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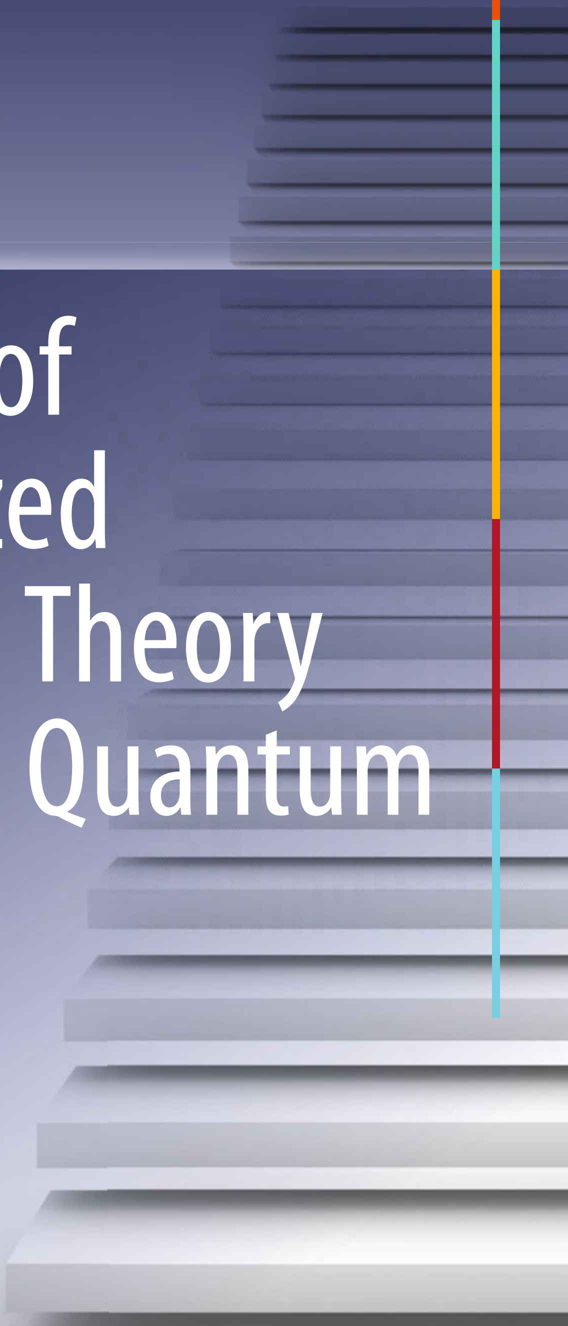
Utilization of Renormalized Mean-Field Theory upon Novel Quantum Materials



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Utilization of Renormalized Mean-Field Theory upon Novel Quantum Materials

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Supervisor's Foreword

Searching for a new state of the matter has always been many physicists' research goal. After the discovery of the high-temperature superconductor (HTS) about 30 years ago, its microscopic mechanism is still under debate due to the fact that several so-called competing orders like charge and spin density waves have been found along with the superconductivity. Many believe that its precursor, the Mott insulator, may be responsible for the microscopic properties. However, as we know the relevance of Mott physics in cuprates has been greatly under debate for many years and even questioned recently by some physicists like R. B. Laughlin (PRB **89**, 035134 (2014)). Some completely abandon the strong coupling approach and others have argued that the strong correlation only provides a renormalization of the dispersion of quasiparticles. Although we do not exclude the possibility that weak coupling manages its underlying physics, we have shown in our works that for all the hole doping relevant for cuprate phase diagram, the Mott Physics provides a very strong renormalization of local chemical potential so that it can vary from site to site without costs of energies. Thus, the charge ordered states is a natural consequence of Mott physics and it goes beyond just simple renormalization of dispersion.

The usual way to produce charge orders or charge/spin density wave is through special Fermi surface features like surface nesting or hot spots with very strong antiferromagnetic scattering. Hence, the strong correlated $t-J$ model seems to be not a viable model and one must invoke new extra interactions to explain the so-called "competing phases". But we have presented a theory based on a well-known and accepted $t-J$ model of cuprates and it reproduces almost all the important results like special bond-order symmetry, local density of states, two gaps, the Fermi arc, etc. More importantly, our method of producing charge density waves (CDW) is not due to Fermi surface nesting or hot spots. Although some of our results have been reported before, they mostly focused on a particular hole doping level of 0.125 and used different parameters or models and therefore, it is unclear how generic the results were. Especially, it is not clear if the pattern is as what observed by experiments. Now with our work, we have presented many more quantitative evidences that the charge order is a consequence of strong correlation.

Another non-trivial superconducting phase that may provide hints for us in discovering the physics of high T_c materials is the famous Fulde–Ferrell and Larkin–Ovchinnikov state. Coincidently, it has not been firmly established by experiments for more than 50 years since its first theoretical prediction. This state has superconducting electrons paired with a finite total momentum to account for the presence of competing magnetic field. It has a modulation of pairing order in real space, i.e. a pair density wave (PDW). In the meanwhile, the mystery about the pseudogap phase for the high T_c cuprates, which occupies a huge area in the phase diagram overlapping with the superconducting dome, has existed for almost 25 years for the reason that not only there is no satisfactory explanation, but also the experiments seem to document more and more complex phenomena. In this work, we propose a particular kind of PDW to be responsible for most of the novel spectra in the pseudogap phase. At lower temperature, this state also has a pairing order parameter with total momentum zero besides a finite momentum pairing order. This is the first theoretical work, which is able to account for the doping and temperature dependence of the spectra for both the superconducting and pseudogap phases of the high temperature superconductors. As a result, we have strengthened greatly the likelihood that the PDW states are the basis in the pseudogap phase of cuprates if we neglect phase fluctuation and disorder. We have also mentioned a mechanism to verify our prediction and to isolate the Fulde–Ferrell and Larkin–Ovchinnikov state.

In summary, we have pointed out that the cause of these orders comes from the strongly correlated nature of this material. Therefore, they are instead intertwined and are not competing in our interpretation. Furthermore, there is a new pairing order composed of Cooper pair with a finite center-of-mass momentum. It should be pointed out that although our theory is based on a mean-field approach, more and more much accurate numerical methods have obtained similar solutions as ours. The simplicity and intuitive picture emerged from our mean-field approach provides an important basis to unravel the mystery of HTS.

Taipei, Taiwan
December 2018

Prof. Ting-Kuo Lee

Abstract

This thesis aims at utilizing the strongly correlated t –J Hamiltonian for better understanding the microscopic pictures of certain condensed matter scenario. One of the long existing issues in the Hubbard model and its extreme version, t –J model, lies in the fact that there is not an analytical way of solving them. Therefore, when dealing with these models, numerical approaches become very crucial. In this thesis, we will present one of the methods called renormalized mean-field theory (RMFT) and exploit it upon the t –J model. Thanks to the concept proposed by Gutzwiller, all we have to do is to try to include the correlation of electrons, which is mainly the most difficult part, with several renormalization factors. After obtaining the correct form of these factors, we can apply the routine mean-field theory in solving for the Hamiltonian, which is the principal methodology throughout this thesis.

Next, the physical systems that we are interested in consist of two parts. The mystery of High-Tc superconductivity comes first. After 30 years of its discovery, people still cannot settle for a complete microscopic theory in describing this exotic phenomenon. However, with more and more experimental equipment with higher accuracy nowadays, lots of behaviors of copper-oxide superconductor (also known as cuprate) have been revealed. Those discoveries can definitely help us better understand its microscopic mechanism. Therefore, from the theoretical side, to compare the calculated data with experiments leads us to know whether our theory is on the right track or not. We have produced tons of data and made a decent comparison which will be shown in the main text.

The second system we are curious about is the mechanism of electrons under magnetic field. The Hofstadter butterfly along with its Hamiltonian, the Harper-Hofstadter model have achieved great success in describing free electrons' movement with lattice present under the influence of external magnetic field. Thus, it will be also interesting to ask the question: what will happen if the electrons are correlated. Our RMFT for t –J Hamiltonian, by adding an additional phase in the hopping term, happens to serve as a great preliminary model for answering this question. We will compare the results of ours with our collaborators', who solved this model by a different approach, the exact diagonalization (ED). Together with our calculations, we proposed several discoveries which might be realized by the cold atom experiments in the future.

Keywords Strongly correlated systems · $t-J$ model · RMFT

Parts of this thesis have been published in the following journal articles:

[1] W. Tu and T. K. Lee. Genesis of charge orders in high temperature superconductors. *Scientific Reports* **6**, 18675 (2016).

[2] P. Choubey, W. Tu, T. K. Lee, and P. J. Hirschfeld. Incommensurate charge ordered states in the $t - t' - J$ model. *New Journal of Physics* **19**, 013028 (2017).

[3] W. Tu, F. Schindler, T. Neupert, and D. Poilblanc. Competing orders in the Hofstadter $t - J$ model. *Physical Review B***97**, 035154 (2018).

[4] W. Tu and T. K. Lee. Evolution of Pairing Orders between Pseudogap and Superconducting Phases of Cuprate Superconductors. *Scientific Reports* **9**, 1719 (2019).

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Second, Dr. Didier Poilblanc also taught me a lot. The academic environment in Taiwan is not that open compared with that in Europe where scientists from different countries can easily meet each other. Thanks for his acceptance of my request of a joint-degree thesis, I got the chance to conduct research in France and therefore obtained many opportunities discussing physical topics with other outstanding scientists. To learn how to express my idea properly is crucial in becoming an independent physicist and during the time in France those are among all what I got to learn the most. I think it is fair to say that he led me on the track of becoming an independent researcher from just an apprentice of physics. Thus, I want to thank Didier for not only teaching me a lot of academic knowledge, but also those chances he granted me for interacting with other experts in this field.

Plus, our co-workers mean a lot to me since they were willing to spare time collaborating with us upon certain issues. I would like to thank Dr. Peayush Choubey and Dr. Peter J. Hirschfeld from the University of Florida for participating in the work of analyzing STS results in detail with Wannier function. Dr. Peng-Jen