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Delaunay Polytopes and the Pauli Principle

Consider the integer lattice Z^d, and a lattice polytope P in Z^d. Then, P is Delaunay if it can be circumscribed by an empty ellipsoid E, where there are no lattice points interior to E, and the only Z^d-elements on the boundary are the vertices of P. The empty ellipsoid E determines an inhomogeneous quadratic function up to a scale factor. In general there are many empty ellipsoids that circumscribe P, each determining a single ray of quadratic functions. The collection of all such rays is a relatively open cone of quadratic functions, the inhomogeneous domain $D(P)$, of the Delaunay polytope P.

If the vertices of P are $(0,1)$-vectors, then these can be interpreted as giving partial information on a quantum system of electrons that are distributed amongst d one-particle states. Each $(0,1)$-vector is a vector of occupation numbers, component k telling whether state k is occupied or unoccupied; the occupation numbers are limited to 0 or 1 by the Pauli principle. By taking averages we have a more general situation; the components belong to the unit interval and give the probability that state k is occupied. With this quantum interpretation each quadratic function in the domain $D(P)$ corresponds to a Hamiltonian operator on the state space of the quantum system, and the vertices of the Delaunay polytope label a basis for the degenerate ground state of this Hamiltonian.

Besides the probability distribution for the electrons, it is also useful to determine the joint probability distributions for pairs of electrons, and possibly even higher order distributions of electrons. I will describe how pair probability distributions can be described within the present framework, and how the convex set of all pair probability distributions can be described using the family of operators corresponding to the elements of $D(P)$. I will relate this discussion to some questions in quantum information theory.