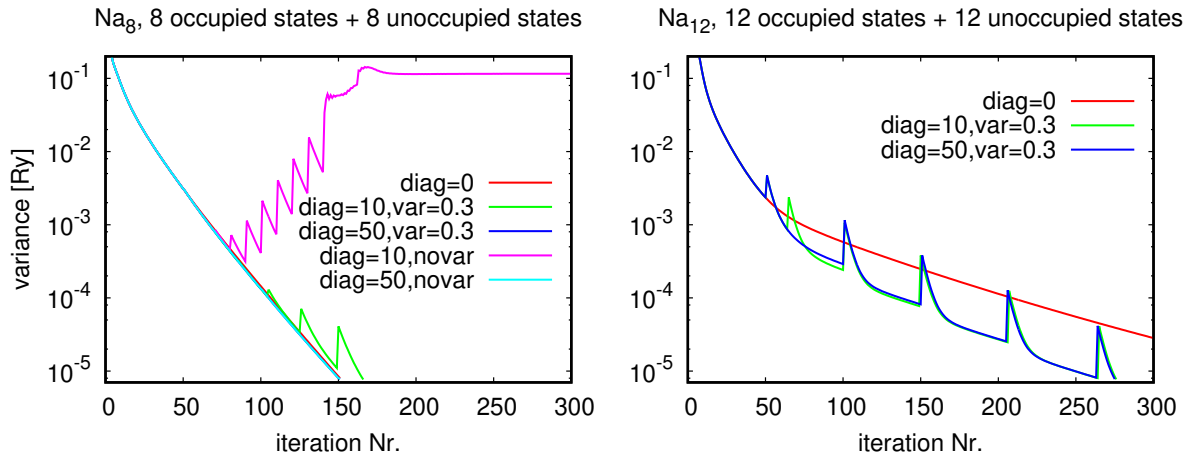
# Static iterations in 3D code – speed and (in-)stability

Discussion file: QDD project

15. May 2019

The static iteration in the triaxial cluster code "QDD" is based on accelerated gradient iteration. To speed up, one can invoke an occasional exact diagonalization of the actual mean-field Hamiltonian. The modulus for this action is the parameter `ifhamdiag`. It is supposed to improve convergence if the pool of s.p. states contains also a couple of unoccupied states. In the nuclear 3D code, this strategy works so efficiently that one uses `ifhamdiag`=1 as standard. This turns out to be nod the case for molecules/clusters. The problem is analyzed here using the test case of $Na_8$ and $Na_{12}$ with ionic background.




The above figure shows the evolution of total variance (r.m.s. average of s.p. variances) with iterations. We look first at the left panel, showing results from $Na_8$. The parameter `ifhamdiag` is abbreviated by the label "diag". The parameter "(no)var" stands for a stabilizing criterion explained below. At the moment, we concentrate on "novar" which means that diagonalization is done strictly at every "diag" iteration. Reference is the case "diag=0" which is straightforward damped gradient iteration without diagonalization steps. It converges steadily and fast. Switching to very occasional diagonalization with "diag=50,novar" improves a tiny bit. Calling for more diagonalization with "diag=10,novar" destroys convergence completely. The hindrance is the interplay with the update of mean field. Diagonalization in the subspace changes the mean field suddenly. Even if that may be only a little, the perturbation has not calmed down sufficiently before the next diagonalization step such that perturbations accumulate.

The solution is, of course, to choose the proper distance between diagonalizations. However, this distance depends on the system and it is asking to much from a standard

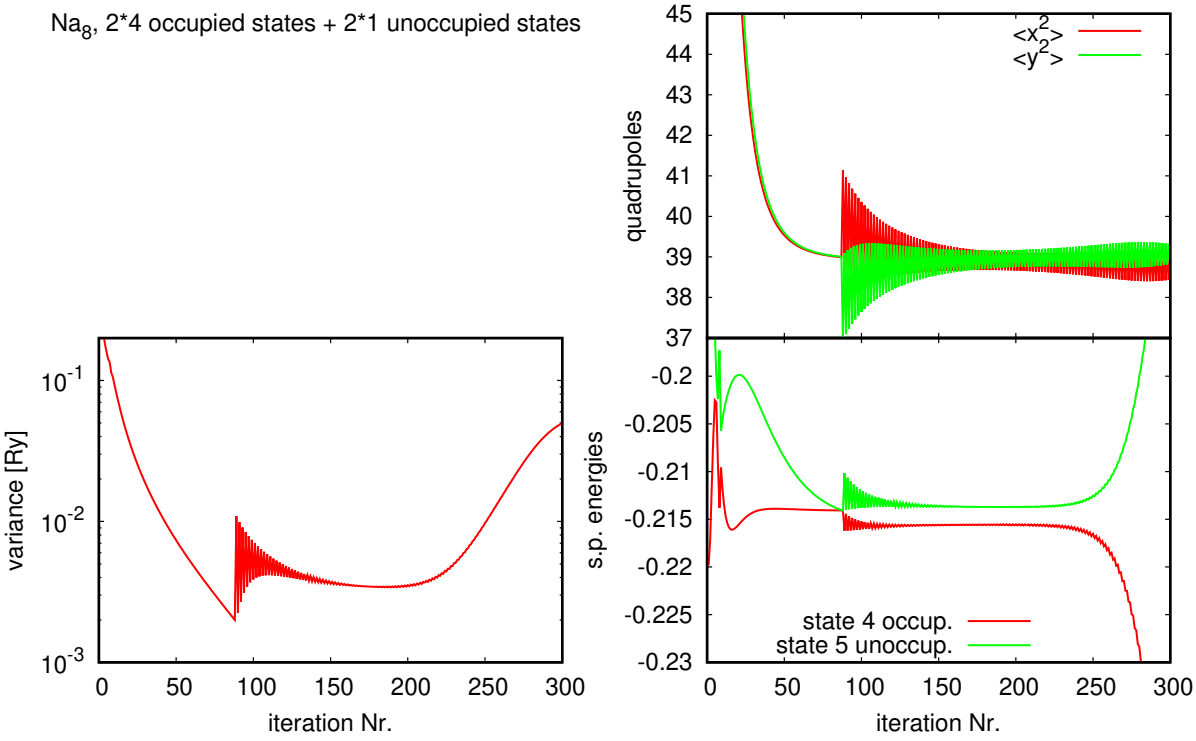
user to fiddle around with `ifhamdiag`. The idea is to let the system check how far recovery from perturbation went. To this end, we introduce a new input parameter `variance_gain` which is the factor about which the variance has to shrink since the last diagonalization before a next diagonalization can become effective. The criterion for a new diagonalization step is then set by two measures, first, `ifhamdiag` gradient steps have to done, and second the actual variance must fulfill

$$\texttt{variance} < \texttt{variance\_gain} * \texttt{variance\_old} \tag{1}$$

where `variance_old` is the variance at the last iteration step before previous diagonalization. The figure above abbreviates var=`variance_gain`. A factor of about 1/3 was found to be efficient. The figure above shows two cases with "var=0.3" and both finally converge well. Still, we see for "diag=10" that the turmoil generated by too often diagonalization causes slight delays in the late phase.

One may wonder why to bother about diagonalization if straightforward damped gradient iteration works so well. The answer is given in the right panel of the above figure which shows results from $Na_{12}$. Opposed to $Na_8$ which is a magic cluster, this cluster represents an open shell situation with high level density at the Fermi energy. It is obvious that occasional diagonalization delivers significantly faster convergence even if the diagonalizations spoil for a moment the variance.

Thus far, we could be happy. An unpleasant surprise comes if we chose a situation with fewer unoccupied states. This is demonstrated in the figure below.




It deals with the "magic" $Na_8$ and only 1 extra state above the Fermi energy (in fact, 2 states but spin degenerated) and it uses only the straightforward damped gradient iteration. The effect is dramatic. At some iteration, the variance (left panel) jumps and never recovers. The lower right panel shows that the instability occurs at the very

moment where HOMO and LUMO cross. What then happens is that these two states exchange their properties from one step to the next as can be seen from the fluctuations quadrupole moments (upper right panel). Such a flip-flop iteration is known from molecules with degenerate ground states. It is a surprise in the present case where we know that a closed-shell ground state exists. Even occasional diagonalization cannot cure that dilemma. It seems that the flip-flop iteration hinders the system from going downhill into the minimum. It is likely that the same mechanism is causing the perturbations in the successful cases discussed first. The larger space of unoccupied states softens the problem. Still, there is something to be understood and/or improved.