameters; $(\ell, n = 0,1,2,...)$ and the same positive integral value function of ℓ and n, $i = i(\ell, n)$, is normally used to order both sets (16) and (17).

The Hamiltonian $\underset{\sim}{H}$, in atomic units, is

$$\begin{aligned} \underset{\sim}{H} = &-\left(\frac{\partial^2}{\partial s^2} + \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial t^2}\right) - \frac{2s(u^2-t^2)}{u(s^2-t^2)} \frac{\partial^2}{\partial s \partial u} \\ &- \frac{2t(s^2-u^2)}{u(s^2-t^2)} \frac{\partial^2}{\partial u \partial t} - \frac{4s}{(s^2-t^2)} \frac{\partial}{\partial s} - \frac{2}{u} \frac{\partial}{\partial u} \\ &+ \frac{4t}{(s^2-t^2)} \frac{\partial}{\partial t} - \frac{8s}{(s^2-t^2)} + \frac{1}{u} . \end{aligned} \qquad (18)$$

However, the point of interest is the relation

$$\chi_i(s,t) = (1 + \beta u)^{-1}\, \phi_i(s,t,u) \qquad (19)$$

between χ_i, ϕ_i and the correlation function $(1 + \beta u)$ that contains the distinguishing parameter β. (The parameter α is common to both sets $\{\phi_i\}$ and $\{\chi_i\}$ and is thus of no consequence in determining the difference between them. It is given a fixed value $\alpha = 1.85$ [3,10] which compares well with its variationally derived value $\alpha = 1.860$, $\gamma = -0.260$ from correlated Hylleraas function [13] $\phi = e^{-\gamma u} e^{-\alpha s}$ for ground state helium atom.) Because of its similarity to (15), Eq.(19) equally raises question (Q).

III. NESTED HILBERT SPACE

This section contains a brief review of the concepts and properties of nested Hilbert space relevant for our purpose. The main theorem is proved in the appendix; for other details see Grossman [11].

A linear transformation E_{db} from an infinitely dimensional, separable Hilbert space H_b into another Hilbert space H_d is called a nesting if it is bounded, injective, and its range is dense in H_d (e.g. if $\phi^{(b)} \in H_b$, then there exists one $\phi^{(d)} \in H_d$ such that $\phi^{(d)} = E_{db}\, \phi^{(b)}$). Its adjoint, $(E_{db})^*_{bd}$, defined by

$$(\varphi^{(b)}, (E_{db})^*_{bd}\, \phi^{(d)}) = (E_{db}\, \varphi^{(b)}, \phi^{(d)}) \tag{20}$$

is also a nesting. Note that at the left-hand side of (20) the scalar product is in H_b and it is in H_d at the right-hand side.

The polar decomposition of E_{db}, given by

$$\left.\begin{aligned} E_{db} &= U_{db}\, [E_{db}]_{bb} \\ \text{where}\qquad [E_{db}]_{bb} &= [(E_{db})^*_{bd}\, E_{db}]^{1/2} \end{aligned}\right\} \tag{21}$$

is injective and U_{db} is unitary. If E_{db} and E_{ad} are nestings, then their product $E_{ad}\, E_{db}$ is a nesting from H_b into H_a. $E_{bb} = 1$ is the identity in H_b.

Let I be a partially ordered set that is directed to the right, has an order-reversing involution $b \leftrightarrow -b \equiv \bar b$ and contains an element 0 such that $\bar 0 = 0$. For every $b \in I$, let V_b be a vector space. Define an equivalence relation in the disjoint union $\bigcup_{b\in I} V_b$ by writing $\phi^{(b)} \sim \phi^{(a)}$ (where $\phi^{(b)} \in V_b$, $\phi^{(a)} \in V_a$) if and only if there exists a $d \geq a,b$ such that $E_{db}\, \phi^{(b)} = E_{da}\, \phi^{(a)}$. The set of classes to which $\bigcup_{b\in I} V_b$ is thus decomposed forms a vector space denoted by V_I and called the algebraic inductive limit of the vector spaces V_b with respect to E_{db} and I ;

i.e.
$$V_I = [V_b\ ;\ E_{db}\ ;\ I] \quad . \tag{22}$$

For every $b \in I$, define the natural embedding operator of V_b into V_I by

$$\phi^{(I)} = E_{Ib}\, \phi^{(b)} \quad , \tag{23}$$

where $\phi^{(I)} \in V_I$, $\phi^{(b)} \in V_b$; (i.e. for every $\phi^{(b)} \in V_b$, E_{Ib} associates the same $\phi^{(b)}$ considered as an element of V_I) and call $\phi^{(b)}$ the representative of $\phi^{(I)}$ in V_b.

The algebraic inductive limit $H_I = [H_b;\ E_{db}\ ;\ I]$ of a family of Hilbert spaces H_b is called a nested Hilbert space if the following conditions are satisfied:

(i) If b and d are any two elements of I, then there exists an $a \leq b,d$ such that

$$E_{Ia}\, H_a = E_{Ib}\, H_b \cap E_{Id}\, H_d \quad ; \tag{24}$$

(ii) For every $b \in I$, there exists a unitary mapping $U_{\bar b b}$ from H_b onto $H_{\bar b}$ such that

$$\left.\begin{aligned} U_{\bar 0 0} &= 1 \\ E_{\bar b \bar d} &= U_{\bar b b}\, (E_{db})^*_{bd}\, U_{d \bar d} \end{aligned}\right\} \tag{25}$$

$$(b \in I;\ d \geq b)\ .$$

3.1 Nested Hilbert space H_I associated with a given Hilbert space H_0

Let $\{\phi_i^{(0)}\}$ ($i = 0,1,2,\ldots$) be the orthonormal basis of a given Hilbert space H_0 and I the set of all sequences of strictly positive numbers. Hence $b \in I$ implies $b = \{b(i)\}$ is a sequence of numbers with $b(i) > 0$ for all i. Defining the partial order in I by $d \geq b$ implies $d(i) \geq b(i)$, and the order reversing involution is defined by

$$\bar b(i) = \frac{1}{b(i)} \qquad \text{for all } i \ . \tag{26}$$

Note that for $0 = \bar 0$ to obtain, $0(i)$ must be equal to one for all i.

For every $b \in I$ let V_b be the vector space of all finite linear combinations of the vectors $\{\phi_i^{(0)}\}$ with scalar product defined by

$$(\phi^{(b)}, \varphi^{(b)}) = \sum \alpha_i^*\, b^{-2}(i)\, \beta_i \ , \tag{27}$$

where $\phi^{(b)} = \sum_i \alpha_i \phi_i^{(0)}$; $\varphi^{(b)} = \sum_i \beta_i \phi_i^{(0)}$ are elements of V_b.

Denote by H_b, the Hilbert space obtained by completing V_b with respect to the scalar product (27), and by E_{db} the natural embedding of H_b into H_d for all $d \gg b$ that belong to I. Observe, from (27), that the scalar product in H_b has the form of the scalar product in H_0

$$\text{i.e.} \quad (\phi^{(0)}, \varphi^{(0)}) = \sum_i \alpha_i^* \beta_i \quad , \tag{28}$$

where $\phi^{(0)} = \sum_i \alpha_i \phi_i^{(0)}$; $\varphi^{(0)} = \sum_i \beta_i \phi_i^{(0)}$ are now elements of H_0; but the sequence $\{b(i)\}$ effects the possibility of defining the scalar product between two functions both of which belong to H_b while they need not belong to H_0.

The algebraic inductive limit $H_I = [H_b; E_{db}; I]$ is the nested Hilbert space associated to H_0. It follows from the relation $\phi_i^{(I)} = E_{Ib} \phi_i^{(b)}$ that the vectors $\phi_i^{(I)} = E_{I0} \phi_i^{(0)}$ in H_I have representation $\phi_i^{(b)}$ in H_b whose orthonormal basis can be shown from (27) and (28) to be the set

$$\{e_i^{(b)}\} = \{b(i) \phi_i^{(b)}\} \quad , \quad (i = 0,1,2,\dots) \quad . \tag{29}$$

From now on we make the simplifying assumption that the order in I is total (i.e. all pairs of its elements are comparable). In particular, every other element is comparable with the zero element, $0 = \bar{0}$. The scalar product of $\phi^{(b)} \in H_b$ and $\varphi^{(0)} \in H_0$ is then a bilinear functional $B(\phi^{(b)}, \varphi^{(0)})$ on H_b and H_0; and for its correct evaluation, we need the nesting E_{b0} or its adjoint $(E_{b0})^*_{0b}$, so that

$$\begin{aligned} B(\phi^{(b)}, \varphi^{(0)}) &= ((E_{b0})^*_{0b} \phi^{(b)}, \varphi^{(0)}) \\ &= (\phi^{(b)}, E_{b0} \varphi^{(0)}) \end{aligned} \tag{30}$$

is obtained by taking scalar product either in H_0 or in H_b. In practise, we still prefer to expand $\phi^{(b)} \in H_b$ as linear combination of the orthonormal basis vectors $\{\phi_i^{(0)}\}$ of H_0 and take scalar product in H_0; hence we need the nesting $(E_{b0})^*_{0b}$ at least.

IV. THE EXAMPLES IN TERMS OF NESTED HILBERT SPACE

The preceding section allowed us to construct a nested Hilbert space, H_I, from a given Hilbert space H_0. The family of Hilbert spaces, employed in the construction, come in pairs H_b, $H_{\bar{b}}$ through the order-reversing involution defined for all elements $b \in I$ (the set of all totally ordered sequences of strictly positive numbers); just like the nestings E_{db}, $(E_{db})^*_{bd}$ for any pair of elements $d, b \in I$ with $d \gg b$. In this section we need only the family $b \in I$ with $b \gg 0$; and shall realize the corresponding Hilbert space, H_b, as the space of classes of real valued functions $L^2(\mathbb{R}^N, \tau)$ defined on N-dimensional space, measurable and square integrable with respect to the measure τ, with the usual scalar product.

4.1 The quartic oscillator

In Eq.(15) denote $\chi_i'(x)$ by $\phi_i^{(b)}(x)$ and $\phi_i(x)$ by $\phi_i^{(0)}(x)$ so that, in the notation of Sec.III, this equation becomes

$$\phi_i^{(b)}(x) = \exp[-\tfrac{1}{2}(2b + b^2) x^2] \; \phi_i^{(0)}(x) \quad . \tag{15a}$$

Identify $\phi_i^{(b)}$ as an element of $H_b \neq H_0$ and $\{\phi_i^{(0)}\}$ remains the set of orthonormal basis of H_0, while the nestings E_{b0} and its adjoint $(E_{b0})^*_{0b}$ are, respectively, realized on $\mathbb{R}$ as

$$E_{b0}(x) = \exp[-\tfrac{1}{2}(2b + b^2) x^2] \quad , \tag{31}$$

$$(E_{b0})^*_{0b}(x) = \exp[\tfrac{1}{2}(2b + b^2) x^2] \quad . \tag{32}$$

Now, the integral

$$\int_{-\infty}^{\infty} |\phi_i^{(b)}(x)|^2 dx = \int_{-\infty}^{\infty} \exp[-(2b+b^2)x^2] \, |\phi_i^{(0)}(x)|^2 dx$$

is defined for all real values of b. Therefore if $H_0 = L^2(\mathbb{R}, \tau)$, then we can identify H_b with $H_b = L^2(\mathbb{R}, \mu) = L^2(\mathbb{R}, b^{-2}\tau)$ since the Lebesque measure μ in H_b is related to the Lebesque measure in H_0 through the function $b^{-2}(x)$ (i.e. $d\mu(x) = b^{-2}(x)\,dx$), where

$$b(x) = \exp[\tfrac{1}{2}(2b + b^2) x^2] \quad . \tag{33}$$

Note that b(x) is a continuous function on $\mathbb{R}$, takes strictly positive values and is therefore an element of I since it satisfies the total ordering in I although I is now a sequence of equal numbers, for fixed x.

Thus the direct answer to (Q) is that H_b is not indentical with H_0. In fact for $b \geqslant 0$, the assertion $H_b \supseteq H_0$ is a direct consequence of a lemma [11] that if d,b are elements of I and $d \geqslant b$ then $E_{Id} H_d \supseteq E_{Ib} H_b$, where E_{Id}, E_{Ib} are, respectively, the ,embedding operators of H_d and H_b into the resulting nested Hilbert space, H_I, of the family of Hilbert spaces. Furthermore, the relations

$$
\begin{aligned}
e_i^{(b)}(x) &= \exp[\tfrac{1}{2}(2b+b^2)x^2]\,\phi_i^{(b)}(x) \\
&= \exp[\tfrac{1}{2}(2b+b^2)x^2]\left\{\exp[-\tfrac{1}{2}(2b+b^2)x^2]\,\phi_i^{(0)}(x)\right\} \\
&= \phi_i^{(0)}(x)
\end{aligned}
$$

show that H_b is sufficiently spanned by the orthonormal basis of H_0. This is expected because H_b is the completion of V_b, a vector space of all finite linear combinations of the vectors $\{\phi_i^{(0)}\}$ with scalar product defined by (27). It confirms the nesting $E_{b0}(x)$ of (31) as a natural embedding of H_0 into H_b (i.e. E_{b0} associates the same vector $\phi_i^{(0)}$ belonging to H_0 as an element of H_b) and that $H_0 \subseteq H_b$.

The effect of Gram-Schmidt orthogonalization of the set of vectors $\{\phi_i^{(b)}(x)\}$ is to produce the orthonormal set $\{\chi_i(x)\}$ of (12),but the integrals

$$
\begin{aligned}
\int_{-\infty}^{\infty}|\chi_i(x)|^2 dx &= \int_{-\infty}^{\infty}\left|(1+b)^{1/2}\phi_i^{(0)}[(1+b)x]\right|^2 dx \\
&= \int_{-\infty}^{\infty}|\phi_i^{(0)}(y)|^2 dy ,
\end{aligned}
$$

where $y = (1+b)x$, show that (12) spans the Hilbert space $H_c = L^2(\mathbb{R},(1+b)\tau)$ which corresponds to the result of a simple choice of another element $c \in I$ given by

$$c = (1+b)^{-1/2} \tag{34}$$

with $b > -1$.

Again, $e_i^{(c)}(x) = c\,\chi_i(x) = (1+b)^{-1/2}[(1+b)^{1/2}\,\phi_i^{(0)}(x)] = \phi_i^{(0)}(x)$ imply that H_c is spanned by the orthonormal basis H_0; also $H_0 \subsetneq H_c$ and H_c contains or is contained in H_b according to whether c is greater or less than b. The nesting E_{c0} and its adjoint $(E_{c0})^*_{0c}$ are

$$E_{c0} = (1+b)^{1/2} , \tag{35}$$

$$(E_{c0})^*_{0c} = (1+b)^{-1/2} . \tag{36}$$

Considerations based on Eq.(33) show that continuous functions taking strictly positive values qualify as elements of I; but since elements of type (34) are used in computations under consideration [6], we restrict our attention to this. The method of moments requires different subspaces of the same Hilbert space. The spaces H_c and H_0 are not identical except when $b = 0$ (making $c = 1 = \bar{c}$ by (26) and definition of H_0). Using finite sets $\{\chi_i\}_{i=0}^{N-1}$, $\{\phi_i\}_{i=0}^{N-1}$ that are operative in H_c and H_0, respectively, cannot therefore be strictly interpreted as spanning different subspaces of the same Hilbert space. The facts that $H_0 \subseteq H_c$ and both are effectively spanned by the set $\{\phi_i^{(0)}\}$ allow convergence of the method of moments calculations in the "mixed" Hilbert spaces H_0 and H_c. Such calculations invariably do not evaluate the bilinear functions $B(\phi^{(c)}, \phi^{(0)})$ involved correctly - by not employing the adjoint nesting operator $(E_{c0})^*_{0c}$ - but this operator as identified in Eq.(36) happens to be a constant in the problem and therefore does not lead to error in the solution of the determinant equation (7). Yet, monotonically decreasing and comparable convergence rate is demonstrably obtained when computations are performed in the same Hilbert space. See Table 2 of Ref.6 reproduced below. Also, Eqs.(36), (30) and (10) give the M_i numbers for H_0 and H_c as

$$M_i = (\chi_i(x), \phi_i^{(0)}(x)) = (1+b)^{1/2} = c^{-1} \text{ for all } i.$$

All the suggested functions [9] of the M_i's attain their maximum values with that of M_1. But $M_i = 1$ for all i when $b = 0$, so that $c = 1$ and H_c is then identical with H_0 as noted earlier.

4.2 The helium atom

The same analysis for the quartic oscillator can be repeated for the helium atom computations. Eq.(17) defines independent functions in $\mathbb{R}^3$. Denote their orthonormalized version by $\phi_i^{(0)}(s,t,u)$ and the independent functions $(1+\beta u)\,\phi_i^{(0)}(s,t,u)$ by $\phi_i^{(\beta)}(s,t,u)$ so that Eq.(19) becomes

$$\phi_i^{(0)}(s,t,u) = \frac{1}{(1+\beta u)}\,\phi_i^{(\beta)}(s,t,u) \tag{19a}$$

Table 2 of Ref.6

Five lowest energy levels of even symmetry for the quartic oscillator for several b values and two expansion lengths (in reduced units).

b \ N	5 Energy	Δ a/	10 Energy	Δ a/
	1.06001	− 0.00035	1.06036	0.00000
	8.23358	+ 0.77883	7.44488	− 0.01082
-0.5	34.0870	+ 17.825	17.7236	+ 1.4162
	123.246	+ 96.718	43.0658	+16.537
	389.574	+351.65	105.331	+67.408
	1.06131	+ 0.00095	1.06038	+ 0.00002
	7.47162	+ 0.01588	7.45574	+ 0.00004
0.0 b/	18.8204	+ 2.5586	16.2764	+ 0.0146
	52.9084	+ 26.380	26.7249	+ 0.1946
	155.988	+118.07	43.7714	+ 5.8484
	1.06035	− 0.00001	1.06036	0.00000
	7.44909	− 0.00661	7.45570	0.00000
0.5	16.0913	− 0.1705	16.2619	+ 0.00001
	26.7146	+ 0.1861	26.5234	− 0.0051
	60.7854	+ 22.862	37.8807	− 0.0423
	1.06024	− 0.00012	1.06036	0.00000
	7.43185	− 0.02385	7.45570	0.00000
1.0	16.2217	− 0.0410	16.2619	+ 0.0001
	im. c/	−	26.5305	+ 0.0020
	im.	−	37.8988	− 0.0242
	1.03565	− 0.02471	1.06028	− 0.00008
	6.66191	− 0.79379	7.44980	− 0.00590
2.0	20.3303	+ 4.0685	15.2584	− 1.0034
	im.	−	24.2594	− 2.2691
	im.	−	33.0093	− 4.9137

a/ $\Delta = E_n - E^{exact}$, E^{exact}: very accurate results of Reid [12].

b/ Results of the variational Ritz method.

c/ im. - complex root.

Identify the set $\{\phi_i^{(0)}\}$ as the orthonormal basis of $H_0 = L^2(\mathbb{R}^3,\tau)$, the set $\{\phi_i^{(\beta)}\}$ as independent functions in $H_\beta = L^2(\mathbb{R}^3,(1+\beta u)\tau)$, and the realization of the nestings $E_{\beta 0}$ and $(E_{\beta 0})^*_{0\beta}$ in $\mathbb{R}^3$ as

$$E_{\beta 0}(s,t,u) = (1 + \beta u) \quad , \tag{37}$$

$$(E_{\beta 0})^*_{0\beta}\,(s,t,u) = (1 + \beta u)^{-1} \quad . \tag{38}$$

This is justified because the function

$$\beta(u) = (1 + \beta u) \tag{39}$$

with $\beta \geqslant 0$ is continuous in $\mathbb{R}^3$, and both $\beta(u)$ and $\bar{\beta}(u) = \frac{1}{\beta(u)} = (1 + \beta u)^{-1}$ take strictly positive values, since $0 \leqslant u \leqslant \infty$; therefore β is an element of I (though $\beta(u)$, like b(x) of the quartic oscillator, is a sequence of equal numbers, for fixed u).

H_β and H_0 are not the same Hilbert space except when $\beta = 0$ (and $\beta(u) = 1 = \bar{\beta}(u)$ for all u). Method of moments calculations in the mixed spaces H_β and H_0 converge because H_0 is naturally embedded in H_β and both are sufficiently spanned by $\{\phi_i^{(0)}\}$. It is again significant that calculations with $\beta = 0.29$ converge faster than with $\beta = 0.5$ (i e. when $H_{0.29} \subseteq H_{0.5}$). Table 4 of [10] corresponds to our choice of ϕ_i and χ_i as in Eqs.(16) and (17), respectively, and shows that for N = 20, the helium atom ground state energy value with $\beta = 0.5$ is -2.91445 a.u.; with $\beta = 0.29$ it is -2.90314 a.u., while its "exact" value is -2.903724 a.u. No doubt, the convergence would have been comparably fast and monotonically decreasing when $\beta = 0$ (i.e. when H_β becomes identical with H_0).

4.3 Remarks

In both examples, and in fact generally, the situation remains unchanged when we use the nested Hilbert space H_I instead of the intermediate Hilbert spaces H_b , because the nesting operator E_{I0} from H_0 into H_I is defined for every $\phi^{(0)} \in H_0$, continuous, has dense range in H_I and is injective. Even when the range of E_{I0} is not the whole of H_I (i.e. E_{I0} is a proper nesting operator), as long as we make the usual stipulation that our problem be solved in a given Hilbert space H_0, then E_{I0} (as a natural embedding operator of H_0 into H_I) causes the basis set $\{\phi_i^{(0)}\}$ of H_0 to span the effective part of H_I

necessary for the problem. Recall that $\phi_i^{(I)} = E_{I0}\ \phi_i^{(0)}$ so that formally $e_i^{(I)} = I(i)\ E_{I0}\ \phi_i^{(0)}$ for all i; hence even in H_I, the best results for our problem are obtained when E_{I0} becomes the identity nesting.

The non-monotonic convergence of the method of moments together with the question of best value for parameters usually present in the realization of the basis vectors would appear to be simultaneously solved if indeed the sets $\{\chi_i\}$ and $\{\phi_i\}$ of vectors span the same Hilbert space H_0. This is confirmed by the examples where in the attempt to span the same Hilbert space H_0 we obtain the best results, the chosen sets $\{\chi_i\}$, $\{\phi_i\}$ become identical and the method of moments reduces to the variational method. All the difficulties experienced inthe practical application of the method of moments thus appear to be fundamentally connected with our inability to realize the same Hilbert space $H_0 = L^2(\mathbb{R}^N,\tau)$ by two really distinct but measure-equivalent orthonormal basis sets.

Where the method has to be used, as in the examples considered, (i.e. as an alternative to the variational method), then the error involved (relative to the error the variational method would have produced) is identified with the difference between the identity nesting E_{00} and the nesting $(E_{b0})^*_{0b}$, which is easily determined from the respective measure τ_b and τ_0 of the realizations of the Hilbert spaces H_b and H_0, and is a more practical form of evaluating errors of the method of moments than the M_i numbers or any function of them. Eq.(36) illustrates this point. For minimum relative error we have $E_{00} - (E_{c0})^*_{0c} = 1 - (1 + b)^{-1/2} = 0$, and this implies that $b = 0$ with $H_c \equiv H_0$. $H_c \neq H_0$ for any other allowed value of b. In fact, as $b \to \infty$, the relative error tends to its maximum value 1. The same deduction obtains from Eq.(38) and both show that in general $(E_{b0})^*_{0b}(x)$, as a function of the space of their realization, $x \in \mathbb{R}^N$, are continuous and satisfy

$$0 < (E_{b0})^*_{0b} \leq 1 \quad ;$$

just like the M_i numbers of Eq.(10).

We conclude as follows:

1. The basis functions being employed in the application of the method of moments are seen, through correspondence established between the parameters they contain and the sequence of Hilbert spaces in nested Hilbert space, not to span the same Hilbert space as required in theory.

2. The results are therefore always less accurate than the variational method; the relative error, which depends on the parameters, is associated with the difference between the corresponding nesting operators and tends to zero with the values of the parameters that cause the basis sets to span the same Hilbert space.

3. The question, as to which of the two methods (variational or moments) is the better one, if conditions required by the latter in theory are truely realized, thus appears open.

p.s. Method of moments computations for the quartic oscillator, using two distinct but measure-invariant orthonormal basis sets of the $L^2(\mathbb{R},\tau)$ space, is now in progress and results will be published on completion.

V. NESTED VERSUS RIGGED HILBERT SPACE

Interpretation of the method of moments in terms of rigged Hilbert space appears, at first sight, to be equally possible. The theory of rigged Hilbert space is based on topological concepts. For details see [14,15,16], but it is briefly as follows.

Starting from a linear topological space V, in which a topology is introduced by a norm, a <u>countably normed space</u> V_φ, is defined as a linear topological space such that the neighbourhoods $U_{\rho,\theta}(0)$ of the zero element are given by a denumerable number of comparable, compatible norms with

$$\|v\|_1 \leq \|v\|_2 \leq \cdots, \leq \|v\|_\rho \leq \cdots \qquad \text{for all } v \in V \quad ,$$

where $U_{\rho,\theta}(0) = \{v \mid \|v\|_\rho < \frac{1}{\theta}\}$, $\theta > 0$ and ρ are positive integers; and which is complete with respect to the topology given by $U_{\rho,\theta}(0)$. A countably normed Hilbert space H_φ, is thus the topological limit of a sequence I, of normed Hilbert spaces H_ρ, with norm given by scalar product, $\|v\|_\rho = \sqrt{(v,v)_\rho}$, but in which the elements $\rho \in I$ are positive integers by definition, instead of real numbers as in nested Hilbert space. This creates the first difficulty.

To construct a rigged Hilbert space, a scalar product $(\cdot,\cdot)$ is further introduced into H_φ, to produce a <u>nuclear countably normed Hilbert space</u> (still denoted by the same symbol H_φ), if in addition to the usual properties of scalar product, this scalar product is such that $\lim_{n\to\infty} g_\varphi^{(n)} = g_\varphi$ with respect to the topology in H_φ

$$\Rightarrow \lim_{n\to\infty} (f_\varphi, g_\varphi^{(n)}) = (f_\varphi, g_\varphi) \tag{40}$$

for all $g_\varphi^{(n)}$, g_φ, $f_\varphi \in H_\varphi$.

The second difficulty is connected with the fact that the completion of H_φ with respect to the norm, $\| \ \| = \sqrt{(\cdot,\cdot)}$, produced by this scalar product, is what actually corresponds to the Hilbert space H_0 of our problems.

Condition (40) implies the existence of a continuous, linear, one-to-one operator $\underset{\sim}{T}$ (the properties of which are responsible for the name, nuclear) mapping H_φ into H_0; thus acting as the nesting operator $(E_{I0})^*_{0I}$. Because the topology of H_φ is stronger than the relative topology induced by H_0 on H_φ, H_φ is strictly a subspace of H_0. What should correspond to $H_{\bar\varphi}$ (through the order-reversing involution on I) in a nested Hilbert space approach, is H_{φ^x} , here defined as the space of continuous antilinear functionals on H_φ. Because $H_0 = H_{0^x}$ (i.e. $0 = 0^x$) we have the rigged Hilbert space as the triplet of spaces $H_\varphi \subset H_0 \subset H_{\varphi^x}$. The lack of symmetry between H_φ and H_{φ^x} notwithstanding, identification of H_φ with H_I of nested Hilbert space implies that only $\underset{\sim}{T}$ (corresponding to the nesting $(E_{I0})^*_{0I}$), the nuclear operators $\underset{\sim}{T}_n$ (corresponding to $(E_{In})^*_{nI}$) for integral $n \neq 0$ and $\underset{\sim}{T}^\ell_n$ (corresponding to $(E_{\ell n})^*_{n\ell}$) for integral n,ℓ with $n = \ell - 1$ and $\ell \neq 1$, are defined; irrespective of the linear topological space V, with which we start.

Recall the significance of the elements $b \in I$ in Eq.(29) and the role of the nesting $(E_{b0})^*_{0b}$ for all real values of $b \in I$ in Subsec.4.3. The corresponding quantities $\underset{\sim}{T}^\rho_0$ remain undefined for non-integral values of ρ in the rigged Hilbert space interpretation; and it is the source of the third difficulty. Finally, $H_\varphi \subset H_0$, whereas we need the possibility of $H_\varphi \equiv H_0$, when the best results are obtained in the examples considered, although the method of moments then reduces to the variational method. Even if these difficulties are somehow overcomed, interpretation of the method of moments in terms of rigged Hilbert space will apparently not be as simple nor comprehensive as is the case with nested Hilbert space interpretation.

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APPENDIX

This appendix contains the proof, by adaptation of the methods of Grossmann (1966), of the main

Theorem: The algebraic induction limit $H_I = [H_b; E_{db}; I]$ is a nested Hilbert space.

Proof: First, we prove a

Lemma: Suppose b and d are any two elements of I and a is defined as $a(i) = \min(b(i), d(i))$ for all i. If α_i is a sequence of numbers such that the series $\sum_i \alpha_i \phi_i^{(b)}$ and $\sum_i \alpha_i \phi_i^{(d)}$ are strongly convergent in H_b and H_d, respectively, then the series $\sum_i \alpha_i \phi_i^{(a)}$ is also strongly convergent.

Proof: From (29) $\|\phi_i^{(b)}\| = b^{-1}(i)$ and the set $\{\phi_i^{(b)}\}$ is orthogonal. Therefore, if Σ' denotes summation over a finite linear combination of the set of vectors, then

$$\| \sum_i{}' \alpha_i \phi_i^{(b)} \|^2 = \sum_i{}' |\alpha_i|^2 b^{-2}(i) ,$$

$$\| \sum_i{}' \alpha_i \phi_i^{(d)} \|^2 = \sum_i{}' |\alpha_i|^2 d^{-2}(i) .$$

Hence $$\| \sum_i{}' \alpha_i \phi_i^{(a)} \|^2 = \sum_i{}' |\alpha_i|^2 a^{-2}(i) \leq \sum_i{}' |\alpha_i|^2 (b^{-2}(i) + d^{-2}(i))$$

$$= \| \sum_i{}' \alpha_i \phi_i^{(b)} \| + \| \sum_i{}' \alpha_i \phi_i^{(d)} \|^2 .$$

$\therefore$ If the partial sums of $\sum_i \alpha_i \phi_i^{(b)}$ and of $\sum_i \alpha_i \phi_i^{(d)}$ are Cauchy sequences, then the partial sums of $\sum_i \alpha_i \phi_i^{(a)}$ are also Cauchy sequences. But H_a is complete, hence the series $\sum_i \alpha_i \phi_i^{(a)}$ is strongly convergent. ∎

Next, suppose $\phi^{(I)} \in E_{Ib} H_b \cap E_{Id} H_d$, where E_{Ib}, E_{Id} are natural embeddings of H_b, H_d, respectively, into H_I. From (27), (29) and the lemma above, it follows that the strongly convergent expansions $\phi^{(b)} = \sum_i \alpha_i \phi_i^{(b)}$ and $\phi^{(d)} = \sum_i \alpha_i \phi_i^{(d)}$ are vectors in H_b and H_d, respectively, and the series $\phi^{(a')} = \sum_i \alpha_i \phi_i^{(a)}$ is strongly convergent in H_a. But $E_{ba} \phi^{(a')} = \sum_i \alpha_i E_{ba} \phi_i^{(a)} = \sum_i \alpha_i \phi_i^{(b)} = \phi^{(b)}$; showing that $\phi^{(a')}$ should be denoted by $\phi^{(a)}$ and is the representation of $\phi^{(I)}$ in H_a. Hence $\phi^{(I)}$ $E_{Ia} H_a$ and

$$E_{Ia} H_a \supseteq E_{Ib} H_b \cap E_{Id} H_d \quad .$$

Eq.(24) is thus also satisfied.

To satisfy Eq.(25), consider the vectors in H_I, given by

$$\phi_i^{(I)} = E_{I0} \phi_i^{(0)} \tag{A.1}$$

and also the vectors in H_b and H_d, given, respectively, by

$$e_i^{(b)} = b(i) \phi_i^{(I)} \quad ; \quad e_i^{(d)} = d(i) \phi_i^{(I)} \tag{A.2}$$

for every $b, d \in I$, with $d > b$.

From (A.1) and (A.2), define the nesting E_{db} by

$$E_{db} \, e_i^{(b)} = \frac{b(i)}{d(i)} \, e_i^{(d)} \quad . \tag{A.3}$$

Then it follows from (20), (29) and (A.3) that

$$(E_{db})^*_{bd} \, e_i^{(d)} = \frac{b(i)}{d(i)} \, e_i^{(b)} \quad . \tag{A.4}$$

Define a unitary mapping $U_{\bar b b}$ from H_b onto $H_{\bar b}$ as

$$U_{\bar b b} \, e_i^{(b)} = e_i^{(\bar b)} \tag{A.5}$$

by linear extension and closure.

Since $\bar 0 = 0$, then by (A.5), $U_{\bar 0 0} = 1$. Also from (26), (A.5), (A.3) and (A.4), it follows that

$$U_{\bar b b} (E_{db})^*_{bd} U_{d \bar d} \, e_i^{(\bar d)} = U_{\bar b b} (E_{db})^*_{bd} U_{d \bar d} U_{\bar d d} \, e_i^{(d)}$$

$$= U_{\bar b b} (E_{db})^*_{bd} \, e_i^{(d)} = U_{\bar b b} \left(\frac{b(i)}{d(i)} e_i^{(b)} \right) = \frac{b(i)}{d(i)} \left(U_{\bar b b} \, e_i^{(b)} \right) ,$$

and that

$$E_{\bar b \bar d} \, e_i^{(\bar d)} = \frac{\bar d(i)}{\bar b(i)} \, e_i^{(\bar b)} = \frac{b(i)}{d(i)} \left(U_{\bar b b} \, e_i^{(b)} \right) ;$$

showing that

$$E_{\bar b \bar d} \, e_i^{(\bar d)} = U_{\bar b b} (E_{db})^*_{bd} U_{d \bar d} \, e_i^{(\bar d)}$$

for every i. Hence Eq.(25) is satisfied. ■

Note that a general element $b \in I$ can now be taken as $b(x)$ of (33), c of (34) or β of (39) and each satisfies the definitions in the proof of the theorem.

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