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Commutators and Self-Adjointness of Hamiltonian Operators

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Abstract. A time dependent approach to self-adjointness is presented and it is applied to quantum mechanical Hamiltonians which are not semi-bounded. Sufficient conditions are given for self-adjointness of Schrödinger and Dirac Hamiltonians with potentials which are unbounded at infinity. The method is the introduction of an auxiliary operator $N \geqq 0$ whose rate of change (commutator with the Hamiltonian) is bounded by a multiple of N.

1. Introduction

Let $\mathscr{H}$ be a Hilbert space and H be a Hermitian operator acting in $\mathscr{H}$. That is, H is a linear transformation (defined on a dense linear subspace $\mathscr{D}(H) \subset \mathscr{H}$ and taking values in $\mathscr{H}$) such that $\langle Hf, g\rangle = \langle f, Hg\rangle$ for all f and g in $\mathscr{D}(H)$.

The Schrödinger equation associated with H is $i\frac{du(t)}{dt} = Hu(t)$. The initial value problem with initial condition $u(0) = f$ has the formal solution $u(t) = \exp(-itH)f$, but it is possible that the series expansion for the exponential does not converge for sufficiently many vectors in $\mathscr{D}(H)$ to determine a unitary operator $\exp(-itH)$.

The exponential of a self-adjoint operator, however, is uniquely determined (by the spectral theorem). Thus any self-adjoint extension of H leads to a solution of the initial value problem for the Schrödinger equation. The typical quantum mechanical Hamiltonian is a real operator (that is, it commutes with some conjugation), so it has self-adjoint extensions. The problem that remains is whether H has a unique self-adjoint extension.

If H is the sum of (positive) kinetic energy and potential energy terms, the Schrödinger equation describes a particle moving in configuration space under the influence of forces determined by the potential energy. If the potential energy is unbounded below, the kinetic energy