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Long Range Atomic Potentials in Thomas-Fermi Theory

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Abstract. We prove that the interaction among neutral atoms in Thomas-Fermi theory behaves, for large separation l, like Γl^{-7}. The constant Γ is independent of the atomic nuclear charges, but does depend on the relative positions of the nuclei. We also show that Γ is not a simple sum of pair terms, i.e. in TF theory three and higher body terms persist into the asymptotic (in l) region.

I. Introduction

We investigate the interaction among neutral atoms in Thomas-Fermi (TF) theory and prove that the interaction is asymptotically (const.) l^{-7} for large separation, l. The non-neutral case will not be discussed because there the interaction is asymptotically (const.) l^{-1} for elementary electrostatic reasons.

The TF theory is defined as follows (see [1] for a complete discussion and the basic theorems): Define the functional

$$\mathscr{E}(\varrho)=\tfrac{3}{5}\int \varrho(x)^{5/3}dx-\int V(x)\varrho(x)dx+\tfrac{1}{2}\iint \varrho(x)\varrho(y)|x-y|^{-1}dxdy+U$$

$$V(x)=\sum_{j=1}^{k} z_j|x-R_j|^{-1} \tag{1.1}$$

$$U=\sum_{1\leq i<j\leq k} z_i z_j|R_i-R_j|^{-1}$$

for positive functions $\varrho(x)$ on $\mathbb{R}^3$ in $L^{5/3}\cap L^1$. $\mathscr{E}(\varrho)$ is the functional appropriate to a system consisting of k nuclei of charges $z_i>0$ and located at $R_i\in\mathbb{R}^3$. The TF energy is defined to be

$$e(z_1,\ldots,z_k;\,R_1,\ldots,R_k)=\min_{\varrho}\mathscr{E}(\varrho) \tag{1.2}$$

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