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Symmetry Breaking for a Non-linear Schrödinger Equation

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Abstract. We define a notion of stability for molecular states and show that the stable ground states of a molecular Hamiltonian are not unique (break rotational symmetry) if the atomic masses are greater than certain finite critical values. The stable ground states are stationary with respect to a new non-linear Schrödinger equation, which is exactly soluble in certain simple cases.

§ 1. Introduction

There has been some interest recently [2, 12, 13] in the problem of the quantum-mechanical justification of the concept of molecular structure. The problem is to explain why it is that in most situations, excluding possibly those of extreme isolation, the wave function of a molecule seems to be not an eigenstate of the Hamiltonian, but one of a class of slowly time varying states which are more stable in some sense.

In this paper we propose a precise definition of stability and prove the existence of stable ground states (Sect. 2). In Sect. 3 we show that for large enough atomic masses and typical two-body interactions the stable ground states are not unique. The breaking of the rotational symmetry of the Hamiltonian which occurs is closely related to the problem of molecular structure, as was pointed out by Woolley [12]. We study the anharmonic oscillator in some detail and show that reflection symmetry (parity) breaking does not occur for small masses and that there is an associated phase transition for finite values of the various parameters.

Having proved in Sect. 2 that the stable ground states satisfy a certain non-linear Schrödinger equation, we devote Sects. 4 and 5 to an analysis of the associated time-dependent one-body Schrödinger equation. Although non-linear we show that it is exactly soluble even in three space dimensions, and clarify some geometrical properties of the solution related to the Euclidean symmetry of the equation. Finally in Sects. 6 and 7 we sketch two possible approaches to the "derivation" of the non-linear Schrödinger equation, firstly using a second quantised linear Hamiltonian describing the interaction of an atom with an external phonon field, and secondly by reference to a collective model of nuclear structure.

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