Three particles constraint as linear inequalities in v2DM optimization

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The idea of using the two-particle reduced density matrix (2DM) in a variational method to determine the groundstate energy of a many body quantum mechanical system has a long history. The energy of an N-body system with two-particle interaction is completely expressed by the 2DM, opening the door to quantum mechanics without wavefunctions. The main challenge in using the 2DM as a basis object is the so-called N-representability: a relevant 2DM should be derivable from a physical wavefunction. This problem is hard, in fact it has been proven to be QMA complete. However, we do have a set of necessary but not sufficient constraints in the two-particle space (the so-called $\mathcal{P}$, $\mathcal{Q}$ and $\mathcal{G}$ constraints) and in the three-particle space ($\mathcal{T}_1$ and $\mathcal{T}_2$ constraints). With these matrix positivity constraints, the problem of finding the ground-state energy reduces to a semidefinite optimization problem (sdp). There are several algorithms known to solve these problems.

When using only the two-particle constraints, a good approximation to the ground-state energy is found for only a limited number of systems; in general the three-particle constraints are necessary to find an acceptable ground-state energy. The problem is that the complexity of the problem with two-particle constraints scales like M^6 (with M the number of single particle states), while the scaling with three-particle constraints included is M^9. An interesting idea is to use some information of the three-particle space to improve the energy, without fully applying the $\mathcal{T}_1$ or $\mathcal{T}_2$ conditions, thereby avoiding the M^9 complexity. Since the T1 and T2 matrix are sparse, we can efficiently calculate their lowest eigenvalues and eigenvectors using a Lanczos algorithm. We can use these (negative) eigenvalues and eigenvectors as linear inequality constraints on the 2DM. The idea is then to apply the $\mathcal{P}$, $\mathcal{Q}$ and $\mathcal{G}$ conditions in full, and iteratively apply only the lowest eigenvalues of the $\mathcal{T}_1$ and $\mathcal{T}_2$ matrices. First tests with a barrier method program show that even applying a single eigenvalue of $\mathcal{T}_1$ or $\mathcal{T}_2$ gives a considerable improvement of the energy. We are currently trying this idea on a primal-dual and a barrier point program. Further, we are investigating the cutting plane method as a alternative to these traditional sdp methods. The cutting plane method is not an interior-point method, but finds the solution to the problem by decreasing the solution space with hyperplanes cuts. This makes it ideal for our purposes. It is also capable of handling large number of constraints much more easily than the traditional methods.

The hope is then to find an efficient algorithm that yields an energy between $\mathcal{P}$, $\mathcal{Q}$, $\mathcal{G}$ and full blown conditions $\mathcal{P}$, $\mathcal{Q}$, $\mathcal{G}$, $\mathcal{T}_1$, $\mathcal{T}_2$.