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Review Article

Zero Temperature Numerical Studies of Multiband Lattice Models of Strongly Correlated Electrons

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Abstract. Relative to single-band models, multiband models of strongly interacting electron systems are of growing interest because of their wider range of novel phenomena and their closer match to the electronic structure of real materials. In this brief review we discuss the physics of three multiband models (the three-band Hubbard, the periodic Anderson, and the Falicov-Kimball models) that was obtained by numerical simulations at zero temperature. We first give heuristic descriptions of the three principal numerical methods (the Lanczos, the density matrix renormalization group, and the constrained-path Monte Carlo methods). We then present generalized versions of the models and discuss the measurables most often associated with them. Finally, we summarize the results of their ground state numerical studies. While each model was developed to study specific phenomena, unexpected phenomena, usually of a subtle quantum mechanical nature, are often exhibited. Just as often, the predictions of the numerical simulations differ from those of mean-field theories.

Key words: Lanczos method; density matrix renormalization group; constrained-path Monte Carlo; three-band Hubbard model; periodic Anderson model; Falicov-Kimball model

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1 Introduction

As a tool for understanding the properties of strongly correlated electron systems, numerical methods are both an opportunity and a challenge. They are an opportunity because in only a few cases are the simplest models of such systems exactly solvable. By producing very accurate solutions and thereby filling the gap between an exact solution and an uncontrolled approximation, these methods are thus an importantly useful way to advance the understanding of the properties of these models. What has been significant is their frequent revelations of unexpected and important new physics that standard perturbation and mean-field theories unfortunately often miss. The challenge is finding numerical algorithms that work well.

In this review we will be concerned only with results produced by three current common methods for producing the zero temperature energy and wavefunction of certain strongly correlated electron models. In general, there are three classes of zero temperature numerical methods: Krylov space [1,2], density-matrix renormalization group (DMRG) [3], and projector Monte Carlo methods. From the wavefunction that each estimates, a variety of physical properties, other than the energy, are easily calculated.

The Monte Carlo method allows the largest system sizes to be studied but with an accuracy that is in general several orders of magnitude less than the other two. The infamous fermion sign problem [4], manifested by the statistical variance of the numerical solution becoming exponentially large as the size of the system simulated becomes large, plagues these algorithms. The DMRG method, particularly in one dimension, allows the study of the next largest system sizes with a high degree of accuracy. For just the basic qualitative picture of the models's possible phases, as opposed to extrapolating its properties to the thermodynamics limit, a particular Krylov space method, the Lanczos method [1,2], is often the method of choice. Although often called the exact diagonalization method (ED), it actually only produces a variational upper bound to the ground state energy of the model. The accuracy of the method however is usually outstanding, being nearly full floating point precision.

In this review we will only present recent results of zero temperature numerical studies of the three-band Hubbard, periodic Anderson, and Falicov-Kimball models. All three are multiband models. The three-band Hubbard obtains multiband stature from having three single orbital atoms per unit cell. It is inherently two-dimensional, being proposed to model the CuO_2 planes in high temperature superconductors. For this model the numerical simulations have focused on the behavior the d-wave paring correlation function as a function of the model's parameter. Here, the results are obtained by use of a particular projector Monte Carlo method, the constrained-path Monte Carlo method (CPMC) [5–7]. This method is also the primary tool for the results presented for the periodic Anderson model. The focus of these results will be magnetic properties, particularly its ferromagnetic properties. The model which shows the most novel physics is the Falicov-Kimball model. For the simplest version of the model, a combination of analytic work using strong coupling theory and numerical work using the ED and CPMC methods, has demonstrated the