Preface

This thesis covers most of my work in the field of ultracold atoms loaded in optical lattices. This thesis can be divided into five different parts. In Chapter 1, after a brief introduction to the field of optical lattices I review the fundamental aspects pertaining to the physics of systems in periodic potentials and a short overview of the experiments on ultracold atoms in an optical lattice.

In Chapter 2 we develop an inhomogeneous mean-field theory for the extended Bose-Hubbard model with a quadratic, confining potential. In the absence of this potential, our mean-field theory yields the phase diagram of the homogeneous extended Bose-Hubbard model. This phase diagram shows a superfluid (SF) phase and lobes of Mott-insulator (MI), density-wave (DW), and supersolid (SS) phases in the plane of the chemical potential μ and on-site repulsion U; we present phase diagrams for representative values of V, the repulsive energy for bosons on nearest-neighbor sites. We demonstrate that, when the confining potential is present, superfluid and density-wave order parameters are nonuniform; in particular, we obtain, for a few representative values of parameters, spherical shells of SF, MI, DW, and SS phases. We explore the implications of our study for experiments on cold-atom dipolar condensates in optical lattices in a confining potential.

In Chapter 3 we present an extensive study of Mott insulator (MI) and superfluid (SF) shells in Bose-Hubbard (BH) models for bosons in optical lattices with harmonic traps. For this we develop an inhomogeneous mean-field theory. Our results for the BH model with one type of spinless bosons agrees quantitatively with quantum Monte Carlo (QMC) simulations. Our approach is numerically less intensive than such simulations, so we are able to perform calculations on experimentally realistic, large three-dimensional(3D) systems, explore a wide range of parameter values, and make direct contact with a variety of experimental measurements. We also generalize our inhomogeneous mean-field theory to study BH models with harmonic traps and (a) two species of bosons or (b) spin-1 bosons. With two species of bosons we obtain rich phase diagrams with a variety of SF and MI phases and associated shells, when we include a quadratic confining potential. For the spin-1 BH model we show, in a representative case, that the system can display alternating shells of polar SF and MI phases; and we make interesting predictions for experiments in such systems. . In Chapter 4 we carry out an extensive study of the phase diagrams of the extended Bose Hubbard model, with a mean filling of one boson per site, in one dimension by using the density matrix renormalization group and show that it contains Superfluid (SF), Mott-insulator (MI), density-wave (DW) and Haldaneinsulator (HI) phases. We show that the critical exponents and central charge for the HI-DW, MI-HI and SF-MI transitions are consistent with those for models in the two-dimensional Ising, Gaussian, and Berezinskii-Kosterlitz-Thouless (BKT) universality classes, respectively; and we suggest that the SF-HI transition may be more exotic than a simple BKT transition. We show explicitly that different boundary conditions lead to different phase diagrams.

In Chapter 5 we obtain the excitation spectra of the following three generalized of Bose-Hubbard (BH) models: (1) a two-species generalization of the spinless BH model, (2) a single-species, spin-1 BH model, and (3) the extended Bose-Hubbard model (EBH) for spinless interacting bosons of one species. In all the phases of these models we show how to obtain excitation spectra by using the random phase approximation (RPA). We compare the results of our work with earlier studies of related models and discuss implications for experiments.

References:

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2- Bose-Hubbard models in confining potentials: Inhomogeneous mean-field theory, R.V. Pai, J.M. Kurdestany, K. Sheshadri and R. Pandit, Phys. Rev. B **85**, 214524 (2012).

3- **Phases, transitions, and boundary conditions in a model of interacting bosons**, J.M. Kurdestany, R.V. Pai, S. Mukerjee and R. Pandit, **arXiv:1211.5202v1**.

4- Random-Phase-Approximation Excitation Spectra for Bose-Hubbard Models, J.M. Kurdestany, R.V. Pai and R. Pandit, to be published.