

# Variational density matrix study of the one-dimensional Hubbard model: The need for three-particle constraints

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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 stringent 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:

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

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

$$B_{ab(S_{ab})c}^{\dagger S} = \frac{1}{\sqrt{1 + \delta_{ab}}} \left[ [a_a^\dagger \otimes a_b^\dagger]^{S_{ab}} \otimes a_c^\dagger \right]^S.$$

This object contains three-particle information but has the third spatial-index diagonal, thus keeping all 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.