Commun. math. Phys. 33, 293—304 (1973)

Solution of the Hartree-Fock Equations*

G. Fonte, R. Mignani and G. Schiffrer
Istituto di Fisica Teorica dell'Università, Catania (Italy)

Received December 4, 1972; in revised form May 16, 1973

Abstract. We suggest to use the Newton iteration method for constructing a (locally unique) solution of the atomic and nuclear Hartree-Fock equations for an arbitrary number of particles. Our proposal is based on a theorem by Kantorovič and rests on the following points: 1) the two-body potential must satisfy a boundedness condition; 2) the zero-order approximation, used to start the iteration sequence, must satisfy certain conditions, to be proved numerically. Condition 1) holds, for instance, for all local potentials, defined by a bounded function and for a class of nonlocal potentials; it does not hold for local potentials, behaving as $1/r$ near the origin.

1. Introduction

Although the Hartree-Fock theory is known since the earliest years of quantum mechanics [1] and has been extensively used in atomic [2] and in nuclear physics [3], no rigorous and general treatment of the related equations has appeared so far in the literature. This gap has been filled only partially by some more recent papers [4–6]. Refs. [4] and [5][1] are mathematically rigorous, but deal only with systems of two identical fermions plus another particle, the former reference with harmonic oscillator interactions, the latter with Coulomb ones (helium atom). In Ref. [6], the problem of computing a solution, proving its local uniqueness and estimating the error due to the finiteness of the iteration, has been solved for the nucleus ^{16}O in a subspace spanned by a finite harmonic oscillator basis, using the Newton method of successive approximations in the generalized form and with the convergence conditions of Kantorovič [7, 8][2]. The aim of the present paper is to contribute to a better mathematical understanding of the problem, by extending the theory of Ref. [6] to an infinite-dimensional space and presenting it independently of any

* This work has been supported in part by Istituto Nazionale di Fisica Nucleare (Sezione di Catania) and by Centro Siciliano di Fisica Nucleare e di Struttura della Materia (Catania).

[1] We thank the referee for bringing to our attention this paper.

[2] Russian references are translitterated according to the international convention, recommended in Suppl. Nuovo Cim. **1**, 387 (1955).