Spin projection energies in RHF: application to quantum dots

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In the last years both Hartree-Fock (HF) and density functional theory (DFT) have been extensively applied to study different properties in a variety of electronic nanostructures with occupations that range from moderate to large number of electrons, for which more exact methods, such as exact diagonalization, quantum Monte Carlo or configuration interaction, are not feasible. The importance of correlations in circular quantum dots depends on the so-called Wigner parameter (R_W), which is a measure of the relative strength between electron-electron interaction and external confinement. Whereas for high density (weak interaction) a single-particle picture is valid and the system can be adequately described within a space restricted mean field formalism (RHF, RDFT), for low density (strong interaction) the electronic structure is more adequately described by allowing the electrons to localize, forming a so-called Wigner molecule, similar to that found in the 2D electron gas in the strong correlation limit [1]. In this latter case it has been shown that a space unrestricted formalism (UHF, UDFT) can provide a better description of the electronic structure [2,3]. A common drawback in all mean field calculations lies in its failure to work with good total spin states, *i.e.* eigenstates of the $\hat{S}^2$ operator. Spin symmetry, as well as rotational symmetry for UHF, restoration methods have proved to be a valuable technique, which led to improved energy estimates and at the same time is able to provide predictions for total spin and orbital angular momentum [3,4].

In this work we concentrate on the spin symmetry restoration technique [5], based on the evaluation of the spin projection operator acting on a Slater determinant (SD) with the help of the Sanibel coefficients [3,6]. This total spin eigenstate is simply expressed as a linear combination of a big new set of SD's obtained by performing all possible spin-exchange operations over the initial state. This state can then be used to estimate different physical quantities through the calculation of appropriate expectation values. We apply this formalism to circularly confined quantum dots, described within RHF, and show how the corresponding expectation values for the total energy and several other observables can be efficiently computed for an arbitrary number of electrons. The predictions for the total spin projection (S, S_z) corresponding to the lowest energy solution are discussed as a function of R_W and the strength of a vertically applied magnetic field. The projected total energies are also compared with their RHF counterparts, and explicit expressions for the evaluation of expectation values of arbitrary, but spin-independent, one- and two-body operators are provided. As an example we compute the particle density variation in the different spin channels.

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