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Self-consistent field theory of collisions: Orbital equations with asymptotic sources and self-averaged potentials

Y.K. Hahn

TRG/SWH 5916 Old Greenway Drive, Glen Allen, VA 23059, USA

HIGHLIGHTS

- First extension of HF to scattering states, with proper asymptotic conditions.
- Orbital equations with asymptotic sources and integrable orbital solutions.
- Construction of self-averaged potentials, and orbital energy fixing.
- Channel coupling and configuration mixing, involving the new orbitals.
- Critical evaluation of the continuum HF and its improvements.

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ABSTRACT

The self-consistent field theory of collisions is formulated, incorporating the unique dynamics generated by the self-averaged potentials. The bound state Hartree–Fock approach is extended for the first time to scattering states, by properly resolving the principal difficulties of *non-integrable* continuum orbitals and imposing complex *asymptotic conditions*. The recently developed asymptotic source theory provides the natural theoretical basis, as the asymptotic conditions are completely transferred to the source terms and the new scattering function is made *fully integrable*. The scattering solutions can then be directly expressed in terms of bound state HF configurations, establishing the relationship between the bound and scattering state solutions. Alternatively, the *integrable* spin orbitals are generated by constructing the individual orbital equations that contain asymptotic sources and self-averaged potentials. However, the orbital energies are *not* determined by the equations, and a special channel energy fixing procedure is developed to secure the solutions. It is also shown that the variational construction of the orbital equations has intrinsic ambiguities that are generally

E-mail address: ykhahn22@verizon.net.

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associated with the self-consistent approach. On the other hand, when a small subset of open channels is included in the source term, the solutions are only *partially integrable*, but the individual open channels can then be treated more simply by properly selecting the orbital energies. The configuration mixing and channel coupling are then necessary to complete the solution. The new theory improves the earlier continuum HF model.

1. Introduction

The concept of self-consistent field (SCF) is intuitively appealing as much as operationally effective, as it generates its own *unique dynamics*. The individual orbitals are distorted by the presence of rest of the particles, whose orbitals are the very ones being calculated in a self-consistent bootstrap. Thus, the Hartree- and Hartree–Fock (HF) methods [1,2] and their variations have been one of the most effective and widely applied approaches for treating the many-body atomic and nuclear *bound* systems [3,4]. The HF methods are especially effective when they are formulated in the single particle representation. Similar theories have also been extensively developed in plasma and solid state physics [5,6], where the periodic conditions apply. Since the SCF's for the individual particles are generated by averaging the interaction potentials over the *integrable density* of residual particles, the system being treated is assumed to be in a state which is either box-normalizable or locally confined, so that its wave functions are integrable. The *excited* state configurations are also generated by the HF, without explicitly requiring the usual orthogonalization procedure, mainly because of their differential forms.

The principal purpose of this paper is to incorporate the SCF concept in describing scattering processes with diverse asymptotic channels. As is well-known, the scattering functions are by definition defuse, so that the scattering system is not directly amenable to SCF treatment, unless some crucial adjustments are made to 'localize' the system. The main difficulties to be resolved are: (i) The continuum orbitals are *not integrable*, so that the averaging of the interactions to generate SCF cannot be carried out. Integrable orbitals are needed. (ii) The scattering states require complex *asymptotic boundary conditions* for the various outgoing waves, instead of simple decaying behavior in the bound state case. Furthermore, (iii) the use of single particle orbitals is not convenient as the SCF potentials distort them, even in the asymptotic region where the boundary conditions require 'free' orbitals. (iv) When one or more sub-clusters appear asymptotically, strong localizations/correlations are required. (v) The orthogonality among the open channels breaks down, and the unitarity requirements must also be satisfied. Mainly because of these difficulties, the SCF concept has never been fully adopted to scattering systems, and is conspicuously absent from the scattering theory literature [7,8].

The continuum shell model [9–11] was one of the first systematic attempts to extend the bound state theory to scattering states, where presumably the shell model potentials represent effective SCF. But, the difficulties noted above complicate the theory. More recently, the continuum Hartree–Fock theory was formulated [12,13], in which an amputation procedure was introduced to generate integrable orbitals for the limited projection purpose. The theory has been applied to elastic and breakup reactions, showing that the SCF concept is *effective* in describing collision dynamics, as illustrated in Fig. 1, but weak in satisfying the asymptotic conditions. A critical summary is given in Appendices A and B.

In this paper, the SCF theory of collision (SCC) is formulated, and the resolution of the difficulties summarized above is discussed in detail, while retaining the unique dynamics generated by the SCF. The recently developed scattering theory with asymptotic sources (SAS) [15] provides a natural theoretical basis for this purpose, and is briefly summarized in Section 2. The SAS is applied in Section 3 to obtain the SCF scattering solutions, firstly in terms of bound state HF configurations. Next, the new orbital equations are derived, which contain the asymptotic source terms and self-averaged potentials.