

Some Remarks about a Trial Wave Function for the Ground State of Two-Electron Atoms

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A trial wave-function for the ground state of two-electron atoms is presented with a pedagogical purpose.

Uma função de onda tentativa para o estado fundamental de átomos com dois elétrons é apresentada com objetivos pedagógicos.

In a recent article a trial wave function for the ground state of two-electron atoms was presented with a pedagogical purpose¹. Such simple two-parameter trial wave function was proposed on physical grounds and has the following form (in a.u.)

$$\psi(r_1, r_2) = N \exp(-\alpha(sr_> + r_<)) ; \quad r_1 \neq r_2 \quad (1)$$

For the special case when $r_1 = r_2$

$$\psi(r_1, r_2) = N \exp[-\alpha(s+1)(r_1 + r_2)/2] \quad (2)$$

where α and s are variational parameters and

$$r_> = \max(r_1, r_2) \quad ; \quad r_< = \min(r_1, r_2)$$

The numerical results for the first four members of the helium isoelectronic sequence yield very good results with an evaluation procedure almost as simple as that corresponding to a one-parameter variational calculation. The authors remark that the chosen wave function

preserves the symmetry between the coordinates r_1 and r_2 of the two electrons. In this note we want to discuss this point more thoroughly because it is very interesting with regard to the indistinguishability principle of identical particles and may be useful in the courses in quantum mechanics.

The authors compare the wave function (1) with the Hylleraas-like function

$$\psi(r_1, r_2) = M \exp[-\alpha^1(r_1+r_2)] (1 + c|r_1-r_2|) \quad (3)$$

and note that (1) may be looked upon as a generalization of (3). But it is useful to compare the wave function (1) with Eckart's wave function²

$$\psi(r_1, r_2) = P \{ \exp[-\gamma(\beta r_1 + r_2)] + \exp[-\gamma(\beta r_2 + r_1)] \} \quad (4)$$

which is based on the same physical grounds as those given by Srivastava and Bhaduri¹. The wave function (4) may be written as a function of coordinates $r_>$ and $r_<$

$$\psi(r_>, r_<) = P \{ \exp[-\gamma(\beta r_> + r_<)] + \exp[-\gamma(\beta r_< + r_>)] \} \quad (5)$$

We can see that the wave function (5) is a generalization of the wave function (1). Furthermore (5) preserves not only the symmetry between the coordinates r_1 and r_2 of the two electrons but also between the coordinates $r_>$ and $r_<$, while the wave function (1) does not preserve the latter. From the point of view of the indistinguishability principle of identical particles^{3,4} the following equality must be satisfied for fermions

$$\psi(\xi_1, \xi_2) = -\psi(\xi_2, \xi_1) \quad (6)$$

where ξ_1 and ξ_2 represent the set of three coordinates and the spin projection of each particle. For the particular case of the ground state of two-electron atoms, taking a spin-independent Hamiltonian, Eq.(6) is reduced to

$$\psi(\eta_1, \eta_2) = \psi(\eta_2, \eta_1) \quad (7)$$

where η_1 and η_2 represent the set of three coordinates. Then for every set of coordinates, Eq. (7) must be satisfied, and so the wave function (5) is strictly related to the indistinguishability principle, whereas the wave function (1) is not.

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