Reduced density matrix optimization for strongly correlated systems: a study of the one-dimensional Hubbard model

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In recent years a lot of research has been aimed at determining the second-order density matrix directly through a variational optimization. This is an appealing technique because one can determine all ground-state properties without reference to the wave function. The problem is that one has to find N-representability conditions to force the density matrix to be *physical*, *i.e.* derivable from a N-particle wave function. We have applied this technique to the one-dimensional Hubbard model and found that the standard two-index conditions are not strong enough in the strong-correlation limit. The much heavier three-index conditions are needed to correctly describe this region. In an effort to obtain the same accuracy as with three-index constraints, but at the same time keeping the program computationally tractable, we determined the following object variationally:

$$W^l|^{S(S_{ab};S_{cd})}_{ab;cd} = \sum_i w_i \frac{1}{[\mathcal{S}]^2} \sum_{\mathcal{M}} \langle \Psi^N_{\mathcal{SM},i} | {B^\dagger}^S_{ab(S_{ab})l} \; B^S_{cd(S_{cd})l} | \Psi^N_{\mathcal{SM},i} \rangle \ ,$$

with $B^\dagger$ the spin-coupled three-particle creation operator:

$${B^\dagger}^S_{ab(S_{ab})c} = \frac{1}{\sqrt{1+\delta_{ab}}} \left[\left[a^\dagger_a \otimes a^\dagger_b \right]^{S_{ab}} \otimes a^\dagger_c \right]^S \ .$$

This object contains three-particle information but has the third spatial-index diagonal, thus keeping al the calculations on two-particle space. One can derive six independent N-representability constraints for this object. Imposing these we found that they yield the same level of accuracy as the three-index conditions, while requiring less computational resources.