Variational Approaches to the *N*-Representability Problem

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The *N*-representability problem is reformulated as a max-min problem, where the inner minimization is over the energy and the outer maximization is with respect to a single *N*-representability constraint. This construction seems to be extremely general; it can be used to derive *N*-representability constraints for the electron density, electron pair density, and multi-electron distribution functions. It can be used to derive *N*-representability constraints for the Wigner distribution (or other quasiprobability distributions). It can be used to derive *N*-representability constraints for reduced density matrices. In its most general incarnation, the max-min principle says that if the energy is a convex function of the descriptor q and q^* is an element of the dual to the space of the descriptor, then the ground state energy can be found using a variational procedure like:

$$E_{g.s.} = \underbrace{\max_{q^*}} \; \underbrace{\min_{\{q | q^* q \geq E_{q^*}\}}} \; E[q].$$

Aside from its generality and power, the construction lends itself to practical computational implementations. In this context it is important that the energy is a convex functional of the quantity being minimized and a concave functional of the constraint being maximized. This allows one to use Lagrange multipliers (or, even better, augmented Lagrangians) to performed the constrained minimization. Alternatively, the constrained minimization can be restated as a nonlinear equation.

Time permitting, I will conclude with some comments about the structure of the *N*-representability conditions for the two-electron reduced density matrix and how they pertain to more "conventional" quantum chemical methods.

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