Spin contamination in quantum dot RHF states: a phase diagram

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In recent years, semiconductor heterostructures, such as quantum dots and rings, have been the subject of many experimental and theoretical investigations. The success in controlling several system parameters, including shape, size or electron number encourages its potential use in future applications as nanoscale electronic devices. From a theoretical point of view the electronic structure of these systems has been studied using different methods [1]. Quantum Monte Carlo (QMC), configuration interaction (CI) or exact diagonalization (ED) have proved to give quite accurate results for moderate number of electrons $N \leq 13$. For larger electron numbers all these methods become exceedingly demanding for computational purposes and the electronic properties must be analyzed by resorting to simpler approximate methods such as Hartree-Fock (HF) or density functional theory (DFT). Depending on the relative strength of electron-electron interaction versus confinement, represented by the Wigner parameter (R_W), space restricted (RHF, RDFT) or unrestricted (UHF, UDFT) formalisms are more suitable to describe the state of the system [2,3]. In either case the many body wave function is represented by a single Slater determinant which in general is not an eigenstate of the total spin operator $\hat{S}^2$, thus breaking an exact symmetry of the hamiltonian. This failure to describe an adequate spin wave function can be important when trying to explain the dependence of spin properties, like singlet-triplet transitions, with the intensity of an applied magnetic field, as the mixing or *contamination* of different total spin states may result in wrong predictions for these quantities. Methods of spin restoration, pioneered by Löwdin [4] in the 1950s, (see [5] for a recent application to quantum dots), provide a useful way to solve this problem by projecting the mixed spin wave function onto different eigenstates of the total spin operator. In this work we analyze in detail the spin properties of the RHF ground states for parabolically confined quantum dots as a function of two parameters: the intensity of an applied magnetic field (B) and the relative strength of interaction over confinement (R_W). The (B-R_W) spin phase diagram is presented for quantum dots containing different number of electrons, clearly identifying regions where the spin dispersion varies from zero to its maximun allowed value. The same method can also be applied to analyze UHF or DFT states with arbitrarily high number of electrons.

References:

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