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Demonstration of the Gunnarsson-Lundqvist theorem and Lack of Hohenberg-Kohn Theorem for Excited States XIAO-YIN PAN, YU-QI LI, BIAO LI, Ningbo University, VIRAHT SAHNI, Brooklyn College CUNY — By considering two noninteracting fermions in a 1-D infinite square well we demonstrate the following: (a) The GL theorem is satisfied for the lowest excited triplet state. There exists only one potential for this density so that the HK theorem is satisfied for this lowest excited state configuration. (b) For the second excited triplet state, there exists no other potential with the original orbital configuration that reproduces the density. However, (c) for the second excited triplet state, there exist other potentials with orbital configurations different from the original that reproduce the density. Thus, there is no HK theorem for this and other excited states. The orbitals of the other set of potentials are related to the original orbitals by a rotation. The exact new eigenvalues, and solutions for the potentials and orbitals including near and at the boundaries are provided.

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