Commun. math. Phys. 47, 215—219 (1976)

Communications in
Mathematical
Physics

The Thomas-Fermi-Theory as Result of a Strong-Coupling-Limit

Bernhard Baumgartner
Institut für theoretische Physik der Universität Wien, A-1090 Wien, Austria

Abstract. The energy of non-relativistic neutral atoms is shown to approach asymptotically the Thomas-Fermi-energy, when the charge of the nucleus tends to infinity.

I. Introduction

As is well known, the Thomas-Fermi- (T.F.-) theory for atoms results by treating the electrons as a locally ideal Fermi-gas in the mean field created by the nucleus and the other electrons. We show that this scheme becomes correct if we take the limit of infinitely large atoms in nonrelativistic quantummechanics. (This result has also been announced by Lieb and Simon [1].) First we show that the ground-state-energy in a mean-field-theory, which supplies us with lower bounds to the energy of atoms, tends to the T.F.-energy. In the second step the density in ground states of related Hamiltonians is shown to converge in a certain sense to the T.F.-density. Finally we take the expectation value of the nonrelativistic Hamiltonian for atoms in the above mentioned ground state and show that it also gives asymptotically the T.F.-energy.

II. The Limit of a Lower Bound

We use a Hamiltonian, which gives lower bounds to the energies of atoms, recently found by P. Hertel et al. [2]:

$$\begin{aligned} h_N = \sum_{i=1}^{N} & (P_i^2/2m - N|x_i|^{-1} + \phi_N(x_i) \\ & - \tfrac{1}{2}\{\int \phi_N(x) n_N(x) d^3x + 3N\,(\pi/N \int n_N(x)^2 d^3x)^{1/3}\}, \end{aligned} \tag{1}$$

$$\phi_N(x) = \int |x-y|^{-1} n_N(y) d^3y\,, \tag{2}$$