Charge instabilities and topological phases in the extended Hubbard model on the honeycomb lattice with enlarged unit cell

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We study spontaneous symmetry breaking in a system of spinless fermions in the Honeycomb lattice paying special emphasis to the role of an enlarged unit cell on time reversal symmetry broken phases. We use a tight binding model with nearest neighbor hopping $t$ and Hubbard interaction $V_1$ and $V_2$ and extract the phase diagram as a function of electron density and interaction within a mean field variational approach. The analysis completes the previous work done in Phys. Rev. Lett. 107, 106402 (2011) where phases with non–trivial topological properties were found with only a nearest neighbor interaction $V_1$ in the absence of charge decouplings. We see that the topological phases are suppressed by the presence of metallic charge density fluctuations. The addition of the next to nearest neighbor interaction $V_2$ restores the topological non-trivial phases.

I. INTRODUCTION

Topological phases of matter are a new paradigm in condensed matter physics.1114 These phases evade a standard classification in terms of local order parameters and broken symmetries, being described by topological invariants. In addition to the obvious interest from a fundamental viewpoint, the robustness of topological properties against certain local perturbations make these phases appealing also in applied physics. The recently discovered time reversal invariant topological insulators are a raising star in the family, with topological invariants protected against non magnetic disorder by time reversal symmetry $(T)$.15 Together with time reversal invariant topological insulators, the TQ$1$ quantum Hall insulating state is the paradigmatic example of a topological phase.5 The non trivial topology is in this case driven by an external magnetic field which breaks $T$. In quantum anomalous Hall (QAH) insulators, another example of a topological phase, $T$ is broken spontaneously, and a quantized anomalous Hall (AH) conductivity arises in the absence of any external magnetic field.9 When the Fermi level does not fall into the bulk band gap there is a non quantized contribution to the AH conductivity characterized as a property of the Fermi surface through its Berry phase and the systems are termed topological Fermi liquids.1115

The Honeycomb lattice is perhaps the best studied case for its special properties.1112 It is bipartite and yet due to its topology it is easily amenable to frustration. It is fair to say that the pioneer works proposing this lattice as a “condensed matter simulation of a three-dimensional anomaly”16–18, together with the analysis of the spin orbit in graphene done in refs. 19–21 opened the modern field of topological insulators. In these pioneering works the breaking of time reversal symmetry that allowed the topological non–trivial phases was explicitly put in the Hamiltonian in the form of complex hopping parameters. The non interacting behavior of the topological phases in the insulating family is at present fairly well understood, and the attention is now shifting to the effect of electron-electron interactions on these phases.22,23 and to the nature of the phase transitions between topological and ordinary phases (see 24 and references therein). In most cases following the original work by Haldane2 breaking $T$ is associated with bond order (complex hoppings) originating finite flux states.25–27 In this later context the electron spin is not meant to be a key ingredient, contrary to the topological insulators known to date where the strong spin-orbit coupling is responsible for the non trivial topology. Focusing in the two-dimensional (2D) case, and using spinless fermionic models, the strategy then is to search for spontaneously broken $T$ phases showing an AH or QAH effect driven by Coulomb interactions.

A realization of the Haldane model through electron-electron interactions was obtained at mean field level in the honeycomb lattice in refs. 22–24 by adding second neighbor Coulomb interactions. Other proposals involve more complex lattices which allow for intracell fluxes, as the checkerboard, the Kagome, or the decorated honeycomb,26–28 $T$–broken superconducting states have also been proposed recently on the honeycomb lattice.29–31

In a recent publication32 we proposed enlarging the unit cell of simple lattice models as an alternative way to drive the spontaneous appearance of phases with broken $T$. We explored as an example the nearest neighbor (NN) tight binding model for spinless fermions interacting through a NN Coulomb interaction in the honeycomb lattice. Our main motivation was the idea that enlarging the unit cell – to enable for instance Kekulé type of distortions – would allow for non–trivial topological phases without the necessity to go to longer range hopping or interactions. We also focussed on a region of high doping near the Van Hove singularity where short range electronic interactions
are enhanced and give rise to interesting phases. For this purpose we considered a minimal model and restricted the mean field decoupling to order parameters of the type $< a_i^+ b_j >$ ignoring possible charge ordered phases with order parameters of the type $< c_i^+ c_j >$. The result was that $\mathcal{T}$–broken phases with interesting topological features appeared at large fillings above the Van Hove filling for reasonable values of the interaction. The most interesting region of the phase diagram occurred around the commensurate value $n = 1$ corresponding to have one electrons per enlarged (six atoms) unit cell. There the system was insulating above a critical value of the NN Hubbard interaction $V \equiv V_1$. In this work we complete the former analysis by allowing charge decouplings in the mean field equations. We find that charge inhomogeneous phases dominate the phase diagram in the region where $\mathcal{T}$ broken phases occurred. $\mathcal{T}$ broken phases reemerge and are stabilized by the addition of a next nearest neighbor (NNN) interaction $V_2$. The results then are similar to these obtained at half filling in the pioneer work of Ref. 25 in the sense that $V_2 \neq 0$ is needed to stabilize non-trivial phases. In the present work, however, we have found that the high doping $\mathcal{T}$–broken phases are stabilized for $V_2 \ll V_1$ while at half filling $V_2 > V_1$ is required.

The article is organized as follows: In section II we describe the model and the method of calculation. In Sec. III we explain the phase diagram where for completeness, and to compare with previous results, we present also the situation at half filling IIIA. In Sec. IIIB we analyze the modification introduced in the $V_2 = 0$ case by the charge decoupling at higher fillings. We will see that the charge modulated phases wash out the topologically non–trivial phases. Finally we see how these are restored by the inclusion of the second neighbor interaction and describe the $\mathcal{T}$ broken phases and their band structure. In Sec. IV we summarize the situation and discuss some open problems. The Appendix contains the technical details of the calculation.

II. MODEL

We consider the model describing spinless electrons on the honeycomb lattice,

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + V_1 \sum_{\langle i,j \rangle} n_i n_j + V_2 \sum_{\langle \langle i,j \rangle \rangle} n_i n_j$$

(1)

where $t$ is the NN hopping, and $V_1$ and $V_2$ the NN and NNN repulsion, all of them real. The operator $c_i^\dagger$ ($c_i$) creates (annihilates) a fermion at site $i$, the number operator is $n_i = c_i^\dagger c_i$, and the sums run over either NN sites $\langle i,j \rangle$ or NNN sites $\langle \langle i,j \rangle \rangle$.

We use a 6–atom unit cell to allow for finite flux also in NN loops, and not only in NNN loops. The basis vectors can be chosen as $a_1 = \frac{a}{\sqrt{3}} (-\sqrt{3}, 1)$ and $a_2 = \frac{a}{\sqrt{3}} (\sqrt{3}, 1)$, and their counterparts in reciprocal space are $b_1 = \frac{2\pi}{3\sqrt{3}a} (-1, \sqrt{3})$ and $b_2 = \frac{2\pi}{3\sqrt{3}a} (1, \sqrt{3})$. The number of Fourier components of local operators is six, $a_i^\dagger k = \frac{1}{\sqrt{N}} \sum_{\langle i \in A \rangle} c_i^\dagger e^{i k \cdot r_i}$ and

Figure 1: Unit cell and mean field parameters of our model. In each panel we show 9 distinct effective hoppings, making up a total of 27 (see appendix A).
where summation over repeated indices is assumed (thus the factor \(1/2\) in the last two terms), with \(i, j = 1, 2, 3\), and where we have defined the 3 × 3 matrices

\[
\gamma_q = \begin{pmatrix}
1 & e^{-ia_2 \cdot q} & 1 \\
e^{-ia_1 \cdot q} & 1 & e^{i(a_1+a_2) \cdot q} \\
e^{-ia_1 \cdot q} & e^{ia_1 \cdot q} & 1
\end{pmatrix},
\]

\[
\alpha_q = \begin{pmatrix}
0 & 1 + e^{iq(a_1+a_2)} & 1 + e^{-iq(a_1+a_2) + e^{iqa_2}} \\
1 + e^{-iq(a_1+a_2) + e^{iqa_2}} & 0 & 1 + e^{iq(a_1+a_2) + e^{-iqa_2}} \\
1 + e^{-iq(a_1+a_2)} & 1 + e^{iq(a_1+a_2) + e^{iqa_2}} & 0
\end{pmatrix},
\]

\[
\beta_q = \begin{pmatrix}
0 & 1 + e^{iq(a_1+a_2)} & 1 + e^{-iq(a_1+a_2) + e^{iqa_2}} \\
1 + e^{-iq(a_1+a_2)} & 0 & 1 + e^{-iq(a_1+a_2) + e^{-iqa_2}} \\
1 + e^{iq(a_1+a_2)} & 1 + e^{iq(a_1+a_2) + e^{iqa_2}} & 0
\end{pmatrix}.
\]

Note that while \(\alpha_q\) and \(\beta_q\) are hermitian, the matrix \(\gamma_q\) is not.

### III. PHASE DIAGRAM

The phase diagram of the model is obtained within the variational mean field approach. The details of the mean field decoupling and related equations are extensively explained in Appendix A. In brief, we replace the four fermion interaction terms in Eq. (2) with bilinears which, when written in real space, can be interpreted as the most general hopping and potential energy terms compatible with the reduced translational symmetry of the lattice (6 atom unit cell). In total there are 9 NN (ξ) and 18 NNN (9 per sublattice, \(\chi^A\) and \(\chi^B\)) complex hopping parameters, which are depicted in Fig. 1. In addition there are 6 local energy terms (3 per sublattice, \(\rho^A\) and \(\rho^B\)), of which only 5 are independent due to charge conservation. See Appendix A1 for details.

Using the variational mean field approach one finds the set of 33 = 3 × 9 + 6 mean field equations which, complemented by charge conservation, determine the mean field parameters and the chemical potential \(\mu\) (see Appendix A2 and A3). The mean field equations read as,

\[
\xi_{ij} = -\frac{V_1}{N} \sum_k \gamma_{ij}^k \langle \xi_i^j(k) \xi_{i}^j(k) \rangle_{MF},
\]

\[
\lambda^A_{i,j} = -\frac{V_2}{N} \sum_k \lambda^A_{i,j} \langle \lambda^A_{i,j}(k) \lambda_{i}^A(k) \rangle_{MF},
\]

\[
\lambda^B_{i,j} = -\frac{V_2}{N} \sum_k \lambda^B_{i,j} \langle \lambda^B_{i,j}(k) \lambda_{i}^B(k) \rangle_{MF},
\]

\[
\rho_i^A = V_1 n_B + 3V_2 n_A - 3V \cdot 2n_i^A,
\]

\[
\rho_i^B = V_1 n_A + 3V_2 n_B - 3V \cdot 2n_i^B,
\]

where \(\lambda^A_{i,j} \) and \(\lambda^B_{i,j} \) are phase factors analogous to \(\gamma^j_{i} \) defined in Eq. (3), \(n_i^c = \frac{1}{N} \sum_k \langle \xi_i^c(k) \xi_{i}^c(k) \rangle_{MF}\) and \(n_c = \sum_{i=1}^{3} n_i^c\) with \(c = A, B\). Detailed expressions for these matrices can be found in the appendix A2. The notation \(\langle \cdots \rangle_{MF}\) means average in the macrocanonical ensemble taking the mean field Hamiltonian in the Boltzmann factor.
In order to obtain the mean field phase diagram we solve the mean field equations self consistently, (see Appendix A3) and take the solution (if more than one is obtained) which minimizes the free energy in Eq. (A10) (see Appendix A4). Care must be taken with charge like order parameters, Eqs. (9) and (10). Due to the frustration introduced by NNN interaction, these order parameters may flow to a non-selfconsistent solution where the charge like order parameters in different sublattices interchange at each step. Apart from this subtlety, getting a solution is straightforward.

We will analyze first the phase diagram obtained at half filling which is interesting on its own and later discuss the modification introduced in the $V_2 = 0$ case by the charge decoupling. We will see that the charge modulated phases wash out the topologically non–trivial phases. Finally we see how these are restored by the inclusion of the second neighbor interaction.

A. Half-filling

Let us first analyze the half-filled case, where $n \equiv n_A + n_B - 3 = 0$. This case provides a test to the present mean field analysis, since a similar approach, also using a 6–atom unit cell, has been taken in ref. 29. For comparison, we show the phase diagram obtained in ref. 29 in the left panel of Fig. 2. In the right panel of Fig. 2 we can see the phase diagram of the present work (we use the same color code). We plot the different phases (that will be described in what follows) as a function of the interaction strength $V_1$ and $V_2$ in units of the hopping parameter $t$. The half filled case was first explored in the original lattice in ref. 25 and non–trivial topological phases were already encountered for values of the interaction $V_2 > V_1$.

For $V_1 \lesssim 1.5t$ and $V_2 \lesssim 2t$ the two phase diagrams coincide. For $V_1 \gtrsim 1.5t$, however, we find that the semi-metallic (SM) and the charge density wave (CDW) phases are robust against the Kekulé phase. The Kekulé phase is characterized by an alternating bond strength as shown schematically in the inset of the left hand side of Fig. 3. This distortion is important in the physics of graphene because it opens a gap in the spectrum breaking the translational symmetry of the original Honeycomb lattice while preserving time reversal ($\mathcal{T}$) and inversion ($\mathcal{I}$) symmetries. It also plays a key role in the models of charge fractionalization in the Honeycomb lattice. In our approach the Kekulé phase only appears at much higher $V_1$ and $V_2$. For $V_2 \gtrsim 2t$ a new phase sets in, not predicted in ref. 29. This is a charge density wave with reduced rotational symmetry; to distinguish from CDW we denote it as charge modulated with modulation also over the sublattice (CMs). In the CDW there is a charge imbalance between sublattices, but no inhomogeneity over the sublattice: the charge–like order parameters $(\rho^A_1, \rho^B_1, \rho^A_2, \rho^B_2, \rho^A_3, \rho^B_3)$ take the form $(\rho, -\rho, \rho, -\rho, \rho, -\rho)$. For CMs, however, the charge is modulated also over the sublattice and the charge like order parameters take the form $(\rho, -\rho, \rho, -\rho, -\Delta, \rho + \Delta)$. We note that for $V_2 \gtrsim V_1$ such modulation is naturally expected from a classical point of view (remember that the Hartree contribution has a classical interpretation): The staggered charge modulation of CDW minimizes the energy coming from NN repulsion, but it does not affect the
for topological phases we have centered our attention in the doping region around the commensurate value in the phase diagram around renormalization of the hopping with the Pomeranchuk symmetry. This is similar to the (CM+RS) phase that occurs most favorable phase. At larger values of the interaction (CM+P) the charge modulated phase is accompanied of a Van Hove filling \( n = 0.75 \) and for very small values of the interaction where the Pomeranchuk instability is still the phases were stabilized before (left hand side of Fig. 3). The charge decoupling leaves only a small region around the n > 1 that was discussed in the previous section.

The new T− broken phases discussed at length in the text; (K) Kekulé distortion with hopping renormalization as shown in the inset; (K+P) coexistence of Kekulé and Pomeranchuk distortions; (T-I) and (T-II) T− broken phases discussed at length in the text; (RS) broken symmetry state with real hopping parameters, the distortion is neither Kekulé type nor Pomeranchuk (reduced symmetry). (Right) Phase diagram with \( V_2 = 0 \) and charge inhomogeneous phases allowed. CM stands for the new charge modulated phase discussed in the text. In the CM+RS phase there is also a real, asymmetric renormalization of the hoppings.

We will now discuss the results obtained for higher dopings. The doped system has been the subject of attention recently due to the experimental availability \(^{31,36-38}\) and to the interesting phases that emerge near the Van Hove filling \(^{31,36,38}\). In ref. \(^{32}\) we have shown that for the Hamiltonian in Eq. (1) with \( V_2 = 0 \), and ignoring charge inhomogeneous phases, T−broken phases show up in the phase diagram \( \Gamma \) vs \( n \). The phase diagram is shown in Fig. 3 (left), where the meaning of the various phases are described. The dominant phases in the region of interest above the Van Hove filling (n=0.75 in our units) were a Pomeranchuk instability (P) characterized by rotational symmetry breaking as indicated in the inset, and the T− broken phases denoted by T-I and T-II obtained at 1 \( \lesssim n \lesssim 1.5 \) and \( V_1 \gtrsim 2t \). These phases are the same as those obtained in ref. \(^{32}\).

When charge inhomogeneous phases are allowed we obtain the phase diagram shown in Fig. 3 (right). As can be seen, the T−broken phases are washed out by a charge modulated (CM) phase. This charge modulation corresponds to a charge imbalance between the two sublattices, and is homogeneous over the sublattice; at half-filling this is the CDW discussed in the previous section. This modulation induces a trivial gap between bands 3 and 4 at the Γ point. The system is thus a trivial insulator at \( n = 0 \), where the Fermi level falls into the gap, and is metallic for \( n > 0 \). We see that the CM phase dominates the region of the phase diagram where Pomeranchuk and T−broken phases were stabilized before (left hand side of Fig. 3). The charge decoupling leaves only a small region around the Van Hove filling (n=0.75) and for very small values of the interaction where the Pomeranchuk instability is still the most favorable phase. At larger values of the interaction (CM+P) the charge modulated phase is accompanied of a renormalization of the hopping with the Pomeranchuk symmetry. This is similar to the (CM+RS) phase that occurs in the phase diagram around \( n = 0.75 \) for larger values of the doping and interaction.

A natural way to restore the topologically non–trivial phases is to add a NNN interaction \( V_2 \). Since we are looking for topological phases we have centered our attention in the doping region around the commensurate value \( n = 1 \).

In Fig. 4 we show the phase diagram for \( V_2 > 0 \) obtained at fixed \( n = 1.2 \). Increasing \( V_2 \) frustrates the CM phase, and T−broken phases are recovered. We note that this happens already for \( V_2 \ll V_1 \). If \( V_2 \) is further increased the system falls into the CMs phase (charge modulated with modulation also over the sublattice) already encountered at half-filling that was discussed in the previous section.

The new T− broken phases T-I and T-II are similar to the ones described in ref. \(^{32}\). Fig. 3 shows the real space hopping pattern for T-I and T-II respectively. The direction of the arrows represents the sign of the phase of the given complex hopping. As discussed in ref. \(^{10}\) the possibility of having non-trivial topological phases characterized by a

Figure 3: (Left) Phase diagram with \( V_2 = 0 \) when charge inhomogeneous phases are not allowed. Legend: (S) symmetric phase, i.e. bare graphene with a uniform renormalization of the hopping; (K) Kekulé distortion with hopping renormalization \( \propto V \) vs \( n \). The phase diagram is shown in Fig. 3 (left), where the meaning of the various phases are described. The dominant phases in the region of interest above the Van Hove filling (n=0.75 in our units) were a Pomeranchuk instability (P) characterized by rotational symmetry breaking as indicated in the inset, and the T− broken phases denoted by T-I and T-II obtained at 1 \( \lesssim n \lesssim 1.5 \) and \( V_1 \gtrsim 2t \). These phases are the same as those obtained in ref. \(^{32}\).

B. Higher filling

For larger values of the interaction (CM+P) the charge modulated phase is accompanied of a renormalization of the hopping with the Pomeranchuk symmetry. This is similar to the (CM+RS) phase that occurs in the phase diagram around \( n = 0.75 \) for larger values of the doping and interaction.
finite Hall conductivity in $\mathcal{T}$– broken systems is determined by the discrete symmetries $\mathcal{T}$– and space inversion $\mathcal{I}$– preserved in the system. As happened in the case discussed in ref. \[32\] the T-II phase is still invariant under inversion hence breaking the product $\mathcal{T}\mathcal{I}$ and is in principle topologically non-trivial with finite Hall conductivity.$^{10}$

Fig. 5 shows a typical band structure for the T-I and T-II phases. The T-I case is shown in Fig. 5(left), where as an example we took the point $V_1 = 5t$ and $V_2 = 0.75t$. In the right panel of Fig. 5 we show the T-II case, for $V_1 = 6t$ and $V_2 = 0.75t$. The two figures are very similar to their counterparts when $V_2 = 0$.

The interesting feature is that, unlike what happened there, we do not have any insulating phase away of half filling, even for the commensurate value $n = 1$ whose band structure is very similar to these in Fig. 5.

IV. CONCLUSIONS AND DISCUSSION

One of the important points of this and the related work in ref. \[32\] is the proposal that non trivial topological phases can be spontaneously generated from interactions in lattice fermionic systems when translational symmetry is relaxed, i.e. when phases with enlarged unit cells are allowed. The employment of enlarged unit cell allows for novel intra-cell current patterns emerging from interactions, and thus novel topological phases. We used the Honeycomb lattice with extended Hubbard interaction to exemplify the type of new physics expected. In \[32\] we checked that no topological phase can arise in the original lattice (two atoms unit cell), without including a second nearest neighbor interactions $V_2$ to allow for the formation of the necessary current loops that break time reversal symmetry.

We have completed the analysis of ref. \[32\] including a charge decoupling order parameter. The phase diagram is dominated by charge modulated phases with no particular symmetry and no topological phases were found. The charge modulated phases in the case $V_2 = 0$ are usual CDW phases but we keep the name CM to emphasize the fact that, away from half filling, these phases are metallic. When $V_2 \neq 0$ a different charge modulated phase arise that we denote $CMs$ in which the charge is modulated also over the sublattice and the charge–like order parameters take the form $(\rho, -\rho, \rho, -\rho, -\rho - \Delta, \rho + \Delta)$. An interesting analysis of charge modulated phases in graphene has been done recently in $^{39}$.

In the previous analysis, $^{32}$ there were two special filling values apart from half filling: The Van Hove filling and the commensurate value $n = 1$ corresponding to four electron per enlarged unit cell. Around the VH density the
Figure 6: Mean field band structure in the T-I phase for \( V_1 = 5t \) and \( V_2 = 0.75t \) (left) and in the T-II phase for \( V_1 = 6t \) and \( V_2 = 0.75t \) (right). The middle black hexagon indicates the position of the Fermi level.

system supported a Pomeranchuk deformation and the topological phases were established around the commensurate \( n = 1 \) filling. The system was gapped only at this particular value. In that case we observed a phase separation in the region in the phase space of fillings in between these two values with the two extremes being the stable phases. We have seeing that in the charge modulated phase dominating the phase diagram the \( n = 1 \) case is not special any more: Even though bands 3 and 4 might be non-trivial now (because of \( V_2 \)), the system at \( n = 1 \) is not an insulator no “full” gap develops as the Fermi level always crosses bands 4 and 5 (see Fig. [6]). This behavior can be understood from the strong coupling point of view due to the frustration induced by the competition between \( V_1 \) and \( V_2 \) for the ground state. The situation is similar to the quarter filling case in one and two dimensions where the long-range Coulomb interaction enhances the metallic behavior.

Since this is only a mean field analysis it will be interesting to check the stability of this phases under quantum fluctuations.

Inclusion of an extra coupling to next to nearest neighbors \( V_2 \), restores the topological phases at fillings around \( n = 1 \). This model was already studied in the literature, in particular in ref. [25] where topological phases were found at half filling for values of the interactions \( V_2 > V_1 \). Allowing the charge decoupling that gives rise to the inhomogeneous charge modulation over the sublattice described along this work, favors the \( T^- \) broken phases that now set at lower values of \( V_2 \).

The possibility of superconducting phases have been left out in this analysis. Considering superconducting order parameters embedded in enlarged unit cells might make novel topological superconducting phases emerge opening new routes to realize these, sometimes elusive, phases of matter. Very recent works suggest the formation of an eight-atom unit cell spin density wave close to the van Hove filling ( \( n \sim 0.75 \) in our notation) or topological superconducting order exactly at \( n = 0.75 \). Whether or not these phases dominate close to \( n \sim 1 \) or rather a spin Hall effect is energetically more stable is still an open question. The \( T^- \) broken phases described in this work can be difficult to observe in graphene since they occur at high values of the interaction and filling but they can probably be tested in cold atom experiments with optical lattices.
Acknowledgments

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Appendix A: Mean field analysis

1. Mean field decoupling

The mean field Hamiltonian we propose is

\[ H_{MF} = H_0 + \sum_k \psi_k^\dagger \begin{pmatrix} \rho_1^A & \xi_{11}^A & \chi_{12}^A(k) & e^{i \mathbf{k} \cdot \mathbf{a}_2} \xi_{12} & \chi_{13}^A(k) \\ \xi_{11}^A & \rho_1^B & \xi_{21}^B & \chi_{12}^B(k) & e^{i \mathbf{k} \cdot \mathbf{a}_2} \xi_{21}^B \\ \xi_{21}^A & \rho_2^B & \xi_{22}^B & \chi_{12}^B(k) & e^{i \mathbf{k} \cdot \mathbf{a}_2} \xi_{22}^B \\ \chi_{12}^A(k) & \chi_{12}^B(k) & \xi_{22}^B & \chi_{13}^B(k) & e^{i \mathbf{k} \cdot \mathbf{a}_2} \chi_{13}^B \\ \chi_{13}^A(k) & \chi_{13}^B(k) & \chi_{13}^B(k) & \chi_{13}^B(k) & \xi_{33} \end{pmatrix} \psi_k, \]

with

\[
\begin{align*}
\chi_{12}^A(k) &= \chi_{12}^A + e^{i \mathbf{k} \cdot (\mathbf{a}_1 + \mathbf{a}_2)} \chi_{12} + e^{i \mathbf{k} \cdot \mathbf{a}_2} \chi_{12} \\
\chi_{12}^A(k) &= e^{-i \mathbf{k} \cdot (\mathbf{a}_1 + \mathbf{a}_2)} \chi_{12} + \chi_{12} + e^{-i \mathbf{k} \cdot \mathbf{a}_2} \chi_{12} \\
\chi_{13}^A(k) &= e^{-i \mathbf{k} \cdot \mathbf{a}_2} \chi_{13} + e^{i \mathbf{k} \cdot \mathbf{a}_2} \chi_{13},
\end{align*}
\]

and

\[
\begin{align*}
\chi_{12}^B(k) &= \chi_{12}^B + e^{i \mathbf{k} \cdot \mathbf{a}_2} \chi_{12} + e^{i \mathbf{k} \cdot \mathbf{a}_2} \chi_{12} \\
\chi_{12}^B(k) &= e^{-i \mathbf{k} \cdot \mathbf{a}_2} \chi_{12} + \chi_{12} + e^{-i \mathbf{k} \cdot \mathbf{a}_2} \chi_{12} \\
\chi_{13}^B(k) &= e^{-i \mathbf{k} \cdot \mathbf{a}_2} \chi_{13} + e^{i \mathbf{k} \cdot \mathbf{a}_2} \chi_{13},
\end{align*}
\]

where \( H_0 \) is the bare Hamiltonian, and we use the spinor notation \( \psi_k^\dagger = [a_1^\dagger(k), b_1^\dagger(k), a_2^\dagger(k), b_2^\dagger(k), a_3^\dagger(k), b_3^\dagger(k)] \). In Fig. 1 we show how the 27 mean field parameters making up the Fock contribution can be interpreted as NN or NNN hoppings. The 6 charge like mean field parameters come from the Hartree contribution due to charge imbalance between the six sites of the unit cell. Due to charge conservation only 5 of them are independent.

2. Mean field equations

Minimizing the free energy functional

\[ F[\xi, \chi, \rho] = \langle H \rangle_{MF} - T S_{MF} = F_{MF} + \langle H - H_{MF} \rangle_{MF} \approx \Omega_{MF} + \langle H - H_{MF} \rangle_{MF} + \mu N_e, \]

we obtain the following set of mean field equations:

\[
\begin{align*}
\xi_{ij} &= -\frac{V_i}{N} \sum_q \gamma_{ij}^q \langle b_\dagger_q a_{i,q} \rangle_{MF} \\
\chi_{ij,k}^A &= -\frac{V_2}{N} \sum_q \gamma_{ij}^q \langle a_{j,q} a_{i,q} \rangle_{MF} \\
\chi_{ij,k}^B &= -\frac{V_2}{N} \sum_q \gamma_{ij}^q \langle b_{j,q} b_{i,q} \rangle_{MF} \\
\rho_k^A &= V_1 n^B + 3V_2 n^A - 3V_2 n_i^A \\
\rho_i^B &= V_1 n^A + 3V_2 n^B - 3V_2 n_i^B,
\end{align*}
\]

where we have defined \( n_i = \frac{1}{N} \sum_q \langle c_{i,q}^\dagger c_{i,q} \rangle_{MF} \) and \( n = \sum_{i=1}^3 n_i \), with \( c = a, b \).

It is easy to show, using Eqs. (4)–(5) and (A1)–(A2), that the mean field equation for the effective NNN hoppings can be cast in the \( k \)-independent form

\[
\chi_{ij}^{\Gamma,\delta} = -\frac{V_i}{N} \sum_q \chi_{ij,\Gamma}^q \langle c_{j,q}^\dagger c_{i,q} \rangle_{MF},
\]
with
\[
\lambda_{12, q}^{A,u} = 1, \quad \lambda_{12, q}^{A,d} = e^{-i q (a_1 + a_2)}, \quad \lambda_{12, q}^{A,h} = e^{-i q a_2} \\
\lambda_{23, q}^{A,u} = e^{i q (a_1 + a_2)}, \quad \lambda_{23, q}^{A,d} = 1, \quad \lambda_{23, q}^{A,h} = e^{i q a_1} \\
\lambda_{31, q}^{A,u} = e^{i q a_2}, \quad \lambda_{31, q}^{A,d} = e^{-i q a_1}, \quad \lambda_{31, q}^{A,h} = 1
\]

and
\[
\lambda_{12, q}^{B,h} = 1, \quad \lambda_{12, q}^{B,d} = e^{-i q a_2}, \quad \lambda_{12, q}^{B,u} = e^{i q a_1} \\
\lambda_{23, q}^{B,h} = e^{i q a_2}, \quad \lambda_{23, q}^{B,d} = 1, \quad \lambda_{23, q}^{B,u} = e^{i q (a_1 + a_2)} \\
\lambda_{31, q}^{B,h} = e^{-i q a_1}, \quad \lambda_{31, q}^{B,d} = e^{-i q (a_1 + a_2)}, \quad \lambda_{31, q}^{B,u} = 1.
\]

3. Solving the mean field equation

In order to solve the set of mean field equations given above we need to compute the averages of the form \(\langle b_j^\dagger(q) a_i(q) \rangle_{MF}\). To calculate these averages we introduce the unitary transformation \(U\) which diagonalizes \(H_{MF}(k)\),

\[
U H_{MF}(k) U^\dagger = \text{diag}[\varepsilon_1(k), \ldots, \varepsilon_6(k)].
\]

The new operators \(c_\alpha(k)\) are such that
\[
\begin{bmatrix}
    c_1(k) \\
    c_2(k) \\
    \vdots \\
    c_5(k) \\
    c_6(k)
\end{bmatrix} = U
\begin{bmatrix}
    a_1(k) \\
    b_1(k) \\
    \vdots \\
    a_3(k) \\
    b_3(k)
\end{bmatrix},
\]

and the average \(\langle b_j^\dagger(q) a_i(q) \rangle_{MF}\) and \(\langle c_j^\dagger(q) c_i(q) \rangle_{MF}\) may be written as
\[
\langle b_j^\dagger(q) a_i(q) \rangle_{MF} = \sum_{\alpha} U_{\alpha, 2j} c^\dagger_\alpha(q) \sum_{\beta} U^*_{\beta, 2i-1} c_\beta(q) \langle c_\alpha(q) c_\alpha(q) \rangle_{MF}
\]
\[
= \sum_{\alpha=1}^6 U_{\alpha, 2j} U^*_{\alpha, 2i-1} \langle c^\dagger_\alpha(q) c_\alpha(q) \rangle_{MF}
\]
\[
= \sum_{\alpha=1}^6 U_{\alpha, 2j} U^*_{\alpha, 2i-1} f[\varepsilon_\alpha(q)],
\]

and
\[
\langle a_j^\dagger(q) a_i(q) \rangle_{MF} = \sum_{\alpha=1}^6 U_{\alpha, 2j-1} U^*_{\alpha, 2i-1} f[\varepsilon_\alpha(q)]
\]
\[
\langle b_j^\dagger(q) b_i(q) \rangle_{MF} = \sum_{\alpha=1}^6 U_{\alpha, 2j} U^*_{\alpha, 2i} f[\varepsilon_\alpha(q)],
\]
and the densities \( \langle c_i^\dagger(q)c_i(q) \rangle_{MF} \) as
\[
\langle a_i^\dagger(q)a_i(q) \rangle_{MF} = \sum_{\alpha=1}^{6} |U_{\alpha,2i-1}|^2 f[\varepsilon_\alpha(q)]
\]
\[
\langle b_i^\dagger(q)b_i(q) \rangle_{MF} = \sum_{\alpha=1}^{6} |U_{\alpha,2i}|^2 f[\varepsilon_\alpha(q)],
\]

with
\[
f[\varepsilon_\alpha(q)] = \frac{1}{\exp \beta[\varepsilon_\alpha(q) - \mu] + 1}.
\]

Then we can write the set of mean field equations as,
\[
\xi_{ij} = -\frac{V_1}{N} \sum_q \gamma_{ij}^{\delta} \sum_{\alpha=1}^{6} U_{\alpha,2j-1}^* U_{\alpha,2i-1} f[\varepsilon_\alpha(q)] \tag{A4}
\]
\[
\chi_{ij}^{A,\delta} = -\frac{V_2}{N} \sum_q \lambda_{ij,q}^{A,\delta} \sum_{\alpha=1}^{6} U_{\alpha,2j-1}^* U_{\alpha,2i-1} f[\varepsilon_\alpha(q)] \tag{A5}
\]
\[
\chi_{ij}^{B,\delta} = -\frac{V_2}{N} \sum_q \lambda_{ij,q}^{B,\delta} \sum_{\alpha=1}^{6} U_{\alpha,2j} U_{\alpha,2i-1}^* f[\varepsilon_\alpha(q)] \tag{A6}
\]
\[
\rho_i^A = V_1 n_B^A + 3V_2 n^A - \frac{3V_2}{N} \sum_q \sum_{\alpha=1}^{6} |U_{\alpha,2i-1}|^2 f[\varepsilon_\alpha(q)] \tag{A7}
\]
\[
\rho_i^B = V_1 n^B + 3V_2 n_B^B - \frac{3V_2}{N} \sum_q \sum_{\alpha=1}^{6} |U_{\alpha,2i}|^2 f[\varepsilon_\alpha(q)], \tag{A8}
\]

with
\[
n^A = \frac{1}{N} \sum_q \sum_{i=1}^{3} \sum_{\alpha=1}^{6} |U_{\alpha,2i-1}|^2 f[\varepsilon_\alpha(q)]
\]
\[
n^B = \frac{1}{N} \sum_q \sum_{i=1}^{3} \sum_{\alpha=1}^{6} |U_{\alpha,2i}|^2 f[\varepsilon_\alpha(q)]. \tag{A9}
\]

This set of equations has to be solved self-consistently with the constrain imposed by the Luttinger theorem, which reads (ignoring logarithmic corrections in fermion number \( N_e \)),
\[
3 + n \equiv \frac{N_e}{N} = \int N \frac{\partial \Omega}{\partial \mu} \approx \int N \frac{\partial \Omega_{MF}}{\partial \mu} = \frac{\langle N \rangle_{MF}}{N} = \frac{1}{N} \sum_q \sum_{\alpha} f[\varepsilon_\alpha(q)],
\]
and from which we get \( \mu \) self-consistently.

4. Free energy

To check the stability of possible phases we need the Free energy defined in Eq. (A3). For a given set of converged order parameters we have,
\[
\mathcal{F} = \Omega_{MF} + \mu N_e + \langle \mathcal{H} - \mathcal{H}_{MF} \rangle_{MF}, \tag{A10}
\]
where the mean field grand canonical potential is given by

\[ \Omega_{MF} = -k_B T \sum_{q,\alpha} \ln \left\{ 1 + e^{-\beta [\varepsilon_{\alpha}(q) - \mu]} \right\}, \]

and

\[
\langle \mathcal{H} - \mathcal{H}_{MF} \rangle_{MF} = \frac{V_1}{N} \sum_{i,j} [A_{ij}]^2 - N \sum_{\alpha} (\rho_i^A n_i^A + \rho_i^B n_i^B) - \left( \sum_{i,j} \xi_{ij} A_{ij} + \text{c.c.} \right)
\]

\[
+ \frac{3}{2} \frac{V_2}{N} \sum_{\Gamma = \{A, B\}} \sum_{\delta = \{u, d, h\}} \left( |D^\Gamma_{12}|^2 + |D^\Gamma_{23}|^2 + |D^\Gamma_{31}|^2 \right)
\]

\[
- \frac{V_2}{N} \sum_{\Gamma = \{A, B\}} \sum_{\delta = \{u, d, h\}} \left( \chi^\Gamma_{12} [D^\Gamma_{12}]^* + \chi^\Gamma_{23} [D^\Gamma_{23}]^* + [\chi^\Gamma_{31}]^* D^\Gamma_{31} + \text{c.c.} \right)
\]

where

\[ A_{ij} = \sum_{q,\alpha} (\gamma^q_{ij})^* U_{\alpha,2i-1} U_{\alpha,2j}^* f[\varepsilon_{\alpha}(q)] \]

\[ D^A_{ij} = \sum_{q} \lambda^A_{ij,\alpha} \sum_{\alpha=1}^6 U_{\alpha,2j-1} U_{\alpha,2i-1}^* f[\varepsilon_{\alpha}(q)] \]

\[ D^B_{ij} = \sum_{q} \lambda^B_{ij,\alpha} \sum_{\alpha=1}^6 U_{\alpha,2j} U_{\alpha,2i}^* f[\varepsilon_{\alpha}(q)]. \]