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Dependence of the Thomas-Fermi Energy on the Nuclear Coordinates*

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Abstract. Let $E(R)$, respectively $e(R)$, denote the total energy, respectively the electronic contribution to the energy, in the Thomas-Fermi theory for a system of two fixed nuclei a distance R apart. We prove that $e(R)$ and $-E(R)$ increase as R does. For the case of N fixed nuclei, we prove the monotonicity of e and E under certain displacements of the coordinates of the nuclei. The analogous result for the electronic contribution to the Born-Oppenheimer energy is proved.

1. Introduction

The Thomas-Fermi (TF) theory is defined by the energy functional (in units in which $h^2(8m)^{-1}(3/\pi)^{2/3}=1$ and $|e|=1$, where e and m are the electron charge and mass)

$$\xi(\rho)=\tfrac{3}{5}\int \rho(x)^{5/3}\,dx-\int V(x)\,\rho(x)\,dx+D(\rho,\rho)+U, \tag{1}$$

where

$$D(\rho,\rho)\equiv\tfrac{1}{2}\int \rho(x)\,|x-y|^{-1}\,\rho(y)\,dx\,dy, \tag{2}$$

$$V(x)=\sum_{j=1}^{k} z_j|x-R_j|^{-1}, \tag{3}$$

and

$$U=\sum_{1\leqq i<j\leqq k} z_i z_j|R_i-R_j|^{-1}. \tag{4}$$

Here $z_1,\ldots,z_k\geqq 0$ are the charges of k fixed nuclei located at $R_1,\ldots,R_k$. $\int dx$ is always a three-dimensional integral. $\xi(\rho)$ is defined for electronic densities $\rho(x)\geqq 0$ such that $\int\rho$ and $\int\rho^{5/3}$ are finite. The TF energy for λ (not necessarily an integer) electrons is defined by

$$E(\lambda;\{R_i\})=\inf\{\xi(\rho)\,|\int\rho=\lambda\}. \tag{5}$$

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