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Stability of Finite Subspaces in Density Functional Theory: Application to Simple Atoms P. IZA, Departamento de Física, Escuela Superior Politécnica del Litoral, ESPOL., F.J. TORRES, Departamento de Química e Ingeniería Química, Universidad San Francisco de Quito, USFQ., E. V. LUDEÑA, Center of Nanotechnology Research and Development, CIDNA, Escuela Superior Politécnica del Litoral, ESPOL., Y. CARRILLO, L. RINCÓN, Departamento de Química e Ingeniería Química, Universidad San Francisco de Quito, USFQ., D. ZAMBRANO, Departamento de Física, Escuela Superior Politécnica del Litoral, ESPOL. — The validity of the first Hohenberg-Kohn theorem, namely the one-to-one relationship between an external potential and the one-particle density, is examined; when it is applied to finite subspaces and consider the stability of these subspaces with respect to external potentials. This is done by analyzing the DFT description of some atoms (e.g., H, He, Li and Be) provided by the solution of the Kohn-Sham equation in a finite Gaussian basis set. We show that in the finite subspace generated from the finite basis set, it is possible to construct external potentials that differ from one another by more than a constant but which associate with the same one-particle density. We carry out the specific construction of these potentials for the above atoms using the wave functions resulting from the application of the B3LYP functional.

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