Summary Hartree-Fock Stability of HEG

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I. BACKGROUND

The Hartree-Fock procedure has been implemented the quantum many-body problem since its inception and remains the basis for many more advanced techniques even today. In general, the eigenstates of the Hartree-Fock Hamiltonian are solved self-consistently. However, this procedure ensures only that the solution is stationary with respect to the determined orbitals. A method for determining the stability of a Hartree-Fock solution was proposed by Thouless in 1960[1]. The condition for stability of a Hartree-Fock solution is equivalent to the conditions for unstable (complex frequency) many-body oscillations within the Random Phase Approximation (RPA). The condition was rederived into the expression familiar to quantum chemists by Cizek and Paldus in 1967[2]. Furthermore, the stability equations factorize depending on the symmetry of the Hartree-Fock eigenfunctions. To this end, Seeger and Pople outlined a hierarchical approach to systematically evaluate the stability of HF states in the restricted, unrestricted and generalized Hartree-Fock procedures[3]. Recently, the method has been used to aid the in search for the lowest energy Unrestricted Hartree-Fock (UHF) solutions in molecules, as well as the General Hartree-Fock (GHF) solutions in geometrically frustrated hydrogen rings which cannot conform even to the UHF scheme [4][5].

The presence of GHF solutions to the Homogeneous Electron Gas which have lower energy than the RHF solutions was proven in the landmark paper by Overhauser[6]. Later still, the ground state energies of the electron gas were found to great accuracy by Ceperley and Alder [7]. In the past few years, phase diagrams have been determined for the HEG in 2 and 3 dimensions[8][9][10]

II. REFERENCES

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