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Wave Function Arbitrariness of Noninteracting Fermion Model in Quantal Density Functional Theory[1](QDFT) MARLINA SLAMET, Sacred Heart University, VIRAHT SAHNI, The Graduate School, CUNY — In the QDFT mapping from a *ground* or *excited* state of the interacting system to one of noninteracting fermions in a particular *excited* state with equivalent density, there is an arbitrariness in the wave function of the model system. For example, in the case of a two-electron atom, the mapping to the excited singlet 2^1S state of the model system, there are three wave functions that lead to the *same* density: two single Slater determinants of the orbitals that are eigen functions of only S_z, and a linear combination of Slater determinants of these orbitals that is an eigen function of both S_z and S^2. Neither of the wave functions is more appropriate than the other, since all three wave functions deliver the same density. However, based on the choice of wave function, the structure of the corresponding Fermi and Coulomb holes, and therefore the values of the resulting Pauli and Coulomb correlation energies, will differ. Their sum, the Fermi-Coulomb holes, and the Pauli-Coulomb energy, remains unchanged. The wave function arbitrariness will be demonstrated via the Hooke's atom.

1 *Quantal Density Functional Theory*, V. Sahni (Springer-Verlag, 2004).

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