There are systems which cannot be describe by a simple mean-field state within DFT. Trying to describe them, nonetheless, with DFT runs into strange problems already with the static iteration. Many atoms show this problem. We discuss here as simple example the carbon atom. Figure 1

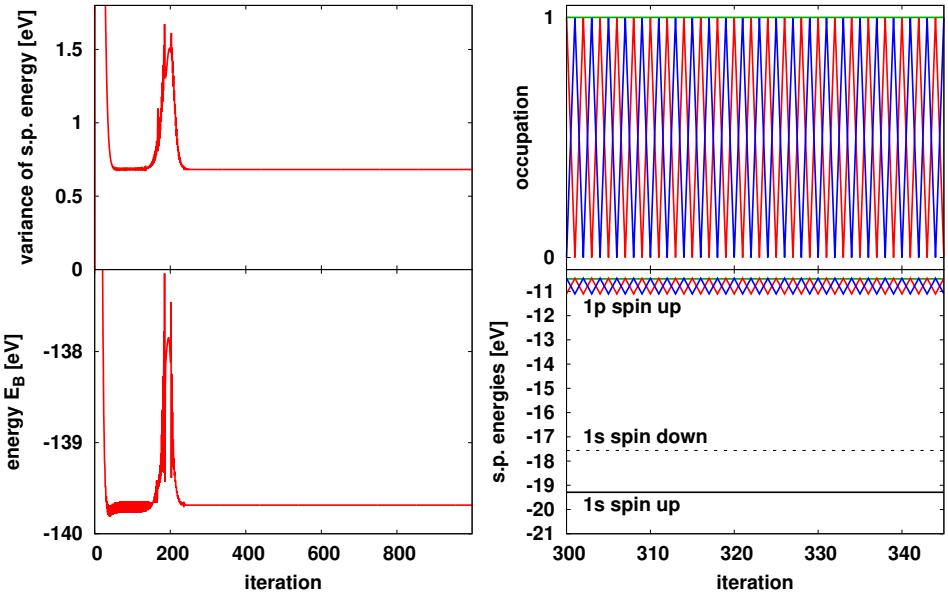

Figure 1: Evolution of static iterations for the C atom as function of iteration number. Lower left: total energy. Upper left: average variance of s.p. energies. Lower right: lowest s.p. energies as indicate. Upper right: Occupation numbers in the spin-up 1p shell.

shows the (non-)convergence pattern of four crucial observables. The total energy in the lower left panel gives the impression of perfect convergence in that it approaches quickly a stable asymptotic value. However, the average variance of s.p. energies (upper left) is stuck at a too large value. Even when playing with iteration parameters, there is no way to reduce the final variance significantly. What happens becomes apparent when looking at the behavior of s.p. energies and occupation numbers in detail. This is done in the two right panels whereby we concentrate on states which have a chance to be occupied. We see that there are two states in the $1p$ shell never stop to exchange occupations from one iteration to the next. Recall that C has total spin 1 in its ground state. The $1s$ shell is occupied by two electron, spin-up and spin-down. The two remaining electrons are both spin-up to form a spin 1 configuration as observed in experiment. The two electrons have three states to fill in the $1p$ shell. Whichever two states we decide to fill the emerging Kohn-Sham field yields s.p. energies which prefer the other configuration (if the states are occupied in energy order as should be done). Such systems as the C atom require correlated states

to obtain a unique ground state. Unfortunately, there is no simple rule to tell in advance when such an unstable situation will occur as soon as one deals with molecules because then the electronic state depends sensitively on the ionic configuration. The user has to be alert to spot the problem if it happens.