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Study of Simulation Cell Size in Mean-Field Studies of Interacting Lattice Models

Yueguang Shi and Warren E. Pickett*

Department of Physics, University of California Davis, Davis CA 95616, USA.

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Abstract. A lattice model of interacting fermions is studied with the principal aim of assessing the dependence of calculated mean-field ground states versus the $N\times N$ lattice size, with $N=16$, 32, and 48. A two band model on the two-dimensional square lattice is simulated, with on-site energies and interaction parameters chosen to represent crystal field split orbitals in the moderately correlated regime. Nearest neighbor hopping leads to the well known van Hove singularities (vHs) of the square lattice. Anomalies in the inverse participation ratio of the eigenstates are found to be associated with the vHs, with their prevalence decreasing inversely with N. For the chosen model, inhomogeneous spin densities are always obtained for the small lattice size $N=16$, with the degree of variation decreasing rapidly for most polarizations as N is increased. Various spin polarizations are treated, and one case in which spin density inhomogeneity persists for the largest lattice size is discussed and analyzed. Coupling of spin density inhomogeneities to charge density variation is minor but evident, and is primarily of intra-orbital origin.

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Key words: Lattice Hamiltonian, mean field, lattice size, moderate interactions.

1 Introduction

The study of inhomogeneous phases in correlated electron systems has long been an area of active investigation, with the spin density wave in chromium providing an early example [1]. Activity increased strongly after the discover of charge density stripes in hole-doped $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ with $x=0.12$ [2], in hole-doped manganites $La_{1-x}Ca_xMnO_3$ [3] and $La_{0.5}Sr_{1.5}MnO_4$ [4], and also hole-doped nickelates $La_2NiO_{4.125}$ [5] and $La_{1.67}Sr_{0.33}NiO_4$ [6]. The classic inhomogeneities, charge density waves (CDW) and spin density waves (SDW) have conventionally been tied to Fermi surface nesting [1], though

*Corresponding author. *Email addresses:* wepickett@ucdavis.edu (W. E. Pickett), ygshi@ucdavis.edu (Y. Shi)

a close connection to CDWs to nesting has been questioned [7]. Density wave states have by definition a specific wavelength λ and direction, hence a specific wavevector $\vec{q}$, $q=|\vec{q}|=2\pi/\lambda$, related to Fermi surface calipers.

Theoretical study of these inhomogeneities began in earnest in response to reported inhomogeneities in cuprates, newly discovered to be high temperature superconductors when hole-doped. These investigations focused on the square lattice Hubbard model doped away from the antiferromagnetic ordered state at half filling and treated in a mean field (Hartree-Fock) manner. Su obtained spin polaron states [8] building on the spin-bag mechanism of electron pairing that had been introduced by Schrieffer, Wen, and Zhang [9]. Machida used an approach somewhat more from the itinerant side and obtained a soliton lattice spin structure and striped charged domain walls [10]. Zaanen and Gunnarsson extended such studies to a two-band model, finding charged magnetic domain walls (charge and associated spin stripes) or a ring of such a wall, depending on the periodicity enforced by 9×10 versus 10×10 periodic lattices [11]. This work may have been the first to indicate the effect of lattice (simulation cell) size and commensurability on the resulting ground states that are obtained. More on such studies, and the methods that were developed, will be discussed in Section 2.

Since this early work, numerous related papers have appeared (some of the early papers have accumulated hundreds of citations), with much of the effort turning to dynamical inhomogeneities or more varied spatial inhomogeneities, and how they impact the properties of strongly correlated electron systems. Nevertheless studies of static charge and spin stripe ground states have persisted, with extensions to more nuanced models aimed at modeling specific classes of materials, viz. manganites versus cuprates versus iron pnictides. Dagotto and coworkers have reported studies on a two orbital model adapted to model the d_{xz}, d_{yz} orbitals of iron pnictides, finding stripes for periodic Hamiltonians and disturbed stripes for cases with quenched-in disorder, such as by Co doping [12, 13]. A recent direction has been to move beyond mean field approaches for multi-orbital models by extending quantum Monte Carlo methods to study such charge and stripe correlations [14, 15]. Meanwhile, experimental investigations have become more detailed, by mapping symmetries of inhomogeneous phases using, for example, advanced spectroscopic imaging [16, 17] in addition to diffraction.

Most previous studies have concentrated on the strongly correlated regime. When interaction effects are strong, effects of the underlying mean field Fermi surface assume less importance; conversely moderately correlated systems may retain instabilities connected to the Fermi surface. In the latter scenario, reasonable sampling of the Fermi surface requires larger simulation cells. This is the feature we address in this paper: for a moderately correlated two-orbital (two-band) lattice model, how does the calculated ground state depend on the lattice size in the simulation.

The organization of the manuscript is as follows. In Section 2 the two band model and methods of treatment are presented. Section 3 presents some baseline results for the density of states (DOS) and the inverse participation ratio of the single particle eigenstates, related to lattice size $N\times N$ with $N=16$,32, and 48. Results for interacting particles