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On the performance of Thomas-Fermi in periodic two-dimensional systems[1] LAZARO CALDERIN, MALCOLM J. STOTT, Department of Physics, Queen's University, Kingston K7L 3N6, Ontario, Canada — The largest missing piece of a completely orbital free Density Functional Theory is the kinetic energy functional $T_s[n]$, and approximations for this are of interest. One of these expands T_s in terms of density gradients with the Thomas-Fermi functional as the first term. But in three-dimensions the expansion appears not to converge, and the sixth and higher order corrections diverge for localized systems. In contrast, a number of authors have shown that the density gradient corrections all vanish in two-dimensions, while numerical test revealed that, even when not exact, TF is a very good approximation. That has been shown for the case of an impurity in a otherwise two-dimensional uniform electron gas. In this work we explore the validity of TF and linear response theory for a periodic two-dimensional system, a system that is likely to be more widely applicable.

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Lazaro Calderin
Department of Physics, Queen's University, Kingston K7L 3N6, Ontario

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