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SOME RESULTS ON THE THOMAS-FERMI-DIRAC-VON WEIZSÄCKER MODEL

C. LE BRIS

Centre de Mathématiques de l'Ecole Polytechnique, 91128 Palaiseau Cedex, France

(Submitted by: P.L. Lions)

Abstract. We study here the Thomas-Fermi-Dirac-von Weizsäcker model of molecular systems. Under some conditions on the number of electrons and on parameters of the model, we prove the existence and uniqueness of the minimum and the convexity of the infimum.

1. Introduction. We study the following minimization problem:

$$I_\lambda = \inf\{E(\rho) : \rho \geq 0, \sqrt{\rho} \in H^1, \int_{\mathbb{R}^3} \rho = \lambda\}, \tag{1.1}$$

where

$$E(\rho) = \int_{\mathbb{R}^3} |\nabla \sqrt{\rho}|^2 + \int_{\mathbb{R}^3} V\rho + c_1 \int_{\mathbb{R}^3} \rho^{5/3} - c_2 \int_{\mathbb{R}^3} \rho^{4/3} + \frac{1}{2} \int\int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|}\, dx\, dy. \tag{1.2}$$

In these formulas, E is the Thomas-Fermi-Dirac-von Weizsäcker energy (TFDW energy in short), ρ represents the electron density, c_1 and c_2 are two nonnegative parameters, V is the coulombian potential created by the nuclei (of total charge Z); that is,

$$V(x) = -\sum_{i=1}^{N} \frac{z_i}{|x - x_i|}$$

with $\sum_{i=1}^N z_i = Z$, $(x_i)_{i=1,\ldots,N}$ fixed. We can also write the problem in terms of $\sqrt{\rho}$:

$$I_\lambda = \inf\{\mathcal{E}(\psi) : \psi \in H^1, \int_{\mathbb{R}^3} \psi^2 = \lambda\}, \tag{1.3}$$

where

$$\begin{aligned} \mathcal{E}(\psi) = &\int_{\mathbb{R}^3} |\nabla\psi|^2 + \int_{\mathbb{R}^3} V\psi^2 + c_1 \int_{\mathbb{R}^3} |\psi|^{10/3} - c_2 \int_{\mathbb{R}^3} |\psi|^{8/3} \\ &+ \frac{1}{2} \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\psi(x)^2\psi(y)^2}{|x-y|}\, dx\, dy. \end{aligned} \tag{1.4}$$

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