B.5. Atomic Theory of Strongly Correlated Systems

B.5.1. Overview

This is a progress report for contract No. DE-FG03-98ER14900, entitled "Atomic Physics of Strongly Correlated Systems," which is a separate grant with Dr. C. D. Lin as the Principal Investigator. After discussing with Dr. Pat Richard and with Dr. Eric Rohlfing, it was decided to merge this grant with the one to the JRM laboratory to create a single grant between DOE BES and Kansas State University in order to streamline the administrative tasks. This portion of the Progress Report covers C.D. Lin's project for the period since January, 1998--at that time the previous Progress Report was submitted. Section 4.9 summarizes projects performed by C.D. Lin's group that were supported by the JRML grant where Dr. Patrick Richard is the P.I.

The main theme of this program has been to develop new theoretical tools to deal with atomic and molecular systems where the standard or conventional theoretical methods are not valid. To some extent we deal with exotic systems, not necessarily because the particles are exotic, but because of the nature of the physical states. Thus we cover doubly excited and triply excited states of atoms. The conventional shell model or the mean-field theory cannot be used to describe such systems. The issues are both conceptual and computational. Not only do we need to find methods to perform the calculations, we also want to be able to provide new ways, or new approximate quantum numbers, for describing such systems. We also look for methods that are more general. We have used the hyperspherical approach extensively, which allows us to cover from typical atomic systems to molecular systems within the same framework. Such an approach has the added advantage that we can then use the same method for systems that are not easily described by either atomic or molecular methods.

In the following we summarize the progress made since January 1998.