Variational determination of the second-order density matrix.

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The variational determination of the density matrix is a technique to determine the ground-state properties of a many-body system without reference to 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.

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

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.

We will give an overview of the structure of the algorithm we have developed to solve the semidefinite program and discuss its application to some physical systems, e.g. the isoelectronic series of Beryllium, Neon and Silicon [1] and potential energy surfaces in diatomic dissociation [2, 3, 4]. We will also discuss the succes of the approach to one dimensional lattice systems such as the Hubbard model.

References

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