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A COMPACT CI WAVEFUNCTION FOR HELIUM AND HYDRIDE ION

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Configuration interaction (CI) and explicit introduction of interelectronic coordinates are approaches commonly employed in obtaining wavefunctions which are more accurate than Hartree Fock. The disadvantage of the CI method is the large number of configurations required while the explicit introduction of interelectronic coordinates causes difficulties in integral evaluation. To overcome these problems the interelectronic coordinates are introduced via correlated Gaussians and the expansion functions taken to be $\underline{\bar{\Phi}}_o$ the self consistent determinant and $\left\{\bar{G}_k^+ \underline{\bar{\Phi}}_o\right\}$ is a function obtained from $\left\{\bar{G}_k^+ \underline{\bar{\Phi}}_o\right\}$ which is constructed using a strong orthogonality projection operator[1], and is expressed entirely in terms of Gaussians and correlated Gaussians. The wavefunction for helium and hydride ion are presented using this method.

Reference

1. Handy, N. C. (1973). *Mol. Phys.*, **26**, 169.