The phase diagram of the Haldane-Falicov-Kimball model

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We provide analytical and numerical results for the phase diagram of the Haldane-Falicov-Kimball model - a model combining topology, interactions and disorder at finite temperatures. By compiling results on the observables of localized and itinerant electrons, we obtain a rich phase diagram on the interaction - temperature plane. Along with known phases, we unveil an insulating charge ordered state with gapless excitations and a temperature-driven gapless topological insulating phase. Intrinsic - temperature generated - disorder, is the key ingredient explaining the unexpected behavior. Our findings support the possibility of temperature-driven gapped and gapless topological insulating phases in systems with a large mass unbalance in fermionic species.

Keywords: topology, disorder, strong correlations, Haldane model, Falicov-Kimball model.

I. INTRODUCTION

The experimental discovery of the integer quantum Hall effect opened the way for a completely new type of phase transitions without spontaneous symmetry breaking: the topological phase transitions. Since then, topology has been the source of many publications due to the very appealing properties that topological insulating materials (TI) hold such as the robustness of their surface conducting states against defects.

More recently, the influence of disorder, interactions and finite temperatures on topological phases of matter has attracted a large theoretical interest in order to better understand the role of topology in real-world materials. Strong interactions were shown to suppress topological phases when magnetic order was induced both for Hubbard-like and spinless nearest-neighbor (NN) interactions. Magnetic ordering was also found to coexist with topological phases to form antiferromagnetic topological insulating phases. Some mean-field studies showed that interactions could, in some cases, induce a topological phase when imposed in a trivial band model, forming the so called topological Mott insulator, that exists in the strong-coupling regime. The existence of this phase outside the mean-field scope has been questioned multiple times and a significant amount of attention has turned to weak coupling interaction-driven topological insulating phases in 2D systems with quadratic band crossing points.

The influence of correlations at finite temperatures on TI has also already been studied. Although thermal fluctuations are responsible for the destruction of topological order when large enough, they can also drive different types of topological phases.

The role of disorder in TI has also been widely studied and it has been found that for 2D systems belonging to the unitary class (for which time-reversal symmetry is broken), disorder effects localize every eigenstate except two bulk extended states that carry opposite Chern numbers in the topological phase. The merge of these states was shown to be associated with the destruction of the topological phase for a sufficiently large disorder strength. Disorder studies on topology also unveiled a new class of TI for which a disorder-induced topological phase transition into a topological phase is possible. These were called topological Anderson insulators (TAI).

The Falicov-Kimball model (FKM) is a limiting case of the Hubbard model for which one of the spin fermion species is infinitely massive, meaning that these fermions - the f-electrons - are immobile. At half-filling, the f-electrons order in a charge ordered state known as the charge density wave (CDW) for every value of the interaction strength between the localized and itinerant electrons. Recently, the full phase diagram of the 2D FK model was obtained with Monte Carlo (MC) techniques and unveiled an Anderson insulating phase overlooked in previous studies. The averaging on configurations of f-electrons sampled with the MC method acts as a disorder potential to itinerant electrons making it possible that their eigenstates become localized without the presence of explicit disorder.

The Haldane model was the first theoretical model of a topological insulator under a zero net magnetic field and studies of this model under the influence of disorder have shown that although the topological phase is robust for small disorder, it can be destroyed for a large enough disorder strength.

In this letter we attain the finite temperature phase diagram of the Haldane-Falicov-Kimball model (HFKM), at half-filling, using the approximate variational mean field and the exact Monte Carlo Metropolis Hastings (MC) methods. This approach provides a way of obtaining unbiased numerical results for a model combining topology, interactions and disorder at finite temperatures. Our main results are summarized in Fig. 1 which depicts the different phases as a function of the temperature, $T$, and of the interaction magnitude, $U$. By computing observables of localized and itinerant electrons, a group of different phases were found: a charge...
density wave (CDW) at low temperatures coexisting with a topological insulating phase (TI) at low $U$ and with a finite superposition with a gapless (GI) and Mott-like (MI) insulating phases. As a central result, the topological phase was found to exist for larger $U$ when $T$ is increased from $T = 0$ and to extend into the gapless region of the phase diagram at higher temperatures, giving rise to a temperature-driven gapless topological insulating phase (GTI). At large temperatures, the HFKM reduces to the Haldane model with binary disorder and the phase transitions lose temperature-dependence. The similarities between MF and MC results imply that the approximation used in the former captures the essential physics of the exact model.

II. MODEL AND METHODS

The Hamiltonian for the HFKM is

$$
H = -t \sum_{(i,j)} c_i^\dagger c_j + i t_2 \sum_{(i,j)} \nu_{ij} c_i^\dagger c_j + h.c. + U \sum_i c_i^\dagger c_i n_{f,i} - \sum_i (\mu_c c_i^\dagger c_i + \mu_f n_{f,i})
$$

(1)

This Hamiltonian depicts a species of itinerant electrons (c-electrons) with creation operators $c_i^\dagger$ and another of localized electrons (f-electrons) whose local density at site $i$ is given by the occupation number $n_{f,i}$. The operators $c_i = c_{i,A}, c_{i,B}$ are defined in the two interpenetrating triangular sublattices $A$ and $B$ that form the honeycomb lattice shown in Fig. 2a, with total volume $V = 2L^2$, where $L$ indicates the linear number of unit cells. The first term is the kinetic energy of the itinerant electrons associated with NN hoppings, with $t$ being the hopping integral for NN. The second term considers Haldane next nearest neighbor (NNN) complex hoppings and $\nu_{ij} = \pm 1$ according to the arrows represented in the honeycomb unit cell in Fig. 2a. The third term describes the local interaction between the localized and itinerant electrons, with $U > 0$. The final term contains the chemical potentials of the itinerant and localized electrons, respectively $\mu_c$ and $\mu_f$. We are studying the model at half-filling for both species - one particle per unit cell - and therefore set $\mu_c = \mu_f = U/2$. In what follows, $t_2 = 0.1t$.

Using the fact that $n_{f,i}$ is a conserved quantity, $n_{f,i} = 0, 1$ can be seen as classical variables and the partition function of the model can be written as

$$
Z = \sum_{\{n_f\}} Tr_{c}[e^{-\beta H(\{n_f\})}] = \sum_{\{n_f\}} e^{-\beta \mathcal{H}(\{n_f\})}
$$

(2)

where

$$
\mathcal{H}(\{n_f\}) = -\frac{U}{2} \sum_i n_{f,i} - \frac{1}{\beta} \sum_i \ln(1 + e^{\beta E_i(\{n_f\})})
$$

(3)

is the effective Hamiltonian obtained after taking the trace over the c-electrons’ degrees of freedom. $\mathcal{H}$ is defined in terms of the eigenvalues $E_i(\{n_f\})$ of $H$ obtained for a fixed configuration of f-electrons, $\{n_f\}$.

Variational mean field. The variational mean field method is based on the Bogoliubov inequality which states that we can define a free energy functional $F$ in

FIG. 1. Phase diagram of the HFKM in the interaction $U$ - temperature $T$ plane obtained with the Monte Carlo Metropolis Hastings (a) and mean field (b) methods. The different phases follow: outside the charge density wave phase (CDW), topological insulator (TI) for small $U$, gapless topological insulator (GTI) and gapless insulator (GI) for intermediary $U$, and Mott-like insulating phase (MI) for large $U$. Inside the CDW phase, phases with similar features as their high temperature counterparts were found and the suffix “/CDW” was added.
terms of a mean field Hamiltonian $H_{MF}$ in such a way that

$$ F \leq F_{MF} + \langle H - H_{MF} \rangle_{MF} \equiv F $$

where $F$ is the exact free energy of the system, $F_{MF}$ is the free energy of the mean field Hamiltonian and $H$ is the effective Hamiltonian defined in expression (3). $H_{MF}$ must depend on a set of variational parameters that are computed in order to better approximate $H$ by minimizing the functional $F$. For the HFKM we propose a Hamiltonian with a single variational parameter $\omega$ given in expression (5)

$$ H_{MF} = -\omega \sum_{i \in A} n_{f,i} + \omega \sum_{i \in B} n_{f,i} $$

In the ordered phase we must have $\omega \neq 0$. In order to compute numerically $\langle H \rangle_{MF}$, exact diagonalization is employed and the average is performed in configurations satisfying $\langle n_{f,i}^{A,B} \rangle = \langle n_{f,i}^{A,B} \rangle_{MF} = n_{FD}(T\beta\omega)$, with $n_{FD}$ being the Fermi-Dirac distribution. The order parameter corresponding to the average staggered occupation on each sublattice is defined as $\delta = \langle n_{f,i}^{A} \rangle_{MF} - \langle n_{f,i}^{B} \rangle_{MF}$.

Monte Carlo. The Monte Carlo Metropolis Hastings is a classical Monte Carlo algorithm that provides a way of generating configurations for a set of classical variables according to the Boltzmann weights of the partition function. In our case, although c-electrons are described by quantum operators, the f-electron densities $n_{f,i}$ commute with the Hamiltonian and can be seen as classical variables. By integrating out the c-electron’s degrees of freedom, we defined the effective Hamiltonian $H$ given in Eq. (3) that is written only in terms of f-electron variables. This provides a means of writing the partition function in a classical way as the sum of the Boltzmann weights $e^{-\beta H(n_{f})}$ and makes it possible to use a classical Monte Carlo method to generate configurations of f-electrons according to these weights.

Observables. For f-electrons, we were interested in obtaining the CDW phase transition, characterized by an order parameter corresponding to the staggered occupation of f-electrons in sublattices $A$ and $B$. For the MC method, the $T_{CDW}(U)$ curve was obtained by fixing $U$ and computing the intersections of $T$-dependent Binder cumulant curves for different system sizes. The Binder cumulants have the special feature of being scale invariant at the critical temperature $T_{CDW}$ as shown in the example of Fig. 2b, providing in this way an unbiased method for computing it.

For the MF method, the $F$-functional curves were obtained as a function of the order parameter $\delta$ for a fixed $U$ and different $T$ near $T_{CDW}$, as shown in the example of Fig. 2a. These curves were fitted to a polynomial with even powers of $\delta$ and the coefficient of $\delta^2$ ($b$ coefficient) was found. Near $T_{CDW}$ and according to the Landau theory of second order phase transitions, this coefficient must be proportional to $(T - T_{CDW})$ and therefore a linear fit on the obtained $b$ coefficients was performed to extract $T_{CDW}$ as shown in the example of Fig 2a.

Both the MF and MC methods provide a way of generating configurations of f-electrons for a given temperature $T$ and interaction strength $U$ according respectively with the mean field and exact Boltzmann weights. The observables of c-electrons can then be computed by averaging on these configurations in both cases. In the MF approximation, the c-electron’s phase transitions lose temperature dependence outside the CDW phase for which every configuration becomes equally probable, corresponding to the limit of the Haldane model with binary disorder. Inside the ordered phase, a phase diagram can be obtained in the $(U, \delta)$ plane and then mapped into the $(U, T)$ plane.

In what regards the observables of c-electrons, we have investigated topological, spectral and localization properties. To study topological properties, the Chern number for both methods was computed with the coupling matrix method introduced in Ref. [55]. In MF, the Recursive method [60] [61] and the Transfer Matrix method (TMM) [62] were employed respectively to compute den-
FIG. 3. a - d, Density of states obtained with the Recursive method through MF for different points of the phase diagram: MI/CDW-(U, T) = (3, 0.1), GI/CDW-(3, 0.145), TI-(1.4, 0.23), GTI-(2.1, 0.23) , GI-(4.9, 0.23) and MI-(5.55, 0.23). Figure d shows a zoomed view of the DOS in figure c near E = 0. e - h, Density of states obtained with exact diagonalization through MC: MI/CDW-(U, T) = (2.5, 0.045), GI/CDW-(2.5, 0.085), TI-(1, 0.2), GTI-(2, 0.2) , GI-(4, 0.2) and MI-(5, 0.2). The DOS plots are shown with a Lorentzian broadening of width 0.01. e, Finite size scaling of the DOS at E = 0 for the point (2.5, 0.085) used in figure b. V0 corresponds to volume of the smallest used system (with L = 8). The DOS(E = 0) was computed in an energy window corresponding to 1% of the full bandwidth for the L = 8 system. This window was reduced proportionally to the system size for larger systems.

sities of states (DOS) and study localization. The TMM method considers a finite system with a fixed large longitudinal dimension N_L and a transverse dimension of size M, which is varied in order to compute the localization length \( \lambda_M \). We study the behavior of \( \lambda_M = \lambda_M / M \) as a function of M: if \( \lambda_M \) decreases with M, the eigenstates are localized in the thermodynamic limit and therefore the system is an insulator; on the contrary, if \( \lambda_M \) increases with M, the eigenstates are extended and the system is metallic; a constant \( \lambda_M \) signals a critical point.

The Recursive and transfer matrix methods often involve large system sizes and were not used with the MC method, which encompasses a much larger computational effort. Exact diagonalization was then chosen in this case to obtain the DOS while the inverse participation ratio (IPR) and level spacing statistics (LSS) methods were employed to study localization.

In our definition, the IPR is computed for a given energy \( E_\alpha \) through \( \text{IPR}_\alpha = \sum_i |\phi_{\alpha i}|^4 \), where \( \phi_{\alpha i} \) is the amplitude of the eigenvector with energy \( E_\alpha \) at site \( i \). An IPR histogram can then be obtained as a function of energy by sampling a large number of MC configurations. The IPR must scale to zero with the system’s volume if we are in the presence of extended states and to a constant if the states are localized.

LSS also provides a simple way of distinguishing between extended and localized states: for extended states level repulsion is expected and the spacings between energy levels assume a Wigner distribution with variance \( \sigma^2 = 0.178 \langle s \rangle^2 \) (for the case of the unitary class to which the HFKM belongs), where \( \langle s \rangle \) is the average value of the level spacing distribution; for localized states, the level spacing distribution acquires a Poisson-like shape with a larger variance [63]. The methodology described in Ref. [63] was followed to obtain LSS results.

III. RESULTS AND DISCUSSION

We now describe every phase in the phase diagram of Fig. [1] (CDW). Below the critical temperature \( T_{\text{CDW}} \), dot-dashed curve in Fig. [1] the f-electrons start ordering in a checkerboard-like pattern, that is, only one of the sublattices will be occupied as represented in the honeycomb unit cell in Fig. [2]a. This phase was already reported for the 2D FKM on a square lattice [52]. For the HFKM, besides the expected trivial gapped CDW phase (MI/CDW), a topological insulating phase with charge ordering (TI/CDW) was found along with a peculiar region for which the c-electron spectrum is gapless inside the CDW phase (GI/CDW).

The TI/CDW phase had already been noticed in Refs. [38, 64] and appears in contrast with the results for the Halkane model with NN interactions for which there is no region of coexistence between the CDW and...
TI phases\cite{11}. Regarding the GI/CDW phase, it was first predicted with MF as it can be seen through the plots of the DOS in Fig. 3, that show a transition between a gapped and gapless regime, and then confirmed with MC - Fig. 3. In MF, the Recursive method enabled the usage of systems up to $L = 10^3$, while in MC, we only reached $L = 16$. Therefore, in order to make sure that the GI/CDW phase was not a finite-size effect, the DOS at $E = 0$ was computed by opening a window around this energy with a length of 1% of the total spectral bandwidth and by counting the number of states inside while decreasing the window’s length proportionally to the system size. An example of this scaling is shown in Fig. 3a, for a point inside the GI/CDW phase, for which it can be seen that the quantity $\text{DOS}(E = 0)$ is stabilized and does not scale to zero. In MF, a very narrow GTI/CDW phase was also predicted (see discussion on the GTI phase below), but was not confirmed with MC.

To better understand the behaviour of the CDW phase transition curve, a mapping to the 2D antiferromagnetic Ising model was made for small and large $U$ and the phase transition curves obtained with a perturbative analysis (see Appendix). These curves were computed up to second order in the perturbation which involves either the terms with $U$ or with the hoppings integrals $t$ and $t_2$ and are shown in Fig. 1 in red. For small $U$, the $T_{\text{CDW}}(U)$ curve is quadratic while for large $U$, it is inversely proportional to $U$.

(TI and GTI). TI is a gapped topological phase, that is, $\text{DOS}(E) = 0$ for $|E| < \Delta_{\text{TOP}}/2$ and $C = 1$, with $\Delta_{\text{TOP}}$ being the topological gap. For $T = 0$, the f-electrons only occupy one of the sublattices and therefore act as a staggered potential to the c-electrons. This means that the topological insulating phase exists between $U = 0$ and $U = 6\sqrt{3}t_f \approx 1$, value at which the gap in the c-electron’s spectrum closes and opens, signaling the topological phase transition. When we increase $T$, the topological phase still exists and extends to larger $U$. This would be expected in that for the Hal-dane model with binary disorder - the large temperature limit - the topological phase is only destroyed for $U \approx 2.7$, meaning there must be a temperature-driven topological phase transition for $1 < U < 2.7$. The corresponding phase transition curves obtained with MF and MC are shown in Fig. 1 (thin red lines). In MF, a phase diagram was obtained in the $(U, \delta)$ plane (Figs. 4a,b) which was then mapped into the $(U, T)$ plane. For MC, the results were directly obtained in the $(U, T)$ plane and some of the Chern number curves used to obtain the topological phase transition are shown in Figs. 4c,d.

If we look at the MF approach alone, the $(U, T)$ phase diagram was obtained through a mapping from the Hal-dane model with binary-like disorder imposed in such a way that the probability of occupation of each sublattice depends on the order parameter $\delta$. The fact that the MF and MC results are very similar implies that the MF picture provides a quite good description of the exact effect of interactions in the topological properties of c-electrons. This strengthens the connection between temperature and disorder effects in the properties c-electrons. By noticing this connection, the thermal-induced topological phase transition occurring for $1 < U < 2.7$ resembles TAI phenomena, for which disorder-induced topological phase transitions into topological phases can occur. In MC, we can see the thermal average on the f-electron configurations acting as a disorder potential to the c-electrons. The consequence is that the topological phase extends into the gapless region of the phase diagram for higher temperatures. In Fig. 5, it can be seen that the topological gap existing in the TI phase is closed in the GTI phase, but we continue having $C = 1$ as it can be seen in figure Fig. 4b. In MF, the results are identical (Fig. 5).

The transition from the GTI into the GI phase is accompanied by the merging of the only two extended states that exist in the spectrum and carry opposite Chern numbers (see discussion on localization below). For the transition into the TI phase, the c-electron’s gap closes and reopens at the phase transition curve and this phenomenon is accompanied by the creation of the two bulk extended states that exist in the topological phases. (GI and MI). Increasing $U$ from the GTI phase leads to an interaction-driven topological phase transition into a trivial gapless insulating phase (GI). If we continue increasing $U$, the c-electron’s spectrum acquires a Mott-
like gap (MI). The DOS inside the GI and MI phases is exemplified in Fig.4, for MC and in Figs.4.d for MF. This phase transition is very similar to the one found for the 2D FKM in Ref. [52].

**Gapless insulators.** Up to this point the reason behind labeling the gapless phases GI and GI/CDW as insulating phases is yet to explain. The Haldane model belongs to the unitary class and therefore any degree of uncorrelated disorder is expected to localize every eigenstate except inside the topological phase, in which two extended states that carry opposite Chern numbers exist. This phase is suppressed when the extended states merge and become also localized.

In MF, the results were mapped from the Haldane model with uncorrelated disorder and no deviations from the universal behaviour of systems belonging to the unitary class is expected. This was confirmed after employing the TMM in the gapless phases. For $U$ in the range of the GI/CDW and GTI phases, the only extended states obtained for $E = 0$ were the ones associated with the topological phase transition. This can be seen in Figs.5,b for which $\Lambda_M$ was computed for different system sizes and for $\delta$ within the gapless region of the phase diagram. Indeed, if we compare Figs.5.a,b with Fig.4.a, we see that the value of $\delta$ associated with the extended states in the former matches the critical value of $\delta$ for which the topological phase transition occurs in the latter.

For the exact model, however, different localization properties can be observed in some cases. Outside the CDW phase, in the GTI and GI phases, the correlations between f-electron occupations decay with a characteristic length $\xi$. For distances larger than $\xi$, the disorder potential felt by the c-electrons becomes uncorrelated. These phases smoothly extend to the high $T$ limit, where disorder effects become equivalent to those of a binary quenched potential and therefore, the type of disorder felt by the c-electrons can be seen as uncorrelated similarly to the MF case. Fig.5 shows LSS results for the GTI and GI phases, for which it can be seen that the variance of the level spacing distributions has the expected value for extended states (thick red line) at two particular energies in the GI phase. Inside the GI phase, this variance is larger than this value for every energy, meaning that all eigenstates are localized.

The IPR was also computed in the GI phase and it is plotted in Figs.5.g. Around $E = 0$ the IPR is almost unchanged with the system size meaning the corresponding states are undoubtedly localized. For higher $|E|$ it is clear that IPR becomes smaller with system size. The unit slope associated with the scaling $IPR \propto V^{-1}$ is shown by the red dashed line in Fig.5.g. It can be seen in this figure that when the IPR scaling is compared with this slope in the doubtful regions, it shows the trend of scaling into a constant, suggesting the presence of localized states for every energy in the GI phase in agreement.
with the LSS results. However, for the GI/CDW phase, Figs. 5a,c,e suggest that although the eigenstates are localized around $E = 0$, there are also regions of extended states. Fig. 5b shows that IPR becomes smaller with $V$ for $-3 \lesssim E \lesssim -1$ (and $1 \lesssim E \lesssim 3$) and Fig. 5d shows for two energies in this interval that the IPR indeed scales with $V^{-1}$ for the used system sizes, opposite to what was observed in the GI phase.

Inside the CDW phase, different localization properties can be observed. The correlation length between f-electrons becomes infinite and c-electrons experience a type of long-range correlated disorder. Long range correlated disorder has been shown to be associated with the emergence of regions of extended states in 2D systems \cite{65,66}. Furthermore, for a range of $U$ within the GI/CDW phase, we have a gapped system at $T = 0$ that separates two bands of extended states. As we increase the temperature, our results suggest that the gap starts being populated by localized states due to thermal fluctuations. The important question is whether or not the extended character of the remaining states is maintained up to the GI/CDW phase. Although our results suggest a positive answer, more work should be done to confirm whether the obtained regions of extended states survive in the thermodynamic limit and if so, to theoretically understand the reasons behind their existence.

**Topology at finite temperatures.** As a final remark on our results, some important comments must be made on the robustness of the obtained topological phases at finite temperatures. For large enough temperatures the topological phases are expected to be completely suppressed as the system must be described by maximally mixed states. For smaller temperatures, however, regarding $k_B T$ does not exceed the separation of the extended states existing in the topological phases, these phases must be robust. Indeed, all the eigenstates inbetween are localized and cannot change the Chern number, similarly to what occurs for the integer quantum Hall effect \cite{68}. Very near the topological phase transition curve in Fig. 1, however, the extended states are close in energy and not much can be said about the robustness of the topological phases. On the other hand, as shown in Fig. 5a, just slightly away from the topological phase transition curve, the extended states already have an energy separation $\Delta E \approx 4 >> k_B T \approx 0.1$. This is the central result of the thesis and suggests the possibility of reaching robust temperature-driven gapped and gapless topological insulating phases.

## IV. CONCLUSION

In this work we introduced the HFKM model, allowing to effectively study the interplay of topology and interactions at finite temperatures, and provided a complete characterization of its phase diagram. An extensive numerical analysis was performed in order to obtain the exact phase diagram of the model. As a central result, we have shown the possibility of having temperature-driven topological phase transitions into gapped and gapless topological insulating phases from a region with no topological order at small temperatures. This unexpected phenomenon was found to have its origin in intrinsic disorder generated by thermal fluctuations. We also found an insulating charge ordered state with gapless excitations. In this phase, spectral regions of extended and localized states seem to coexist due to the long range nature of the interaction-induced disorder potential. If confirmed, the coexistence of spectral regions of extended and localized states would correspond to one of the first examples of a many-body mobility edge in a strong interacting system and may suggest similar phenomena to be present in the case of finite mass-ratio between electronic species.

All the ingredients for the experimental realization of the HFKM with ultracold atoms in optical lattices are separately available: there are recent implementations of mass unbalanced fermions \cite{69,70}; and, the Haldane model has recently been successfully realized \cite{71}. A direct verification of our results should therefore be possible with state-of-the-art technology.

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PERTURBATIVE ANALYSIS

By making a perturbative expansion for the effective Hamiltonian $\mathcal{H}(\{n_f\})$ defined in Eq. 3 it is possible to study the small and large $U$ regions of the phase diagram. This expansion allows us to write the Hamiltonian of the HFKM in the form of an effective 2D antiferromagnetic Ising model that only depends on the f-electrons’ degrees of freedom. In this way, we can see the CDW phase transition curves of the effective Ising models as an approximation of the exact phase transition curve of the HFKM in the limits of concern.

We start by defining the Hamiltonian matrix $H$:

$$H = -t \sum_{\langle i,j \rangle} |i \rangle \langle j | + it_2 \sum_{\langle i,j \rangle} n_{ij} |i \rangle \langle j | + \frac{U}{2} \sum_i s_i |i \rangle \langle i |$$

where we introduced the Ising variables $s_i = 2n_{f,i} - 1 = \pm 1$. The propagator of c-electrons is then simply given by $G = (i\omega_n - H)^{-1}$. Once the HFKM Hamiltonian is quadratic in the c-electron’s fields for a given configuration $\{n_f\}$, the formalism of Gaussian path integrals can be employed to write

$$\mathcal{H} = -\frac{1}{\beta} Tr \ln(-G^{-1}) - \frac{U}{2} \sum_i n_{f,i}$$

where the trace is taken over the fermionic degrees of freedom and was extended to incorporate the sum in the Matsubara frequencies. If we separate $H$ in the unperturbed and perturbed terms, respectively, $H_0$ and $H_1$, we can show that

$$\mathcal{H} = \mathcal{H}_0 - \frac{U}{2} \sum_i n_{f,i} + \frac{1}{\beta} \sum_{k=1}^{\infty} \frac{1}{k} Tr \left[ (G_0 H_1)^k \right]$$

where $G_0^{-1} = i\omega_n - H_0$ and $\mathcal{H}_0 = -\frac{1}{\beta} Tr \ln(-G_0^{-1})$. Eq. 8 provides a useful starting point for our perturbative analysis and can be applied in the small and large $U$ limits. For small $U$, we have that $H_0$ and $H_1$ contain respectively the hopping and $U$ dependent terms in Eq. 6 while for large $U$, they interchange. For the perturbative analysis, the expansion was made up to second order in $H_1$. For small $U$, the obtained effective Ising Hamiltonian $\mathcal{H}_{SU}$ was

$$\mathcal{H}_{SU} = U^2 \sum_{\langle i,j \rangle} J_{ij}(R)s_is_j$$

where the sum is over pairs of neighbors and

$$J_{ij}(R) = \left\{ \begin{array}{ll}
\int_{-\infty}^{+\infty} dw \frac{\Delta^2}{16\pi^{3/2}}(m^2 - \omega^2)K_m^2 \left( \frac{R}{\sqrt{\omega^2 + m^2}} \right), & (i) \\
\int_{-\infty}^{+\infty} dw \frac{\Delta^2}{16\pi^{3/2}}(m^2 + \omega^2)K_m^2 \left( \frac{R}{v \sqrt{\omega^2 + m^2}} \right), & (ii)
\end{array} \right.$$  

In the above expression, $R$ is the absolute distance between sites $i$ and $j$, $m = 3\sqrt{3}a_2/2$ is the Haldane model’s topological gap, $A_0 = 3\sqrt{3}a/2$ is the area of the honeycomb unit cell (with $a$ being the lattice constant) and $v = 3t/2$ is the Fermi velocity. Finally, $K_0$ and $K_1$ are modified Bessel functions of the second kind. Conditions (i) and (ii) correspond respectively to $i$ and $j$ in the same and in different sublattices.

On the other hand, the effective Ising Hamiltonian $\mathcal{H}_{LU}$ for large $U$ is

$$\mathcal{H}_{LU} = \sum_{\langle i,j \rangle} \frac{t^2}{2U} s_is_j + \sum_{\langle\langle i,j \rangle\rangle} \frac{t_2^2}{2U} s_is_j$$

Based on the effective Ising models, the critical temperature curves were estimated and are shown in Fig. 2 along with the numerical results. For small $U$, the critical temperature was estimated up to NNNN and NNN were not considered as they can be neglected for the studied case of $t_2 = 0.1t$. For large $U$, the second term in $\mathcal{H}_{LU}$ can also be neglected for the case of interest.