Stationary Schrodinger equation with density matrices instead of wave functions

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Abstract.

The stationary Schrödinger equation (SSE) can be cast in the form $H\rho_E = E\rho_E$, where H is the system's Hamiltonian and ρ_E is the system's density matrix. We explore the merits of this unconventional form of the SSE, which we refer to as SSE_ρ. For a nondegenerate energy level, ρ_E is merely a projection on the corresponding eigenvector Ψ_E. However, in the case of degeneracy ρ_E in non-unique and not necessarily pure. In fact, it can be an arbitrary mixture of the degenerate pure eigenstates. Importantly, ρ_E can always be chosen to respect all symmetries of the Hamiltonian, even if each pure eigenstate in the corresponding degenerate multiplet spontaneously breaks the symmetries. This and other features of the solutions of the SSE_ρ can prove helpful by easing the notations and providing an unobscured insight in the structure of the eigenstates, as we demonstrate for several exemplary spin systems. Eigenvalue problem for quantum observables other than Hamiltonian can also be formulated in terms of density matrices. We provide an analytical solution to one of them, $\mathbf{S}^2\rho_S = S(S+1)\rho_S$, where $\mathbf{S}$ is the total spin of N spins 1/2, and ρ_S is chosen to be invariant under permutations of spins.