Seminario de análisis matemático y aplicaciones
Analisi matematikoa eta aplikazioak mintegia

Generalization of Lieb's Variational Principle

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ABSTRACT: The ground state energy is one of the most important quantities in quantum chemistry. Computing this energy in many particles systems is a complex - if not impossible - task. It is therefore necessary to resort to approximation methods. In the Hartree-Fock approximation, the infimum is calculated over a subclass of states called Slater determinants. Lieb's variational principle is a fundamental tool to compute this infimum (in the fermionic case). It states that the infimum over Slater determinants equals the infimum over a class of quasifree states which is easier to analyze.

In its original formulation, Lieb's variational principle holds for fermion systems with purely repulsive pair interactions. As a generalization we prove for both fermion and boson systems with semi-bounded Hamiltonian that the infimum of the energy over quasifree states coincides with the infimum over pure quasifree states. In particular, the Hamiltonian is not assumed to preserve the number of particles.

We will present:
- The model which motivated Lieb's work,
- Lieb's original result,
- our generalization,
- the convexity argument leading this generalization.

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