Commun. Math. Phys. 163, 185–215 (1994)

Communications in Mathematical Physics

Local Properties of Coulombic Wave Functions

M. Hoffmann-Ostenhof[1], **T. Hoffmann-Ostenhof**[2,3], **H. Stremnitzer**[4]

[1] Institut für Mathematik, Universität Wien, Strudlhofgasse 4, A-1090 Wien, Austria
[2] Erwin Schrödinger International Institute of Mathematical Physics, Pasteurgasse 6/7, A-1090 Wien, Austria
[3] Institut für Theoretische Chemie, Universität Wien, Währingerstrasse 17, A-1090 Wien, Austria
[4] Institut für Theoretische Physik, Universität Wien, Boltzmanngasse 5, A-1090 Wien, Austria

Received: 16 July 1993

Abstract. We investigate the local behaviour of solutions of a nonrelativistic Schrödinger equation which describe Coulombic systems. Firstly we give a representation theorem for such solutions in the neighbourhood of Coulombic singularities generalizing previous results (Cusp conditions) due to Kato and others. Secondly we investigate the influence of Fermi statistics on the local behaviour of many fermionic wave functions, showing that e.g. an N-electron wave function must have zeros of order at least $N^{4/3}$ for large N.

0. Introduction

In a recent paper [6] the local behaviour of a real valued local solution u to the Schrödinger equation

$$(-\Delta + V)u = 0\,, \qquad x \in \Omega\,, \qquad \Omega \subseteq \mathbf{R}^n\,, \qquad n \geq 3 \tag{0.1}$$

under rather weak assumptions on the real valued potential V was investigated. It was shown that in the neighbourhood of a point $x_0 \in \Omega$, assuming that u vanishes there at most polynomially that

$$u(x) = P_M(x - x_0) + \Phi(x - x_0)\,, \tag{0.2}$$

where $P_M(x) \not\equiv 0$ is a harmonic homogeneous polynomial of degree M and $\Phi(x) = o(|x|^M)$. (See Sect. 1 for a precise statement.)

The purpose of the present paper is twofold. Firstly we give a detailed account of the local behaviour of solutions to the Schrödinger equation for Coulombic systems, e.g. atoms and molecules, especially in the neighbourhood of the singularities of the potential. Secondly (see Sect. 5) we investigate the influences of Fermi statistics on the local behaviour of many particle Fermionic wave functions. These results are consequences of (0.2) and some symmetry considerations and are not tied only to the Coulombic case.

Some of our results were recently announced in [7].