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SOME VARIATIONAL PROPERTIES OF HARMONIC OSCILLATOR WAVE FUNCTIONS*

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ABSTRACT

We study some variational properties of harmonic oscillator wave functions, when the frequency of the oscillator is considered as a variational parameter. Several Variational Theorems relating to matrix elements of an arbitrary Hermitian operator with respect to oscillator functions, and to the overlap of an arbitrary normalizable function with these wave functions, are established.

RESUMEN

Se analizan algunas propiedades de las funciones de onda del oscilador armónico, mediante principios variacionales, cuando se considera a la frecuencia del

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oscilador como el parámetro variacional. Se consideran los elementos de matriz de un operador hermitiano arbitrario con respecto a funciones de oscilador y se establecen algunos teoremas variacionales que satisfacen estos elementos de matriz. Asimismo se demuestran algunos teoremas variacionales que satisface el traslape de una función normalizada arbitraria con las funciones de oscilador.

I. INTRODUCTION

The harmonic oscillator has played a very important role in some of the recent developments in the theory of finite many-body systems, especially in nuclear theory, in which it has been used extensively[1]. This is of course due to the fact that harmonic-oscillator wave functions (HOF) are easy to calculate with, since they have a number of particular properties. Among these, one could mention the symmetry between configuration and momentum space, the existence of the SU_3 symmetry and most important of all, the possibility of separating the relative motion from the center-of-mass motion in the two-body system, which makes the calculation of the nuclear-interaction matrix elements with respect to HOF, quite simple[2].

In this paper we shall discuss some variational properties of the harmonic oscillator which, to the best of our knowledge, have not previously been discussed in the literature. Whenever one uses a set of HOF to solve Schrödinger's equation, the eigenvalues and eigenvectors of the system depend on the frequency ω of the oscillator. In some calculations, this frequency is fixed by a simple comparison between theory and experiment. More frequently, however, ω is used as a free parameter to be determined at the end of the calculation. The properties of the harmonic oscillator we now discuss, are relevant when ω is used as a variational parameter and the calculation follows essentially the ideas of the Ritz variational method[3].

The theorems to be discussed below were first discovered when a variational calculation of the ground-state energy of the hydrogen atom was carried out using a finite set of HOF[4]. After diagonalizing the matrix of the Coulomb Hamiltonian we noticed that if we maximize the overlap of the lowest eigenstate of this matrix

with the ground state HOF, using the frequency of the harmonic oscillator as a variational parameter, then the overlap of this eigenstate with the first excited HOF is zero. This is shown in Fig. 1. In section II we generalize this result, and show that the result is independent of the actual Hamiltonian used, being a property of HOF.

The second type of properties we discuss here has to do with the variational properties of the matrix elements of an Hermitian operator with respect to HOF. These properties are again independent of the specific form of the Hermitian operator O and have to do solely with special characteristics of the harmonic oscillator and its eigenfunctions.

As in the case of the overlap theorem, the variational properties concerning matrix elements of O, were discovered when calculating the ground-state energy of the hydrogen atom, using a finite set of HOF. We realized that when the value of the frequency ω is chosen to get a minimum value for

$$< 00 \mid H \mid 00 >$$

the matrix element

$$< 00 \mid H \mid 10 >$$

vanishes. Here $\mid 00>$ and $\mid 10>$ represent the ground-state and first excited HOF, with quantum numbers $n = 0$, $l = 0$ and $n = 1$, $l = 0$, respectively. In the numerical example we refer to, H is the Coulomb Hamiltonian. If one now uses the value of ω so determined, it is extremely simple to prove that the lowest eigenvalue of the two matrices coincide; one of these matrices is built by using zero-quantum HOF only and the other by including both zero and two-quantum states. This is shown for the Coulomb problem in Fig. 2[5].

II. VARIATIONAL PROPERTY OF THE OVERLAP

Let us consider an arbitrary normalizable function, characterized by angular momentum l and projection m,

$$\Psi_{lm}(r) = \psi_l(r)\, Y_{lm}(\theta, \varphi) \tag{2.1}$$

and the eigenfunction of the harmonic oscillator

$$\Phi_{nlm}(r) = \beta^{3/2}\, \mathcal{R}_{nl}(\beta r)\, Y_{lm}(\theta, \varphi)$$

which corresponds to the principal quantum number n and the same angular quantum numbers as $\Psi_{lm}(r)$. Here $\beta = \sqrt{M\omega/\hbar}$, where M is the oscillator mass.

We define the overlap between Ψ_{lm} and Φ_{nlm} as

$$I_n^l(\beta) = \int \Psi_{lm}^{*}(r)\, \Phi_{nlm}(r)\, d^3r$$

$$= \beta^{3/2} \int_0^{\infty} \psi_l(r)\, \mathcal{R}_{nl}(\beta r)\, r^2 dr \tag{2.2}$$

and consider this overlap integral for all values of n, from zero to a maximum value N. We now form the sum of its squares

$$K_N^l(\beta) = \sum_{n=0}^{N} \left[I_n^l(\beta) \right]^2 . \tag{2.3}$$

If N goes to infinity, since the set of functions Φ_{nlm} is a complete system of orthogonal functions and $\Psi_{lm}(r)$ is normalized, $K_{\infty}^l(\beta) = 1$, independently of the value of β. For any finite value of N, on the other hand, we have

$$0 \leqslant K_N^l(\beta) \leqslant 1 . \tag{2.4}$$

We can now state the generalization of the result mentioned in the introduction, as the following theorem:

If $I_N^l(\beta) \neq 0$, the value of the parameter β that makes $K_N^l(\beta)$ an extremum,

is such that

$$I^{l}_{N+1}(\beta) = 0 \quad . \tag{2.5}$$

In order to prove the theorem, we derive $K^{l}_{N}(\beta)$ and equate the result to zero,

$$\frac{dK^{l}_{N}(\beta)}{d\beta} = 2 \sum_{n=0}^{N} I^{l}_{n}(\beta) \frac{dI^{l}_{n}(\beta)}{d\beta} = 0 \tag{2.6}$$

Since

$$\frac{dI^{l}_{n}(\beta)}{d\beta} = \frac{3}{2} \int_{0}^{\infty} \psi^{*}_{l}(r)\, R_{nl}(\beta r)\, \beta^{1/2}\, r^{2} dr$$

$$+ \int_{0}^{\infty} \psi^{*}_{l}(r) \frac{d}{d(\beta r)} R_{nl}(\beta r) \beta^{3/2} r^{3}\, dr ,$$

the condition given in eq. (2.6) is equivalent to

$$\sum_{n=0}^{N} \sqrt{(2n+2l+3)(2n+2)}\; I^{l}_{n+1} I^{l}_{n} - \sum_{n=1}^{N} \sqrt{(2n+2l+1)2n}\; I^{l}_{n-1} I^{l}_{n} = 0 . \tag{2.8}$$

To obtain this expression, use has been made of the following relation

$$2\beta r \frac{dR_{nl}(\beta r)}{d(\beta r)} = \sqrt{(2n+2l+3)(2n+2)}\; R_{n+1,l} - \sqrt{(2n+2l+1)2n}\; R_{n+1,l} - 3R_{nl} . \tag{2.9}$$

Changing the dummy index from n to $n' - 1$ in the first summation of Eq. (2.8), this equation becomes

$$\sqrt{(2N+2l+1)(2N)}\; \overline{I^{l}_{N} I^{l}_{N+1}} = 0 \tag{2.10}$$

which proves the theorem.

It is clear, from the way the proof goes, that the result is valid for any value of l and for a normalizable function Ψ_{lm} of arbitrary r-dependence.

III. VARIATIONAL PROPERTY OF THE MATRIX ELEMENTS.

We shall now consider the variational properties of the matrix elements of an arbitrary scalar Hermitian operator H, with respect to HOF. If we use Eq. (2.9) it is very simple to prove that

$$
\begin{aligned}
2\beta \frac{d}{d\beta} \langle ml|H|nl\rangle = & \sqrt{(2n+2l+3)(2n+2)}\ \langle ml|H|n+1\ l\rangle \\
& - \sqrt{(2n+2l+1)(2n)}\ \langle ml|H|n-1\ l\rangle \\
& + \sqrt{(2m+2l+3)(2m+2)}\ \langle m+1\ l|H|nl\rangle \\
& - \sqrt{(2m+2l+1)(2m)}\ \langle m-1\ l|H|nl\rangle\ ,
\end{aligned}
\tag{3.1}
$$

which in the case $m = n$, because H is a Hermitian operator, reduces to the following relation,

$$
\begin{aligned}
\beta \frac{d}{d\beta} \langle nl|H|nl\rangle = & \sqrt{(2n+2l+3)(2n+2)}\ \langle nl|H|n+1, l\rangle \\
& - \sqrt{(2n+2l+1)(2n)}\ \langle nl|H|n-1\ l\rangle\ .
\end{aligned}
\tag{3.2}
$$

This result clearly represents the generalization of the variational property of the matrix elements of H, mentioned at the end of the introduction. This is so, since for $n = 0$, the second term in the right-hand side of (3.2) does not exist.

Using the property given in Eq. (3.1) we can prove some variational properties of the spectrum of an arbitrary central Hamiltonian H, when the spectrum is calculated in the finite space generated by a set of N HOF. Let us consider the case of the second cumulant σ^2, as an example. As is well known[6], if we perform a variational calculation of the spectrum of H, and look for the best representation of each eigenstate of H, on the average, in terms of a single HOF, then we should look for the minimum value of σ^2. We now discuss what this will imply.

We define the trace of H by the following equation

$$[T_r\, H]^l_N = \sum_{n=0}^{N} \langle nl | H | nl \rangle \tag{3.3}$$

and the second cumulant σ^2_N, as

$$\sigma^2_N = \frac{1}{N} [T_r\, H^2]^l_N - \frac{1}{N^2} \left\{ [T_r\, H]^l_N \right\}^2 . \tag{3.4}$$

Using Eqs. (3.1) and (3.2) the derivative of σ^2_N with respect to β can be readily calculated; one obtains, after some single algebraic manipulations,

$$\frac{1}{2}\beta \frac{\partial \sigma^2_N}{\partial \beta} = \sqrt{(2N+2l+3)(2N+2)} \sum_{n=0}^{N} \left\{ \frac{1}{N} \langle Nl | H | nl \rangle \langle nl | H | N+1\, l \rangle \right.$$

$$\left. - \frac{1}{N^2} \langle nl | H | nl \rangle \langle Nl | H | N+1, l \rangle \right\} . \tag{3.5}$$

We see from this expression that the derivative of σ^2_N is equal to zero if

$$\langle nl | H | N+1\, l \rangle = 0, \qquad n = 0, 1, \ldots, N . \tag{3.6}$$

In other words, we have $N+1$ independent conditions altogether. As we only have one variational parameter, namely β, conditions (3.6) cannot in general all be fulfilled for the same value of β. One could, however, impose the least square fit condition, namely that

$$\sum_{n=0}^{N} \{ < nl \mid H \mid N+1\ l > \}^2 \tag{3.7}$$

be a minimum, and determine β by this requirement.

IV. CONCLUSION

We see from our discussion that when one is using a set of HOF in a variational calculation, the frequency ω of the harmonic oscillator can be determined by many different criteria. Some of them, as the one mentioned in connection with Eq. (3.7), can be useful in special circumstances. The best criterion will, of course, depend on the type of calculation one wishes to perform.

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REFERENCES

1. K.T.R. Davies, S.J. Krieger and M. Baranger, Nucl. Phys. 84 (1966) 545. P. Kramer and M. Moshinsky, "Group Theory of Harmonic Oscillators and Nuclear Structure", Edited by E.M. Loebl, Academic Press, New York, 1968. T.T.S. Kuo and G.E. Brown, Nucl. Phys. 85 (1966) 87.
2. T.A. Brody and M. Moshinsky, "Tables of Transformation Brackets", Gordon and Breach, New York, 1967.
3. B. Moiseiewitsch, Variational Principles, Interscience Publ., London 1966.
4. M. Dubovoy, Tesis de Físico (U.N.A.M., México 1968).

5. M. Moshinsky and O. Novaro, J. Chem. Phys. 48 (1968) 4162.
W. Yeh, to be published.
6. J.B. French, "Spectral Distributions in Nuclei", Dacca Lectures, 1967.

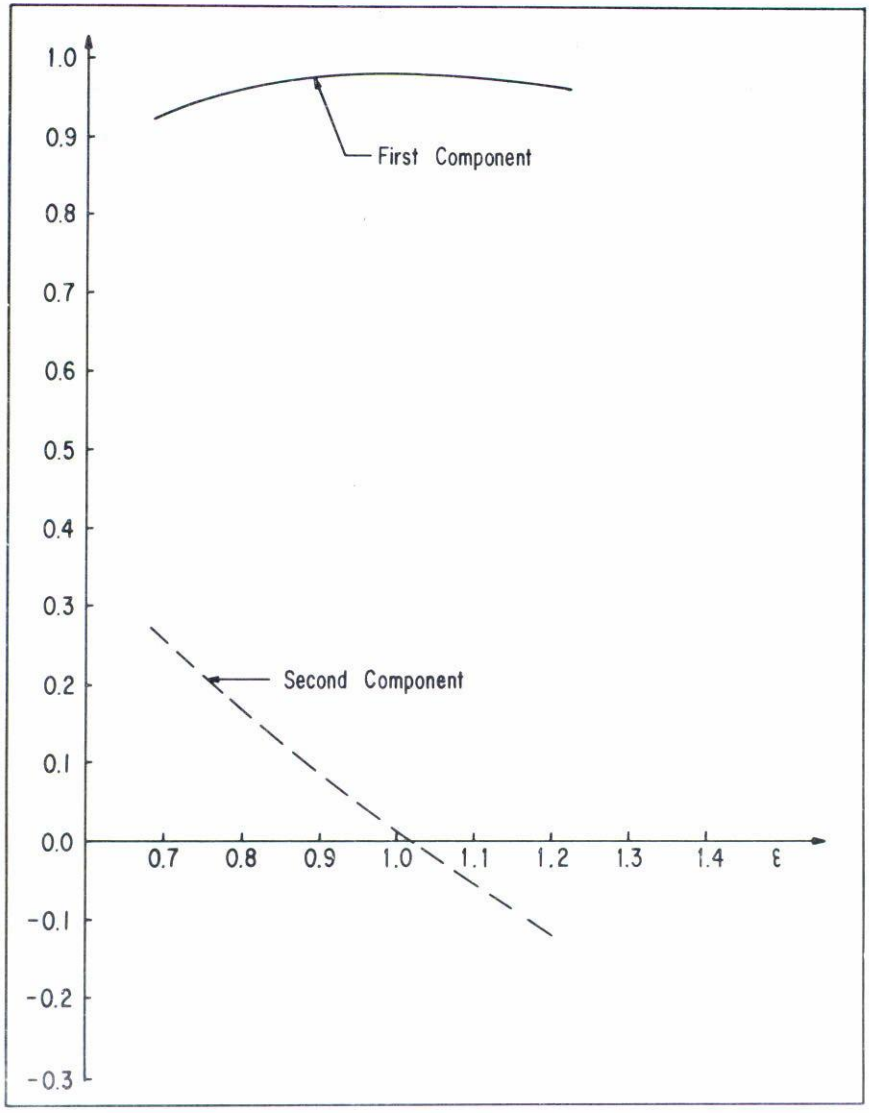

Fig. 1.- Overlap of the ground-state wave function of the Coulomb problem with the zero-quantum state (solid line) and with the two-quantum state (dotted line) as a function of the parameter $\epsilon = [\hbar\omega/(me^4/2\hbar^2)]^{1/2}$ where m and e are the electron mass and charge.

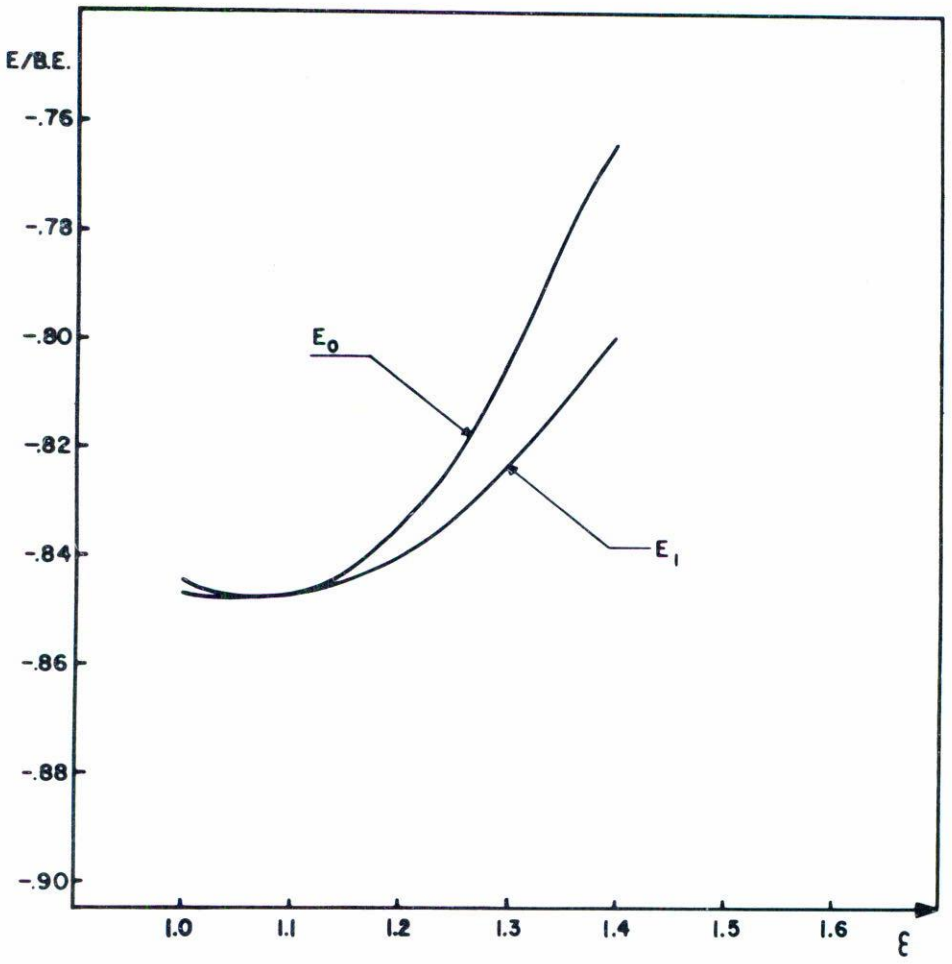

Fig. 2.- Energies E_0 and E_1 for approximations of up to zero and two-quantum states for the hydrogen atom problem as a function of the parameter $\epsilon = [\hbar\omega/(me^4/2\hbar^2)]^{1/2}$. The energy unit is that of the first Bohr orbit.