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Exact Kohn-Sham eigenstates versus quasi-particles in simple models of strongly correlated electrons JAIME FERRER¹, DIEGO CARRASCAL², Departamento de Física, Universidad de Oviedo, Spain — We present analytic expressions for the exact density functional and Kohn-Sham Hamiltonian of simple tight-binding models of correlated electrons. These are the single- and double-site versions of the Anderson, Hubbard and spinless fermion models. The exact exchange and correlation potentials are fully non-local. The analytic expressions allow to compare the Kohn-Sham eigenstates of exact density functional theory with the many-body quasi-particle states of these correlated-electron systems. The exact Kohn-Sham spectrum describes correctly many of the non-trivial features of the many-body quasi-particle spectrum, as for example the precursors of the Kondo peak. However, we find that some pieces of the quasi-particle spectrum are missing because the many-body phase-space for electron and hole excitations is richer.

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