

# Supplemental Material for: 'Theory of nematic charge orders in kagome metals'

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In this Supplemental Material, we present some additional information concerning the quartic interaction of the Ginzburg-Landau potentials and on the mean-field calculation discussed in the main text.

## 1. Quartic interaction of the Ginzburg-Landau potential

The full expression for the quartic part of the Ginzburg-Landau potentials in Eqs. (1),(4)-(5) of the main text reads:

$$\begin{aligned} \mathcal{F}_{\text{quart}} = & \frac{\beta_1}{4} \sum_j \psi_j^4 + \frac{\beta_2}{2} \sum_j \psi_j^4 \cos(4\phi_j) + \frac{\beta_3}{4} \sum_{j,j'>j} \psi_j^2 \psi_{j'}^2 + \frac{\beta_4}{2} \sum_j \psi_j^4 \cos(2\phi_j) \\ & + \frac{\beta_5}{2} \sum_{j,j'>j} \psi_j^2 \psi_{j'}^2 \cos[2(\phi_j + \phi_{j'})] + \frac{\beta_6}{2} \sum_{j,j'>j} \psi_j^2 \psi_{j'}^2 \cos[2(\phi_j - \phi_{j'})] + \frac{\beta_7}{2} \sum_{j,j' \neq j} \psi_j^2 \psi_{j'}^2 \cos(2\phi_{j'}). \end{aligned} \quad (1.1)$$

The quartic potential that appears, e.g., in Eq. (1) of the main text can be obtained from Eq. (1.1) assuming  $\beta_1 = \beta$ ,  $\beta_2 = \beta_3 = \beta_4 = \beta_5 = \beta_6 = \beta_7 = 0$ . This way, it is possible to obtain an analytical expression for the solutions of Eq. (1) of the main text. One can easily derive the full expressions for the potentials in Eqs. (6)-(9) of the main text, even if they are more involved. For brevity, we do not report them here.

## 2. Mean-field analysis

We study the Hamiltonian Eq. (2) of the main text on the kagome lattice in the presence of the field patterns shown in Figs. 1-4. We perform a mean-field decoupling of the interaction [1-3]:

$$n_{i,\uparrow} n_{i,\downarrow} \approx \langle n_{i,\uparrow} \rangle n_{i,\downarrow} + \langle n_{i,\downarrow} \rangle n_{i,\uparrow} - \langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle, \quad (2.1)$$

$$n_i n_j \approx \langle n_i \rangle n_j + \langle n_j \rangle n_i - \langle n_i \rangle \langle n_j \rangle - \sum_{\sigma} (\langle c_{i,\sigma}^{\dagger} c_{j,\sigma} \rangle c_{j,\sigma}^{\dagger} c_{i,\sigma} + \langle c_{j,\sigma}^{\dagger} c_{i,\sigma} \rangle c_{i,\sigma}^{\dagger} c_{j,\sigma} - \langle c_{i,\sigma}^{\dagger} c_{j,\sigma} \rangle \langle c_{j,\sigma}^{\dagger} c_{i,\sigma} \rangle), \quad (2.2)$$

having assumed the symmetry breaking to occur along the spin z direction. We consider two possibilities for the unit cell of the problem depending by the specific pattern for the CBO we analyze, one with 9 atoms ( $\sqrt{3} \times \sqrt{3}$  unit cell) and one with 12 atoms ( $2 \times 2$  unit cell). The number of variation parameters is 54 (of which 36 are complex) in the former and 72 (of which 48 are complex) in the latter case.

After the mean-field decoupling, the Hamiltonian of the problem becomes quadratic, thus it can be easily diagonalized in reciprocal space at each  $\mathbf{k}$  point. Starting from an initial guess for the variational parameters, we can write:

$$H^{\text{MF}} = \sum_{\mathbf{k},\sigma} \psi_{\mathbf{k},\sigma}^{\dagger} \mathcal{H}_{\mathbf{k},\sigma} [\langle n_{i,\sigma'} \rangle, \langle c_{i,\sigma'}^{\dagger} c_{j,\sigma'} \rangle] \psi_{\mathbf{k},\sigma} = \sum_{\mathbf{k},\sigma} \phi_{\mathbf{k},\sigma}^{\dagger} \mathcal{H}_{\mathbf{k},\sigma}^d [\langle n_{i,\sigma'} \rangle, \langle c_{i,\sigma'}^{\dagger} c_{j,\sigma'} \rangle] \phi_{\mathbf{k},\sigma}, \quad (2.3)$$

where  $\mathcal{H}_{\mathbf{k},\sigma} [\langle n_{i,\sigma'} \rangle, \langle c_{i,\sigma'}^{\dagger} c_{j,\sigma'} \rangle]$  is the Bloch Hamiltonian of the problem that depends by all the variational parameters  $\langle n_{i,\sigma'} \rangle$  and  $\langle c_{i,\sigma'}^{\dagger} c_{j,\sigma'} \rangle$ , while  $\psi_{\mathbf{k},\sigma}$  is the reciprocal space spinor with the dimension of the unit cell containing the annihilation operators.  $\mathcal{H}_{\mathbf{k},\sigma}^d [\langle n_{i,\sigma'} \rangle, \langle c_{i,\sigma'}^{\dagger} c_{j,\sigma'} \rangle]$  is the diagonal form of the Bloch Hamiltonian with eigenvalues  $E_{\mathbf{k},\sigma,m}$  on the diagonal and

$$\phi_{\mathbf{k},\sigma} = U_{\mathbf{k},\sigma} [\langle n_{i,\sigma'} \rangle, \langle c_{i,\sigma'}^{\dagger} c_{j,\sigma'} \rangle] \psi_{\mathbf{k},\sigma}, \quad (2.4)$$

is the spinor containing the eigenoperators at point  $\mathbf{k}$  and spin  $\sigma$ , with  $U_{\mathbf{k},\sigma}$  the unitary transformation that transforms  $\psi_{\mathbf{k},\sigma}$  into  $\phi_{\mathbf{k},\sigma}$  (here and in the following, we omit the functional dependence of  $U_{\mathbf{k},\sigma}$  by the variational parameters for conciseness). We compute the expectation value:

$$\begin{aligned} \langle c_{i,\sigma}^\dagger c_{j,\sigma} \rangle &= \frac{1}{A_{BZ}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \langle c_{i,\mathbf{k},\sigma}^\dagger c_{j,\mathbf{k},\sigma} \rangle = \frac{1}{A_{BZ}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \langle (\psi_{\mathbf{k},\sigma}^\dagger)_i (\psi_{\mathbf{k},\sigma})_j \rangle \\ &= \frac{1}{A_{BZ}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \sum_{m,l} \langle (\phi_{\mathbf{k},\sigma}^\dagger)_m (U_{\mathbf{k},\sigma})_{mi} (U_{\mathbf{k},\sigma}^\dagger)_{jl} (\phi_{\mathbf{k},\sigma})_l \rangle \\ &= \frac{1}{A_{BZ}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \sum_m (U_{\mathbf{k},\sigma})_{mi} (U_{\mathbf{k},\sigma}^\dagger)_{jm} f(E_{\mathbf{k},\sigma,m} - \mu). \end{aligned} \quad (2.5)$$

$\mathbf{R}_i$  and  $\mathbf{R}_j$  are the real space positions of the sites  $i$  and  $j$ , respectively,  $A_{BZ}$  is the area of the Brillouin zone and  $f(E_{\mathbf{k},\sigma,m} - \mu)$  is the Fermi distribution function computed at the eigenvalue of the problem shifted by the chemical potential  $\mu$ .  $\mu$  is determined by fixing the number of particles on the unit cell to the desired value (2.5 electrons every three sites at the p-type van Hove singularity).

Eq. (2.5) permits to compute a new value of the variational parameters given the initial guess. By iterating this procedure, we can reach a self consistent solution that generally depends by the original guess. This procedure is analogous to minimizing the free-energy:

$$F = -\frac{1}{A_{BZ}\beta} \sum_{\mathbf{k},\sigma,m} \ln [1 + e^{-\beta(E_{\mathbf{k},\sigma,m} - \mu)}] + \mu N + F^{\text{MF}}, \quad (2.6)$$

with  $N$  the total number of electrons on the unit cell and  $F^{\text{MF}}$  the mean-field free energy:

$$F^{\text{MF}} = -U \sum_i \langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle - V \sum_{\langle i,j \rangle} \langle n_i \rangle \langle n_j \rangle + V \sum_{\langle i,j \rangle, \sigma} \langle c_{i,\sigma}^\dagger c_{j,\sigma} \rangle \langle c_{j,\sigma}^\dagger c_{i,\sigma} \rangle, \quad (2.7)$$

where the summation over the nearest neighbors has to count each bond once.

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- [1] J. Wen, A. Rüegg, C.-C. J. Wang, and G. A. Fiete, Phys. Rev. B **82**, 075125 (2010), URL <https://link.aps.org/doi/10.1103/PhysRevB.82.075125>.
- [2] Q. Liu, H. Yao, and T. Ma, Phys. Rev. B **82**, 045102 (2010), URL <https://link.aps.org/doi/10.1103/PhysRevB.82.045102>.
- [3] M. F. López and J. Merino, Phys. Rev. B **102**, 035157 (2020), URL <https://link.aps.org/doi/10.1103/PhysRevB.102.035157>.