Liquid and Ordered Phases of Geometrical Frustrated Charges

A Monte Carlo study of the Falicov-Kimball model on the triangular lattice

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Liquid phases are states of matter that display no long-range order even at very low temperatures, where usually some kind of symmetry-broken phase is expected. These phases are thought to possess unusual phenomena, such as emergence of effective gauge fields and fractionalization of the original degrees of freedom.

In this project we study interacting electronic systems on the triangular lattice with different filling fractions, which produce different degrees of geometric frustration. For increased frustration one expects liquid-like behavior at low-temperatures. To address this possibility we consider the Falicov-Kimball model: one of the simplest models of strong electron correlations, for which an efficient (classical) Monte Carlo algorithm exists.

At 1/3 filling, where frustration is reduced, we find that for high-temperature there are disordered phases that behave differently according to the interaction strength: for large U there is a Mott insulator; for intermediate U an Anderson insulator; and for low U a weakly-localized phase. For low-temperature there is an ordered phase with a Z_3 symmetry, which for high U leads the order-disorder transition to belong to the same universality class of the two-dimensional Potts model with $q = 3$.

At half-filling, where frustration is high, the results for high-temperature are similar to the ones for 1/3 filling. For low-temperature the regimes found are still mostly inconclusive, but preliminary results seem to point at a potential absence of order. We hope that continuing the work presented here can lead to results that can guide the search for compounds where liquid phases are realized.

1 Introduction

The Falicov-Kimball (FK) Model was introduced in 1969, in an article by Falicov and Kimball [1], to describe metal-insulator transitions for rare earths and transition metals. It has later been proposed as a model for crystallization and for binary alloy systems [2]. It is one of the simplest models of strongly correlated electrons, featuring a set of phases only possible in the presence of interactions. The model was actually discovered earlier by Hubbard as a limiting case of the Hubbard model [3].

The FK model can be thought of as a model of delocalized electrons that move around on a lattice and interact with fixed classical charges. The former are designated as c-electrons and the later as f-electrons. The model is defined on top of a lattice Λ with V lattice sites, which in $2D$ is given by $V = L \times L$, where L is the system's linear size. The Hamiltonian of the simplest version of this model, featuring spinless particles, is given by:

$$H = -\sum_{ij} t_{ij} c_i^\dagger c_j + U \sum_i c_i^\dagger c_i n_{f,i} - \mu_f N_f - \mu_c N_c \ , \tag{1.1}$$

where $c_i^\dagger$ (c_i) represent the creation (annihilation) operator of a c-electron on lattice site i and $n_{f,i}$ the number of f-electrons located there, which can be 0 or 1. The first sum is a tight binding term and represents the kinetic energy of the c-electrons, with t_{ij} being the hopping matrix element which is t for nearest neighbors and 0 otherwise. The second sum represents an on-site interaction between the two species of electrons which is present whenever one of each kind is at the same lattice site, with U being that interaction energy. μ_c and μ_f are the chemical potential of each species and fix their respective particle number N_c and N_f, which are defined as:

$$N_c = \sum_i c_i^\dagger c_i \quad \text{and} \quad N_f = \sum_i n_{f,i} \ . \tag{1.2}$$

Depending on whether $U > 0$ or $U < 0$ the interaction is, respectively, repulsive or attractive, alluding to different physical interpretations. If $U > 0$, the f-electrons can be thought of as belonging to localized f-orbitals of an atom located at a given lattice sites. The c-electrons, on the other hand, belong to orbitals that strongly overlap and so they become delocalized and form a band. If $U < 0$, then what we call f-electrons should be seen as a set of positively charged ions with the c-electrons moving and interacting with the localized potentials generated by the positively charged ions. As shall be seen below there is a symmetry of the model that allows results obtained in one case to be related to results obtained in the other, which means that even though both scenarios are physically different, they are equivalent mathematically. From now on we shall just refer to them as c-electrons and f-electrons.

2 Results

In this section we present our results on the subject. We study the FK model on the triangular lattice using the Metropolis-Hasting algorithm with sequential updates. We

expect that the frustration present on this lattice type might produce changes on the phase diagram obtained previously for the square lattice [4].

We start by presenting the results for filling $\rho_f = 1/3$ and $\rho_c = 2/3$.

2.1 1/3 Filling

The main result of this section is presented in Fig.1, that depics the phase diagram for the FK model at 1/3 filling in the $T - U$ plane.

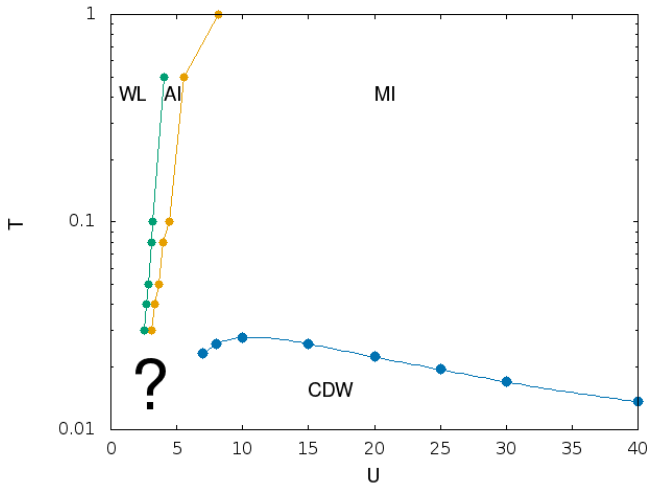


Figure 1: Phase diagram for the Falicov-Kimball model on the triangular lattice with 1/3 filling in the $T - U$ plane, composed of five different regions: a charge density wave (CDW) ordered phase at low temperature and $U \geq 7$. For high temperature there is a Mott insulator (MI) for large values of U, an Anderson insulator (AI) for intermediate ones and a metallic-like (WL) phase for low U. For low temperature and $U < 7$ the results are still inconclusive.

With the exception of the a region low temperature and $U < 7$, where our results are inconclusive, this phase diagram is very similar to the one obtained in Ref. [4] for the square lattice at half-filling, which as was already said was to be expected.

For $U \geq 7$ and low temperature there is a charge density wave (CDW) phase. This ordered phase corresponds to the configurations like the ones shown in Fig.2, the other two low energy states being obtained by translation. Similarly to the checkerboard phase for the square lattice at half-filling, this ordered phase results from a perfect nesting of the Fermi surface that leaves the system susceptible to instabilities that order both species of electron with a certain period.

For high temperature there are three disordered phases that behave differently with respect to the properties of the c-electrons. For low U there is a weakly localized phase with metallic-like behavior and for large U a Mott insulator is observed. For intermediate values there is an Anderson insulator. As was stated in the previous chapter the density

of states (DOS) and the inverse participation ratio (IPR) were used to identify these phases. The Mott insulator is identified by a gap in the DOS around the Fermi surface. The weakly localized phase is identified by an IPR that scales with the volume for states around the Fermi surface, indicating they are delocalized and that the system is not an insulator. For the Anderson phase, even though there is no gap around the Fermi surface, those states are localized and therefore the system behaves as an insulator.

For low temperature and $U < 7$ results are still inconclusive. Some hypothesis for this fact and proposals for further investigation of this region are presented in the conclusion section.

2.2 Z_3 Order Parameter

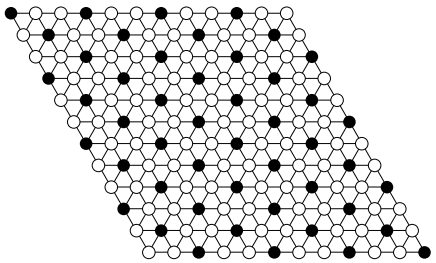


Figure 2: Ground state configuration of the f-electrons at 1/3 filling for the CDW phase.

The CDW phase presented in the phase diagram of Fig.1 has the ground state configuration shown in Fig.2, which corresponds to the f-electrons occupying one of the three sublattices that compose the triangular lattice.

The ground state configurations persist for finite temperatures until a critical value is reached that destroys them. In order to determine the critical temperature of this order-disorder phase transition one has to apply a finite size scaling (FSS) method. Such method, however, requires an order parameter. An appropriate order parameter for this ordered phase is given by

$$\phi = \frac{3}{V} \sum_r e^{i\frac{2\pi}{3}(r_x - r_y)} n_{f,r} \ , \tag{2.1}$$

where r is the lattice label, with r_x being its x and r_y its y coordinate on the lattice, such that $r = r_y L + r_x$. As was stated, there are 3 possible configurations for the ordered phase. There is the one in Fig.2 and the others are obtained by shifting every position by one and two steps to the side. For each of them, ϕ has a different value $\phi = 1, e^{i\frac{2\pi}{3}}, e^{i\frac{4\pi}{3}}$. This is easy to verify: the exponent in (2.1) can only be $\theta = 0, i\frac{2\pi}{3}, i\frac{4\pi}{3} + 2\pi i n$, with n being an integer; a rotation by $2\pi i n$ represents the same complex number. So depending on which ordered configuration we have, only one of this 3 complex numbers is going to be summed. So in the end we get the already stated results for ϕ. If however we have a perfectly disordered configuration then we will have in the sum an equal amount of these 3 complex numbers and so in the end we get $\phi = 0$. Therefore, $\langle|\phi|\rangle = 0$ corresponds

to a disordered phase and $\langle|\phi|\rangle = 1$ to an ordered one. We can thus conclude that this quantity is a good order parameter and we can use it to define the susceptibility $\chi_\phi = \beta V \left(\langle|\phi|^2\rangle - \langle|\phi|\rangle^2\right)$, the Binder cumulant $U_4 = 1 - \langle|\phi|^4\rangle/3\langle|\phi|^2\rangle$ and so on for the remaining quantities mentioned in the previous chapter. This quantities help us to characterize the order-disorder transition in the next section.

2.2.1 Order-disorder phase tnansition and Critical Exponents

The transition line between the ordered phase and the disordered is determined via the crossing point of the Binder cummulant. Simulations were run for several U at low temperature in order to determine the respective critical temperature.

For $U = 30$ a longer simulation was run that allowed for the determination of the critical exponents of the transition which are present in table 1

	ν	γ
Numeric	0.8031(114)	1.4748(329)
Exact	5/6	13/9

Table 1: Comparison between the numeric value of the critical exponents with the exact one.

3 Half-Filling

In this section the results for the half-filling scenario are presented. This case is frustrated and the low temperature picture is expected to be significantly different from the 1/3 filling case. In Fig.3 the phase diagram for the FK model at half-filling in the $T - U$ plane is shown.

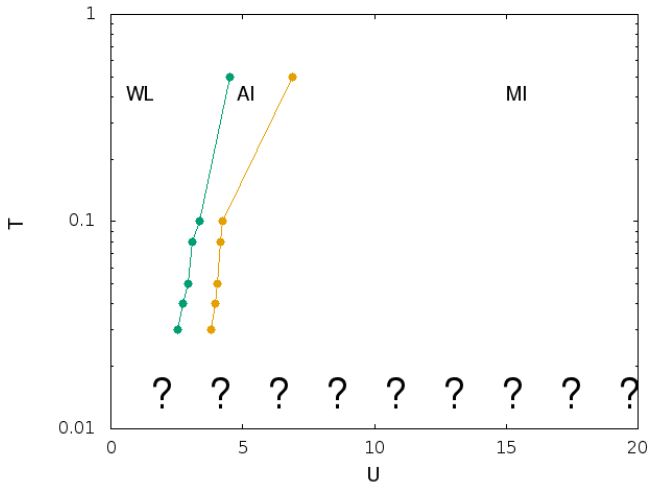


Figure 3: Phase diagram for the Falicov-Kimball model on the triangular lattice with half-filling in the $T - U$ plane, composed of four different regions: For high temperature there is a Mott insulator (MI) for large values of U, an Anderson insulator (AI) for intermediate ones and a metallic-like (WL) phase for low U. For low temperature it is hard to get a definite picture of the phases present.

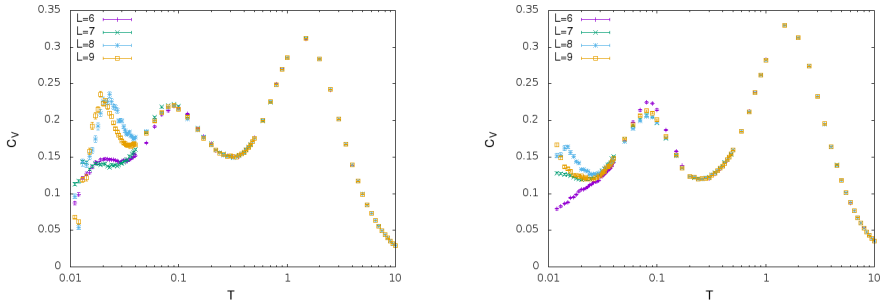
For high temperature the results are very similar to the ones obtained for 1/3 filling in the triangular lattice and the square lattice at half filling. For high temperature and high U there is a Mott insulator, for intermediate U there is an Anderson insulator and at low U there is the metallic-like phase. This similarity is to be expected and in fact we propose that this picture should be very weakly dependent on lattice types or filling fractions. For high U there will always be a gap in the system and if the temperature is high enough for the system to be out of a possible ordered phase, then the only thing left for the system to be is a Mott insulator. When the gap closes for lower U and for high enough temperatures the c-electrons will always see a random potential generated by the f-electrons, which leads to Anderson localization.

For low temperature the results are generally not very conclusive. On one hand this is problematic because it does not allow us to make many solid conclusions. On the other hand, the very fact that the low temperature regime for the half-filling case is hard to analyze is exactly what we set out to find. The fact that the tools employed to characterize the previous case do not work so well here means that what is going on is significantly different and more complex.

We try to complement the picture by looking at the specific heat. Since we do not know what the ordered phase is or if there is even one, we cannot define an order parameter which would help with analyzing the transition. Because of this the only way to locate a possible phase transition or crossover is via the specific heat.

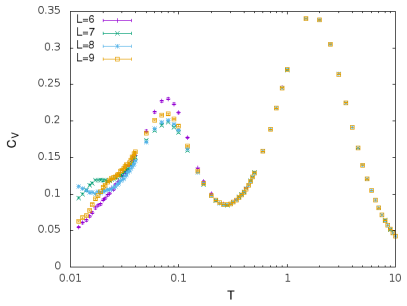
In Fig.4 we show the specific heat for different values of U and different system sizes. For $U = 5$ there is the presence of three bumps in the specific heat. The one for large temperature corresponds to the fact that the system starts to have doubly occupied states.

The other two possess some scaling with the volume which might signal some kind of phase transition. However since most likely the system sizes used are not commensurable with the period of the order (if there is one) the scaling is not perfect. They may also just correspond to crossovers and just mean that the distribution of the states the system occupies somehow changes after going through them. We note that the bump for lowest temperature starts to get pushed for even lower temperatures as U increases and eventually disappears. Besides this nothing very certain was found about it. However for the middle bump there is something that can be said.

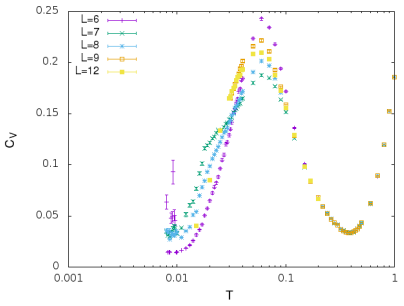


(a) $U = 5$

(b) $U = 6$



(c) $U = 7$



(d) $U = 10$

Figure 4: Specific heat as a function of temperature for different values of U and different system sizes.

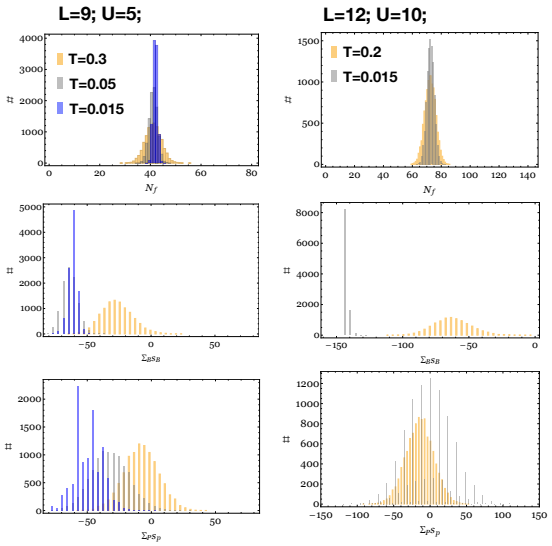


Figure 5: Histograms for the number of f-electrons, the energy distribution of the Ising term and for the triangular plaquettes term. These were computed using the configurations sampled via Monte Carlo for different values of U and T. The temperatures chosen were the ones before and after the bumps in specific heat.

In Fig.5 we show histograms of the antiferromagnetic Ising contributions to the energy along with the contribution from the triangular plaquettes. These are terms from an effective model expansion and the histograms were computed with the configurations sampled via Monte Carlo. There are histograms for $U = 9$: for a temperature lower than the left bump; another for a temperature between the first and the second and another between the second and the third. There is also histograms for $U = 10$ for a temperature before and after the second bump. What is observed is that the distribution of the energy contributions from the Ising term changes significantly when crossing the second bump. This can be seen specially well for $U = 10$. It suggests that with the crossing some constraint is lifted that allows for the population of a greater variety of configurations, which explains the bump in the specific heat. This conclusion also suggests that maybe the lowest temperature bump comes from a similar effect for a different term of the expansion, and since the succeeding terms depend on larger powers of U^{-1}, this would explain why the lowest bump eventually vanishes as U increases. However the histograms for the plaquettes did not allow to make any more conclusions supporting this line of thought.

4 Conclusion

As stated in the very beginning, liquid phases are poorly understood phases of matter that possess some very exotic phenomena. The question that this work set out to answer was whether or not a simple semi-classical model put under geometrical frustration is

capable of displaying the properties of such phases of matter. If so, then a new effective and systematic way of studying them would be open.

To answer this question the Falicov-Kimball model was chosen, since this is one of the simplest models for correlated electron systems and can be simulated efficiently via Monte Carlo. A program that implemented the simulations was developed along with many tools to extract physical observables and tools for numerical analysis.

Results were obtained for two different filling fractions, one frustrated and another not, so the results could be contrasted.

For 1/3 filling the results obtained, except for an inconclusive region were compatible with the ones for the square lattice at half-filling. There was an ordered phase for low temperature and for high temperatures there were weakly localized, Anderson insulator and Mott insulator phases. Inclusively the order-disorder transition also belongs the same universality class a classical model: the Potts model for $q = 3$, whereas for the square lattice it was the Ising model.

For half-filling, the high temperature picture was the same as before and we proposed that this picture should not depend too strongly on lattice types and filling fractions. For low temperature, the results where somewhat inconclusive. We were able to justify the presence of two of the three bumps observed for the specific heat. The remaining one might signal a crossover or a transition to an interesting low temperature phase, as was suggested by the non-uniform structure obtained with the PCA. The fact that the methods used to analyze the 1/3 filling case failed to lead to more solid conclusions for this frustrated scenario is on itself interesting. The goal was to find regimes in the phase diagram that display unusual phenomena that is hard to characterize. Such regimes could be candidates for liquid phases, but further investigation is required to be able to make such strong claims.

Future work shall focus on studying the low temperature regimes obtained for the half-filing. In particular discovering the origin of the lowest temperature bump in the specific heat might provide some insight into the nature of the regime present just before the bump. Given that one of the other bumps was linked directly to the Ising term in the effective model, it would be interesting to simulate the classical models that obtained by truncating that expansion. It might be possible that by adding specific terms of the expansion one might be able to reproduce what was observed for the FK model. This provide an origin for the unknown bump.

It may also be of value to try and come up with methods to identify specifically liquid phases in the phase diagram, since the current approaches are more focused in looking at what liquid phases are not instead of what they are.

References

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