Reduced density matrix optimization using the boundary point

ir. Ward Poelmans

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Abstract

The variational determination of the density matrix is a technique to determine the ground-state properties of a many-body system without using the wave function. The energy is minimized as a function of the second-order density matrix Γ, on the condition that it remains N-representable, i.e.

$$\Gamma_{\alpha\beta;\gamma\delta} = \langle\Psi|a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma|\Psi\rangle$$

There are several necessary conditions known which can be expressed as linear matrixfunctions of Γ that have to remain positive semidefinite. Using these conditions the optimization can be formulated as a so called semidefinite program. There are serveral techniques available to solve a semidefinite program. The boundary point method is the newest technique. For large problems, it's a lot faster then other methods.