spin contamination

In unrestricted Hartree–Fock method, the wavefunctions obtained are eigenfunctions of the Hamiltonian and the spin projection $S_z$ operators, but not eigenfunctions of the $S^2$ operator. As a result, the wavefunctions of the doublet systems are spin-contaminated to some extent by admixtures of quartet, sextet, and higher spin states. The eigenvalues of the $S^2$ operator are given as a measure of the spin contamination.

Source:
PAC, 1999, 71, 1919 (Glossary of terms used in theoretical organic chemistry) on page 1962