CORRELATION INDUCED OPTIMIZATION OF WAVE FUNCTIONS

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9.7 cm

We determine the explicit form of the single-particle wave functions $\{w_i(\mathbf{r})\}$ appearing in the parameters of quantum models such as the Hubbard and the Anderson models. Namely, the rigorous form of the renormalized wave equation is derived by treating the system ground state energy in a correlated state as a functional of $\{w_i(\mathbf{r})\}$ and their derivatives. For the first example - the Hubbard chain - the optimized basis is obtained only **after** the electronic correlations have been included in the rigorous Lieb-Wu solution for the ground state energy. The principal features of the solution are obtained variationally starting from the atomic basis for the s-type wave functions. The results for the ground state energy, the size of the renormalized orbitals, and the intersite-interaction parameters, **all as a function of the lattice constant**, are shown. In the second part, H_2 molecule is treated in the same manner. The renormalized wave equation and the optimized orbitals are obtained for the lowest eigenvalue, to further illustrate the method. The comparison between the relevant quantities for the Hubbard chain and the H_2 system is also made.

13.4 cm

Subject category :

1. Correlated Electrons and High Temperature Superconductors

Presentation mode :
poster

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