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Short Communications

Hypervirial Theorems and Restrictions on Wave Functions

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The conditions that ensure that an optimal variational wave function ϕ under general restricting requirements satisfies the hypervirial theorem are analysed. Application is made to a system where the z-component of angular momentum is a constant of motion and results are discussed in connection with those obtained via symmetry considerations.

Key Words: Hypervirial theorem – Variational wave functions.

An optimal variational wave function ϕ satisfies the equation

$$\langle \delta\phi \,|(H-E)\phi\rangle + \langle \phi \,|(H-E)\delta\phi\rangle = 0. \tag{1}$$

If $\mathrm{i}W\phi$ is a possible variation $\delta\phi$ for a Hermitian operator W, then from Eq. (1) it can be deduced that the diagonal hypervirial theorem

$$\langle \phi|[H, W]|\phi\rangle = 0 \tag{2}$$

is satisfied [1, 2]. Epstein [3] pointed out that when ϕ has a certain symmetry, then the condition $\delta\phi = \mathrm{i}W\phi$ must be replaced by $\delta\phi = \mathrm{i}SW\phi$, where S is the projector onto the symmetry type in question, because possible variations have to obey their intrinsic symmetries. So, we are lead into the variational calculation with restricting conditions. It is the purpose of this note to draw attention to the fact that the symmetry conditions pointed out by Epstein are a particular case of more general restricting conditions. Let us suppose that we wish to optimize a wave function ϕ in a variational way in order to obtain a function belonging to a closed subspace M of the Hilbert space associated with our system. Then it is clear that compatible variations for ϕ must belong to M. Particularly, if W is a linear operator and P_M is

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the projection operator onto M which commutes with H, then

$$\langle\phi|[H, W]|\phi\rangle=\langle\phi|H, \tilde{W}]|\phi\rangle \tag{3}$$

for $\tilde{W}=P_M W P_M$. It is evident that $\mathrm{i}\tilde{W}\phi$ is a possible variation $\delta\phi$, and moreover, in this case, the variational theorem conducts to the hypervirial theorem. When P_M is a projector onto a symmetry type, these results are equivalent to those obtained by Epstein [3] because $\tilde{W}\phi=P_M W\phi$. If $W\phi$ belongs to the subspace orthogonal to M, then $\tilde{W}=0$. According to Chen [4] it is achievable to introduce a variational parameter in a wave function ϕ by applying the evolution operator $U(a, a_0)$, defined as

$$U(a, a_0)\phi(a_0)=\phi(a) \tag{4}$$

which satisfies the equation

$$\frac{\partial U}{\partial a}=A(a)U \tag{5}$$

for A being an anti-Hermitian operator. But there remains as an open question how to introduce such variational parameters when the wave functions have to fulfill certain requirements. The answer is simple due to the possibility of employing the variational wave function

$$\phi^M(a)=P_M\phi(a)=P_M U(a, a_0)\phi(a_0) \tag{6}$$

where

$$\frac{\partial\phi^M}{\partial a}=P_M A\phi^M \tag{7}$$

is a variation for ϕ^M which satisfies the requirement of belonging to M. It is important to note that if ϕ is normalized, then ϕ^M, in general, is not, because

$$\langle\phi^M|\phi^M\rangle\leq\langle\phi|\phi\rangle.$$

When studying certain physical systems, it is found that some operators commute with the Hamiltonian operator H. In his turn, some of these commuting operators are Hermitian and they are associated with constants of motion. In such cases, variational wave functions are searched so as they are eigenfunctions of that kind of operators. Let us assume that the Hermitian operator R commutes with H. Then, applying the Lie identity

$$[H, [R, W]]+[W, [H, R]]+[R, [W, H]]=0 \tag{8}$$

for any linear operator W, we can deduce from previous discussion that the hypervirial theorem

$$\langle\phi|[H, [R, W]]|\phi\rangle=0 \tag{9}$$

will be satisfied. Assuming that our variational wave function is eigenfunction of R with eigenvalue r, then if P_r is the projector onto the subspace of eigenfunctions of

R with eigenvalues r, we have

$$P_r[R, W]\phi = RP_rW\phi - rP_rW\phi = 0. \tag{10}$$

In order to illustrate preceding formal conclusions, we choose as an example that one given by Epstein [3], i.e. a system where the z-component of angular momentum L_z is a constant of motion. Then, if ϕ is eigenfunction of L_z

$$\langle\phi|[L_z, W]|\phi\rangle = 0 \tag{11}$$

and the hypervirial operators are $\{v_{ij} = x_ip_j\}$, we arrive at the tensor virial theorem [5, 6]. First of all we note that

$$[L_z, v_{xx}] = i\hbar v_{xy} \tag{12}$$

so that we are sure that

$$\langle[H, v_{xy}]\rangle = 0. \tag{13}$$

One and the same occurs with the remaining off-diagonal equations. On the other hand, from the equality

$$[L_z, v_{yx}] = i\hbar(v_{yy} - v_{xx}) \tag{14}$$

we can assert that if the theorem is satisfied for v_{xx}, then it is fulfilled for v_{yy} too. In conclusion, if the virial theorem and the equation

$$\langle[H, v_{xx}]\rangle = 0 \tag{15}$$

are satisfied, then all the other equalities which constitute the tensor virial theorem will do the same. But these were the results obtained by Epstein [3] via symmetry considerations.

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