

# Hubbard Model with Staggered Potential

Quantum Many Body Systems and Strongly Correlated Electrons I

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## 1 INTRODUCTION: MEAN-FIELD APPROACH TO HUBBARD INTERACTION

In the present work we will address a mean-field treatment of a particular extension of Hubbard model. This corresponds to a variational optimization of a single Slater-Determinant approximation to the many-body wavefunction, the well-known Hartree-Fock (HF) approximation scheme.<sup>1;2</sup> Thus we expect the method to give reliable results only in the weak-coupling limit of the Hubbard interaction. However, being not HF a perturbative procedure, it is not straightforward to define a relevant dimensionless parameter strictly smaller than unity. Thus we impose a quite indulgent restriction, namely requiring the Hubbard  $U$  to be smaller than the total bandwidth (i.e. the maximum excitation energy) of the corresponding noninteracting model.

The mean-field idea is to recast the number operators appearing in the Hubbard term as:

$$\hat{n}_\sigma = \langle \hat{n}_\sigma \rangle + \delta \hat{n}_\sigma, \quad (1)$$

where we assume  $\langle \hat{n}_{i,\sigma} \rangle$  to be a leading classical term around which we describe some smaller (but still essential for a non-trivial description) quantum fluctuation, by means of the  $\delta \hat{n}_\sigma$  operator. So for each Hubbard term we'll have:

$$\begin{aligned} \hat{n}_\uparrow \hat{n}_\downarrow &= \langle \hat{n}_\uparrow \rangle \langle \hat{n}_\downarrow \rangle + \langle \hat{n}_\uparrow \rangle \delta \hat{n}_\downarrow \\ &\quad + \langle \hat{n}_\downarrow \rangle \delta \hat{n}_\uparrow + \delta \hat{n}_\uparrow \delta \hat{n}_\downarrow \\ &\simeq \langle \hat{n}_\uparrow \rangle \langle \hat{n}_\downarrow \rangle + \langle \hat{n}_\uparrow \rangle \delta \hat{n}_\downarrow + \langle \hat{n}_\downarrow \rangle \delta \hat{n}_\uparrow, \end{aligned} \quad (2)$$

where we have neglected the *correlation of fluctuations* term  $\delta \hat{n}_\uparrow \delta \hat{n}_\downarrow$ . This is the approximation laying at the heart of mean-field theory: we assume a “bulky” classical term and consider only first order quantum correction around it. The latter are quadratic and can be diagonalized within canonical quantization formalism, while the former will be parametrized in terms of appropriate order parameters, guided by some *a priori* knowledge on what physics we expect. A variational determination of these parameters would lead to self-consistency equations through which solve the problem at the HF level.

## 2 THE MODEL

The addressed model is described by the Hamiltonian

$$\hat{H} = -t \sum_{\langle i,j \rangle} \sum_\sigma \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + U \sum_j \hat{n}_{j,\downarrow} \hat{n}_{j,\uparrow} + a \sum_j (-1)^{R_j} \hat{n}_j,$$

The first term is the usual nearest neighbour tight-binding representation of lattice kinetic energy and the second one is the Hubbard model for electron-electron repulsion. The third term is instead a staggered potential coupled with the total electron density  $\hat{n}_i = \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}$ . We can regard it as an alternate shift of the on-site energy of the underlying tight-binding model so that we can interpret our system as an ionic lattice with two inequivalent species<sup>1</sup>.

For dimension  $d = 1$ , assuming periodic boundary conditions (PBCs), we end up with a linear-chain Hamiltonian given by:

$$\hat{H} = -t \sum_{j,\sigma} (\hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \text{h.c.}) + U \sum_j \hat{n}_{j,\downarrow} \hat{n}_{j,\uparrow} + a \sum_j (-1)^j \hat{n}_j$$

assuming  $\hat{c}_{N_{\text{sites}}+1,\sigma} \equiv \hat{c}_{1,\sigma}$ , as our PBC. (3)

Given the ionic nature of the staggered potential term we expect the possibility of nonzero macroscopic polarization, as an order parameter in competition with the well-known antiferromagnetic (AFM) ordering that characterizes the low-temperature physics of pure Hubbard model. A qualitative depiction of the expected behavior of our 1d-chain is reported in fig. 1.

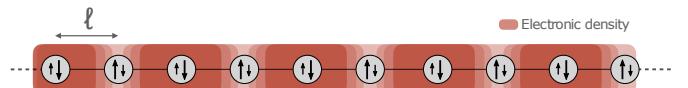


Figure 1: Graphical representation of the expected physics for the 1d-chain model described by eq. (3).

<sup>1</sup>Having a deeper on-site energy in the “odd” sites would favour a higher charge density therein, which we would expect in an ionic lattice.

In the following we shall try to isolate the essential features of this nontrivial ‘‘magnetization vs polarization’’ quantum competition, thus studying the mean-field dynamics of the 1d-chain, at zero temperature and half-filling (fixed number of particles:  $N_{\text{el}} = N_{\text{sites}} =: N$ ).<sup>2</sup>

First of all will be essential to determine the ground state properties of the noninteracting ( $U = 0$ ) version of the model. This issue will be addressed in the next section.

### 3 NONINTERACTING GROUND STATE

The non-interacting Hamiltonian is given by

$$\hat{H}_0 = -t \sum_{j,\sigma} \left( \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \text{h.c.} \right) + a \sum_{j,\sigma} (-1)^j \hat{n}_{j,\sigma}, \quad (4)$$

Introducing the Fourier transforms of the ladder operators

$$\hat{c}_{k,\sigma}^\dagger = \frac{1}{\sqrt{N\ell}} \sum_j e^{-ikj\ell} \hat{c}_{j,\sigma}^\dagger, \quad (5)$$

$$\hat{c}_{j,\sigma}^\dagger = \frac{1}{\sqrt{N\ell}} \sum_k e^{+ikj\ell} \hat{c}_{k,\sigma}^\dagger, \quad (6)$$

we can represent the Hamiltonian (4) in  $k$ -space as:

$$\begin{aligned} H_0 &= -\frac{t}{N\ell} \sum_{j,\sigma} \sum_{k,k'} \left( e^{ikj\ell} e^{-ik'(j+1)\ell} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k',\sigma} + \text{h.c.} \right) \\ &\quad + \frac{a}{N\ell} \sum_{j,\sigma} \sum_{k,k'} (-1)^j e^{i(k-k')j\ell} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k',\sigma} \\ &= \frac{1}{N\ell} \sum_{j,\sigma} \sum_{k,k'} \left[ -t \left( e^{i(k-k')j\ell} e^{-ik'\ell} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k',\sigma} + \text{h.c.} \right) \right. \\ &\quad \left. + a \left( e^{i(k+Q-k')j\ell} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k',\sigma} \right) \right] \\ &= \sum_{k,k',\sigma} \left[ -t \left( e^{-ik'\ell} \delta_{k,k'} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k',\sigma} + \text{h.c.} \right) \right. \\ &\quad \left. + a \left( \delta_{k+Q,k'} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k',\sigma} \right) \right] \\ &= \sum_{k,\sigma} \left[ -2t \cos(k\ell) \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} + a \left( \hat{c}_{k,\sigma}^\dagger \hat{c}_{k+Q,\sigma} \right) \right], \quad (7) \end{aligned}$$

<sup>2</sup>For simplicity we will always assume  $N$  to be even.

where  $Q = \pi/\ell$  is the wave-vector corresponding to double-periodicity staggering, i.e.  $(-1)^j = e^{iQj\ell} = e^{i\pi j}$ .

We can then rewrite the Hamiltonian in the naturally arising  $Q$ -folded Brillouin zone ( $\text{QBZ} = [0, \pi/\ell] = [0, Q]$ ) as:

$$\begin{aligned} \hat{H}_0 &= \sum_{\sigma} \left[ -2t \sum_{k \in \text{BZ}} \cos(k\ell) \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} \right. \\ &\quad \left. + a \left( \sum_{k \in \text{QBZ}} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k+Q,\sigma} + \sum_{k+Q \in \text{QBZ}} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k+Q,\sigma} \right) \right] \\ &= \sum_{\sigma} \left[ \sum_{k \in \text{QBZ}} \left( t_k \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} + t_{k+Q} \hat{c}_{k+Q,\sigma}^\dagger \hat{c}_{k+Q,\sigma} \right) \right. \\ &\quad \left. + a \sum_{k \in \text{QBZ}} \left( c_{k,\sigma}^\dagger \hat{c}_{k+Q,\sigma} + c_{k+Q,\sigma}^\dagger \hat{c}_{k,\sigma} \right) \right], \quad (8) \end{aligned}$$

where we have furthermore introduced a shorthand for the overall hopping term:

$$t_k := -2t \cos(k\ell). \quad (9)$$

\* \* \*

Defining the Hilbert space basis

$$|k\sigma\rangle := \begin{pmatrix} \hat{c}_{k,\sigma}^\dagger \\ \hat{c}_{k+Q,\sigma}^\dagger \end{pmatrix} |0\rangle, \quad (10)$$

we can recast eq. (8) in matrix form as:

$$\hat{H}_0 = \sum_{\sigma} \sum_{\text{QBZ}} \begin{pmatrix} t_k & a \\ a & t_{k+Q} \end{pmatrix} |k\sigma\rangle \langle k\sigma|. \quad (11)$$

Hence, noticing that  $t_{k+Q} = -t_k$  by symmetry and solving the eigenvalue equation

$$\begin{vmatrix} t_k - \varepsilon_k & a \\ a & -t_k - \varepsilon_k \end{vmatrix} = 0, \quad (12)$$

we obtain the single particle energies:

$$\varepsilon_k = \pm \sqrt{t_k^2 + a^2}. \quad (13)$$

In fig. 2 are reported both the  $k$ -dispersion and the  $a$ -dependence of eq. (13). At half-filling we recognize the system as a band-insulator with a valence- to conduction- states gap proportional to the staggered potential strength  $a$  (thus expecting excitations to be exponentially killed at temperatures below the  $a/k_B$  scale).

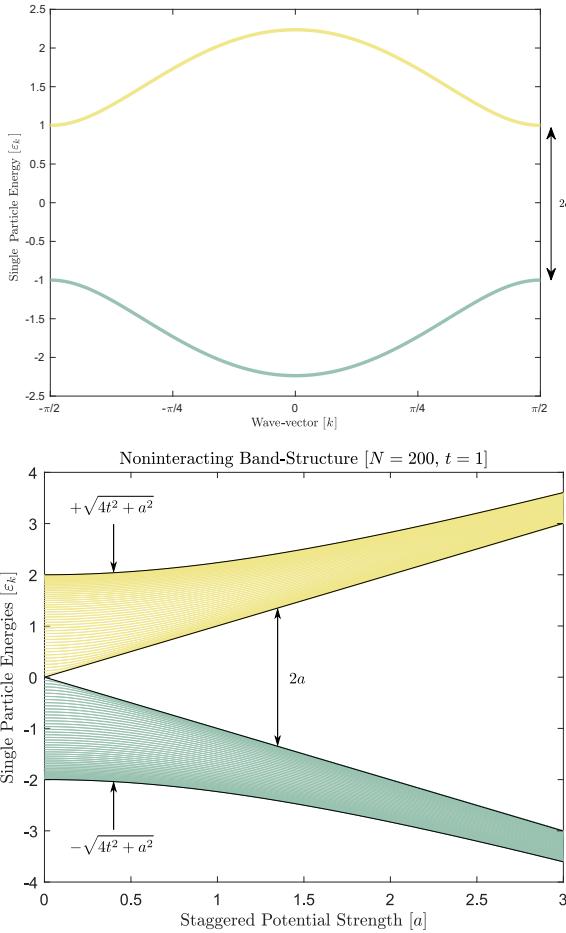


Figure 2: Single particle levels for the noninteracting system (cf. eqs. (4) and (13)). In the upper panel is shown the reciprocal space dispersion of the energies (for  $a = t = 1$ ), while in the lower panel is reported the overall behaviour of the energy bands at varying  $a$  values.

Now we proceed to compute the eigenvectors of the Hamiltonian (8). Defining  $\varepsilon_k^+ := \sqrt{t_k^2 + a^2} =: -\varepsilon_k^-$  we have:

$$\begin{aligned}
 0 &= \begin{pmatrix} t_k - \varepsilon_k^\pm & a \\ a & -t_k - \varepsilon_k^\pm \end{pmatrix} \begin{pmatrix} \cos \theta_k^\pm \\ \sin \theta_k^\pm \end{pmatrix} \\
 &= (t_k - \varepsilon_k^\pm) \cos \theta_k^\pm + a \sin \theta_k^\pm \\
 \implies \cos \theta_k^\pm &= \underbrace{\left( \frac{a}{\varepsilon_k^\pm - t_k} \right)}_{\xi^\pm} \sin \theta_k^\pm. \quad (14)
 \end{aligned}$$

Hence, recognizing that

$$\begin{aligned}
 \xi^+ &:= \frac{a}{\varepsilon^+ - t_k} = \frac{a(\varepsilon^+ + t_k)}{(\varepsilon^+ - t_k)(\varepsilon^+ + t_k)} \\
 &= \frac{a(\varepsilon^+ + t_k)}{t_k^2 + a^2 - t_k^2} = \frac{\varepsilon^+ + t_k}{a} =: -\frac{1}{\xi^-},
 \end{aligned}$$

we can impose

$$\begin{aligned}
 \cos \theta_k^+ &= -\sin \theta_k^- =: \cos \theta_k \\
 \sin \theta_k^+ &= \cos \theta_k^- =: \sin \theta_k
 \end{aligned}$$

so that

$$\tan \theta_k = \frac{1}{\xi^+} = \frac{\sqrt{t_k^2 + a^2} - t_k}{a}.$$

Thus the conduction (+) and valence (-) eigenstates can be written respectively as:

$$|k^+\rangle = \sum_{\sigma} \begin{pmatrix} \cos \theta_k \\ \sin \theta_k \end{pmatrix}^T \begin{pmatrix} \hat{c}_{k,\sigma}^\dagger \\ \hat{c}_{k+Q,\sigma}^\dagger \end{pmatrix} |0\rangle, \quad (15)$$

$$|k^-\rangle = \sum_{\sigma} \begin{pmatrix} -\sin \theta_k \\ \cos \theta_k \end{pmatrix}^T \begin{pmatrix} \hat{c}_{k,\sigma}^\dagger \\ \hat{c}_{k+Q,\sigma}^\dagger \end{pmatrix} |0\rangle, \quad (16)$$

with:

$$\cos \theta_k = \frac{1}{1 + \tan^2 \theta_k} = \frac{a}{\sqrt{a^2 + (\varepsilon_k^+ - t_k)^2}}, \quad (17)$$

$$\sin \theta_k = \frac{\tan \theta_k}{1 + \tan^2 \theta_k} = \frac{\varepsilon_k^+ - t_k}{\sqrt{a^2 + (\varepsilon_k^+ - t_k)^2}}. \quad (18)$$

\* \* \*

At half-filling the ground state of the systems is obtained by filling up the whole valence-band, i.e.

$$\begin{aligned}
 |\text{GS}\rangle &= \frac{1}{\sqrt{N}} \sum_{\text{QBZ}} |k^-\rangle \\
 &= \frac{1}{\sqrt{N}} \sum_{\sigma} \sum_{\text{QBZ}} \begin{pmatrix} -\sin \theta_k \\ \cos \theta_k \end{pmatrix}^T \begin{pmatrix} \hat{c}_{k,\sigma}^\dagger \\ \hat{c}_{k+Q,\sigma}^\dagger \end{pmatrix} |0\rangle. \quad (19)
 \end{aligned}$$

At this point we shall investigate the real space ordering of the noninteracting ground state. As discussed in the previous section we expect some kind of ferroelectricity, i.e. a non zero macroscopic polarization. To verify our guess we shall give a unit-cell<sup>3</sup> definition for the polarization, namely

$$\Delta := \frac{1}{N} \sum_j (-1)^{1+j} \langle \text{GS} | \hat{c}_j^\dagger \hat{c}_j | \text{GS} \rangle \in [-1, 1]. \quad (20)$$

Since the expression in eq. (20) is explicitly constructed to account *odd-site* charges as positive terms and *even-site* charges as negative ones, we expect  $\Delta$  to have the same sign of the staggered potential strength  $a$ , being zero if  $a = 0$ .

Switching to Fourier domain we have:

$$\begin{aligned} \Delta &= -\frac{1}{N} \left\langle \sum_j \frac{(-1)^j}{N\ell} \sum_{k,k'} e^{i(k-k')j\ell} \hat{c}_k^\dagger \hat{c}_{k'} \right\rangle_{\text{GS}} \\ &= -\frac{1}{N} \left\langle \sum_j \frac{1}{N\ell} \sum_{k,k'} e^{i(k-k'+Q)j\ell} \hat{c}_k^\dagger \hat{c}_{k'} \right\rangle_{\text{GS}} \\ &= -\frac{1}{N} \left\langle \sum_{k,k'} \delta_{k+Q,k'} \hat{c}_k^\dagger \hat{c}_{k'} \right\rangle_{\text{GS}} \\ &= -\frac{1}{N} \left\langle \sum_{\text{BZ}} \hat{c}_k^\dagger \hat{c}_{k+Q} \right\rangle_{\text{GS}} \\ &= -\frac{1}{N} \sum_{\text{QBZ}} \left\langle \hat{c}_k^\dagger \hat{c}_{k+Q} + \text{h.c.} \right\rangle_{\text{GS}}. \end{aligned} \quad (21)$$

<sup>3</sup>The definition of macroscopic polarization is quite knotty within periodic boundary conditions. In particular is not really legitimate to identify it with the dipole per unit-cell, since this quantity is not independent on unit-cell choice (which in turn is indeed arbitrary!). The *Modern Theory of Polarization*<sup>3</sup> gives a legitimate formulation in terms of either geometrical phases acquired along  $k$ -space loops, or dipoles between “Wannier centers”. Nevertheless we shall avoid entering this level of detail (although it would be totally possible to do, having a reciprocal space representation of the electronic ground state). Hence, from now on, the term *polarization* is always intended to refer to the *dipole per unit-cell*, despite all the problems this choice leads to. We claim the approach to be legitimate within our scope, for we are interested in any well-defined order parameter to seek in the subsequent mean-field treatment, even if not a true meaningful macroscopic quantity.

Adopting again the Hilbert space basis given in eq. (10) we finally obtain:

$$\begin{aligned} \Delta &= -\frac{1}{N} \sum_{\text{QBZ}} \langle k^- | \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} | k^- \rangle \\ &= -\frac{1}{N} \sum_{\sigma} \sum_{\text{QBZ}} \begin{pmatrix} -\sin \theta_k \\ \cos \theta_k \end{pmatrix}^T \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -\sin \theta_k \\ \cos \theta_k \end{pmatrix} \\ &= -\frac{2}{N} \sum_{\text{QBZ}} (-\sin \theta_k, \cos \theta_k) \begin{pmatrix} \cos \theta_k \\ -\sin \theta_k \end{pmatrix} \\ &= \frac{2}{N} \sum_{\text{QBZ}} 2 \sin \theta_k \cos \theta_k \\ &= \frac{2}{N} \sum_{\text{QBZ}} \frac{2a(\varepsilon_k^+ - t_k)}{a^2 + (\varepsilon_k^+ - t_k)^2} =: \frac{2}{N} \sum_{\text{QBZ}} \Delta_k. \end{aligned} \quad (22)$$

Let's notice that, given<sup>4</sup>

$$\mathbf{i}) \quad \varepsilon_k^+ = \sqrt{a^2 + t_k^2} \geq t_k, \quad \forall a \in \mathbb{R},$$

$$\mathbf{ii}) \quad a^2 + (\varepsilon_k^+ - t_k)^2 \geq 0, \quad \forall a \in \mathbb{R},$$

$$\mathbf{iii}) \quad \lim_{k \rightarrow Q} \Delta_k = \text{sgn}(a), \quad \forall a \in \mathbb{R},$$

$$\mathbf{iv}) \quad \lim_{a \rightarrow 0} \Delta_k = 0, \quad \forall k \neq Q,$$

we can conclude that for any real value of the staggered potential strength  $a$  it holds that:

$$\boxed{\text{sgn}(\Delta) \equiv \text{sgn}(a)}. \quad (23)$$

Thus we have verified that indeed the role of the staggered potential term in the noninteracting Hamiltonian (4) is to introduce a charge polarization in the chain.

<sup>4</sup>Statements i) and ii) follow from basic algebra, while iii) and iv) can be checked by graphical inspection (See fig. 3).

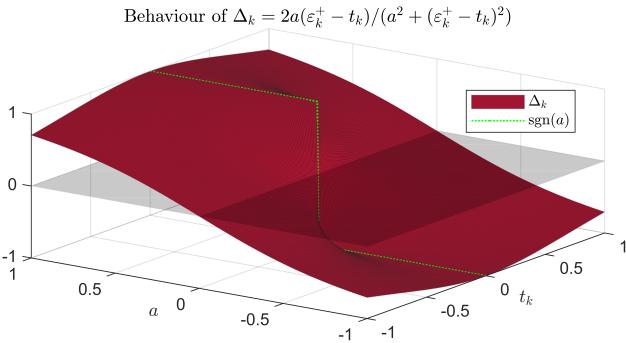


Figure 3: Graphical investigation of the  $a$  and  $t_k$  dependence of the harmonic components of polarization, as defined in eq. (22). It is evident that each  $\Delta_k$  has same sign of  $a$ .

#### 4 MEAN-FIELD TREATMENT OF THE INTERACTION AND SELF-CONSISTENCY EQUATIONS

Having thoroughly investigated the ground state physics of the noninteracting model we shall now introduce the interaction term

$$\hat{H}_U = U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}, \quad (24)$$

so that the complete Hamiltonian of the model (3) is given by  $H = H_0 + H_U$ . Following the mean-field prescription given in eq. (2), we write:

$$\begin{aligned} \hat{H}_U &\simeq U \sum_j \left( \langle \hat{n}_{j,\uparrow} \rangle \langle \hat{n}_{j,\downarrow} \rangle + \langle \hat{n}_{j,\uparrow} \rangle \delta \hat{n}_{j,\downarrow} + \langle \hat{n}_{j,\downarrow} \rangle \delta \hat{n}_{j,\uparrow} \right) \quad (25) \\ &=: E_U + \hat{H}_U^\downarrow + \hat{H}_U^\uparrow \end{aligned}$$

where we have eliminated  $\delta \hat{n}_{j,\sigma} = \hat{n}_{j,\sigma} - \langle \hat{n}_{j,\sigma} \rangle$ , so to have

$$E_U := -U \sum_j \langle \hat{n}_{j,\uparrow} \rangle \langle \hat{n}_{j,\downarrow} \rangle, \quad (26)$$

$$\hat{H}_U^\downarrow := U \sum_j \langle \hat{n}_{j,\uparrow} \rangle \hat{n}_{j,\downarrow}, \quad (27)$$

$$\hat{H}_U^\uparrow := U \sum_j \langle \hat{n}_{j,\downarrow} \rangle \hat{n}_{j,\uparrow}. \quad (28)$$

The first term is a shift of the ground state energy. For now we will not throw it away, for it may contain order-parameter-dependent contributions that will be of course essential in defining the overall energetic competition defining the interacting ground state. The other two are spin-polarized quadratic contributions that can be diagonalized

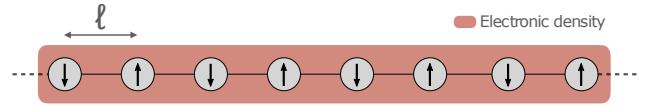


Figure 4: Depiction of the real-space ordering in a Hubbard chain. Total electron density is homogeneous.

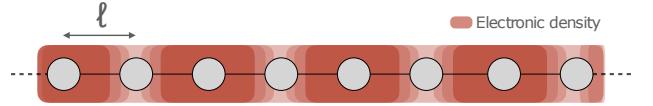


Figure 5: Depiction of the real-space ordering in a noninteracting ionic chain. Total electron density is inhomogeneous.

by means of appropriate canonical transformations. To investigate the issue is crucial to define some *a priori* guess on the expected form of both the ground state averages  $\langle \hat{n}_{j,\sigma} \rangle$ . A good starting point to craft a proper *mean-field ansatz* for our nontrivial model is surely to look at the two simpler ground states we already know:

#### Hubbard Chain

The well-known HF ground state of a half-filled Hubbard chain exhibits an antiferromagnetic ordering that preserves the homogeneity of total electronic density (fig. 4). Hence the standard variational form for the mean-field averages can be determined by combining these two conditions, e.g. in the form<sup>5</sup>

$$\langle \hat{n}_{j,\uparrow} \rangle + \langle \hat{n}_{j,\downarrow} \rangle = 1, \quad \forall j \quad (29)$$

$$\langle \hat{n}_{j,\uparrow} \rangle - \langle \hat{n}_{j,\downarrow} \rangle = (-1)^j m, \quad \text{with } m \in [-1, 1] \quad (30)$$

↓

$$\langle \hat{n}_{j,\uparrow} \rangle = \frac{1 + (-1)^j m}{2}. \quad (31)$$

#### Ionic Chain

As discussed in the previous section the ground state of a noninteracting ionic chain breaks the charge density homogeneity by means of a finite polarization, whose sign is determined by that of the staggered potential strength  $a$  (cf. eq. 20 and fig. 5). If one treated the problem in a variational fashion the ansatz would be

$$\langle \hat{n}_{j,\uparrow} \rangle + \langle \hat{n}_{j,\downarrow} \rangle = 1 + (-1)^{1+j} \Delta, \quad \text{with } \Delta \in [-1, 1]. \quad (32)$$

In order to treat an Hamiltonian in which both tendencies are present (and possibly in mutual competition) we shall

<sup>5</sup>We have adopted a slightly different definition for the variational magnetization  $m$ , with respect to the usual conventions<sup>1;2</sup>. This was done to have the same range as the polarization defined in eq. (20).

then mix the two approaches, namely by taking the AFM condition (30) together with the inhomogeneous total density that characterizes the ionic chain (32). This would lead to a two-variational-parameters ansatz:

$$\begin{cases} \langle \hat{n}_{j,\uparrow} \rangle = \frac{1 + (-1)^{1+j} (\Delta - m)}{2} \\ \langle \hat{n}_{j,\downarrow} \rangle = \frac{1 + (-1)^{1+j} (\Delta + m)}{2} \end{cases} \quad (33)$$

\* \* \*

We proceed now to analyze the consequences of the proposed ansatz (33) on the energy  $E_{\text{U}}$  (26) and the two spin-polarized Hamiltonians  $H_{\text{U}}^{\sigma}$  (27, 28). For the former we just need to evaluate the product of the two spin-polarized averages:

$$\begin{aligned} \langle \hat{n}_{j,\uparrow} \rangle \langle \hat{n}_{j,\downarrow} \rangle &= \frac{[1 - (-1)^j (\Delta - m)][1 - (-1)^j (\Delta + m)]}{4} \\ &= \frac{1 - (-1)^j 2\Delta + (-1)^{2j} [\Delta^2 - m^2]}{4} \\ &= \frac{1}{4} - \frac{(-1)^j \Delta}{2} + \frac{\Delta^2 - m^2}{4}. \end{aligned} \quad (34)$$

The first term is a constant independent on any variational parameter, so that we can reabsorb it in the vacuum energy. The second one has alternating sign on the chain so, recalling its length  $N$  its an even number this contribution will vanish after summing over  $j$ .

The last term is then the relevant one, for it will give rise to a order parameter dependent *many-body shift* of the occupied mean-field single particle levels, namely

$$E_{\text{mb}} = -\frac{UN}{4} (\Delta^2 - m^2). \quad (35)$$

We shall notice that there are actually two contributions to it, with opposite sign. The positive one is coupled to the staggered magnetization of the chain, thus corresponding to the usual *interaction price* to pay for the AFM ordering in a Hubbard chain. But here there is also an energy gain, coupled to the macroscopic polarization of the chain whose origin is to be attributed to the on-site energy shift of the two inequivalent classes of sites.

For future purposes we will also rotate our basis in the space of variational parameters, defining

$$\mu := \frac{\Delta + m}{2}, \quad \delta := \frac{\Delta - m}{2}. \quad (36)$$

In terms of these two new variables the many-body shift will read as  $E_{\text{mb}} = -UN\delta\mu$

Let's discuss then the mean-field form of the spin-polarized Hamiltonians  $H_{\text{U}}^{\sigma}$ . We will again refer to the rotated order parameters (36), with the shorthand notation:

$$\diamondsuit_{\sigma} := \begin{cases} \mu, & \text{if } \sigma = \uparrow \\ \delta, & \text{if } \sigma = \downarrow \end{cases}$$

We have:

$$\begin{aligned} \hat{H}_{\text{U}}^{\sigma} &= U \sum_j \left( \frac{1}{2} + (-1)^{1+j} \diamondsuit_{\sigma} \right) \hat{c}_{j,\sigma}^{\dagger} \hat{c}_{j,\sigma} \\ &= \underbrace{\frac{UN}{2}}_{\text{half-filling}} - U \diamondsuit_{\sigma} \sum_{j,\sigma} (-1)^j \hat{c}_{j,\sigma}^{\dagger} \hat{c}_{j,\sigma}. \end{aligned} \quad (37)$$

The first term is again just a constant energy shift that we can reabsorb in the vacuum energy, while the latter is formally identical to the staggered potential term (refer e.g. to eq. 3), provided the substitution:  $a \mapsto -U\diamondsuit_{\sigma}$ .

Hence, being the noninteracting Hamiltonian also separable in spin-polarized contributions:

$$\begin{aligned} \hat{H}_0 &= \sum_{\sigma} \left[ -t \sum_j \left( \hat{c}_{j,\sigma}^{\dagger} \hat{c}_{j+1,\sigma} + \text{h.c.} \right) + a \sum_j (-1)^j \hat{n}_{j,\sigma} \right] \\ &=: \sum_{\sigma} \hat{H}_0^{\sigma} = \hat{H}_0^{\uparrow} + \hat{H}_0^{\downarrow}, \end{aligned}$$

it becomes clear that the relevant matrix to diagonalize is spin-polarized:

$$\begin{aligned} \hat{H}_{\text{MF}} &:= \sum_{\sigma} \sum_{\text{QBZ}} \left[ \begin{pmatrix} t_k & a \\ a & t_{k+Q} \end{pmatrix} + \begin{pmatrix} 0 & -U\diamondsuit_{\sigma} \\ -U\diamondsuit_{\sigma} & 0 \end{pmatrix} \right] |k\sigma\rangle \langle k\sigma| \\ &= \sum_{\sigma} \sum_{\text{QBZ}} \begin{pmatrix} t_k & a_{\sigma} \\ a_{\sigma} & -t_k \end{pmatrix} |k\sigma\rangle \langle k\sigma|, \quad a_{\sigma} := a - U\diamondsuit_{\sigma}. \end{aligned} \quad (38)$$

Exploiting the formal analogy with eq. (11) we can write all in once the eigenproblem solutions of eq. (38) as:

$$\begin{aligned} E_k &= \sum_{\sigma} E_{k,\sigma} = \pm \sum_{\sigma} \sqrt{\underbrace{t_k^2 + a_{\sigma}^2}_{E_{k,\sigma}^+}} \\ &= \pm \left[ \sqrt{t_k^2 + (a - U\mu)^2} + \sqrt{t_k^2 + (a - U\delta)^2} \right], \end{aligned} \quad (39)$$

$$|k\sigma;+\rangle = \begin{pmatrix} \cos \theta_{k,\sigma} \\ \sin \theta_{k,\sigma} \end{pmatrix}^T \begin{pmatrix} \hat{c}_{k,\sigma}^\dagger \\ \hat{c}_{k+Q,\sigma}^\dagger \end{pmatrix} |0\rangle, \quad (40)$$

$$|k\sigma;-\rangle = \begin{pmatrix} -\sin \theta_{k,\sigma} \\ \cos \theta_{k,\sigma} \end{pmatrix}^T \begin{pmatrix} \hat{c}_{k,\sigma}^\dagger \\ \hat{c}_{k+Q,\sigma}^\dagger \end{pmatrix} |0\rangle, \quad (41)$$

$$\cos \theta_{k,\sigma} = \frac{a_\sigma}{\sqrt{a_\sigma^2 + (E_{k,\sigma}^+ - t_k)^2}}, \quad (42)$$

$$\sin \theta_{k,\sigma} = \frac{E_{k,\sigma}^+ - t_k}{\sqrt{a_\sigma^2 + (E_{k,\sigma}^+ - t_k)^2}}. \quad (43)$$

\* \* \*

The many-body ground state of the system is then

$$|\text{GS}\rangle = \frac{1}{\sqrt{N}} \sum_{\sigma} \sum_{\text{QBZ}} |k\sigma;-\rangle = \frac{1}{\sqrt{N}} \sum_{\sigma} \sum_{\text{QBZ}} \begin{pmatrix} -\sin \theta_{k,\sigma} \\ \cos \theta_{k,\sigma} \end{pmatrix}^T \begin{pmatrix} \hat{c}_{k,\sigma}^\dagger \\ \hat{c}_{k+Q,\sigma}^\dagger \end{pmatrix} |0\rangle, \quad (44)$$

with energy

$$\begin{aligned} E_{\text{GS}} &= E_{\text{MF}} + E_{\text{mb}} \\ &= - \sum_{\sigma} \sum_{\text{QBZ}} E_{k,\sigma}^+ - UN\delta\mu \\ &= \sum_{\text{QBZ}} \left[ \sqrt{t_k^2 + (a - U\mu)^2} + \sqrt{t_k^2 + (a - U\delta)^2} \right] - UN\delta\mu. \end{aligned} \quad (45)$$

To simplify the notation we rescale the variational parameters as  $x := U\mu$  and  $y := U\delta$ , and look for the best ground state by imposing  $\delta E_{\text{GS}}(x, y) = 0$ .

$$\vec{\nabla} E_{\text{GS}}(x, y) = \begin{bmatrix} \sum_{\text{QBZ}} \frac{a - x}{\sqrt{t_k^2 - (a - x)^2}} - \frac{Ny}{U} \\ \sum_{\text{QBZ}} \frac{a - y}{\sqrt{t_k^2 - (a - y)^2}} - \frac{Nx}{U} \end{bmatrix} \quad (46)$$

$$\vec{\nabla} E_{\text{GS}}(x, y) = 0$$



$$\begin{cases} x = \frac{U}{N} \sum_{\text{QBZ}} \frac{a - y}{\sqrt{t_k^2 - (a - y)^2}} \\ y = \frac{U}{N} \sum_{\text{QBZ}} \frac{a - x}{\sqrt{t_k^2 - (a - x)^2}} \end{cases} \quad (47)$$

Minimizing the ground state energy in variational space we have found two inter-coupled equations, that shall be solved iteratively until *selfconsistency*. But before any attempt to solve the general problem one may want to check if the result matches with the two limiting cases:

- The noninteracting ionic chain is trivially recovered by sending  $a_\sigma$  back to  $a$ , in the expression for the eigenstates and energies of the system. The spin dependence disappears, leaving us with the noninteracting expressions, eqs. (13) and (19).
- The traditional Hubbard result can be inspected looking directly at the selfconsistency conditions. Setting  $a$  to zero is equivalent to have  $x = -y = \frac{Um}{2}$ , so eq. (47) reduces to just one condition, namely

$$1 = \frac{1}{N} \sum_{\text{QBZ}} \frac{U}{\sqrt{t_k^2 + (\frac{Um}{2})^2}},$$

the well-known<sup>1;2</sup> selfconsistency equation for a Hubbard chain with magnetization  $m \in [-1, 1]$  (cf. ft.n.<sup>5</sup>).

## 5 ITERATIVE SOLUTION FOR GENERIC $U$ AND $a$

In the present section we will briefly discuss some detail of the iterative routine we have implemented to numerically solve the selfconsistency equations (47). For further details the full listing of the code is available in the appendix. Then we will proceed to present and discuss several results for a full-range span of the variational parameter space. Finally we will address the “small  $a$ ” and “small  $U$ ” asymptotics, i.e. the most trustable (and interesting) mean-field predictions.

### 5.1 IMPLEMENTATION DETAILS

Regarding the iterative algorithm implemented to achieve selfconsistency we want to point out the main choices and consequences:

- The input values for  $a$  and  $U$  have been chosen to be always positive. While for the latter this is constrained choice, for it represents the repulsion between the electrons in the chain, the staggered potential strength could in principle be negative. Nevertheless, by construction of the ansatz (and so by analogy to the non-interacting case) we expect any emerging finite value for the polarization to be negative, for a negative value of  $a$ . This naturally leads to the next point.
- According to lines 23 and 24 of Listing 1 the starting values for  $m$  and  $\Delta$  are extracted from a uniform distribution within the range  $[0, 1]$ . We have excluded negative values for  $\Delta$  because its sign is locked by that of  $a$ , as just discussed. For the magnetization  $m$  the choice might instead appear somewhat arbitrary and restrictive, but it is not the case, for that an opposite sign would just lead to an equivalent broken-symmetry sector (spin-flip of all fermions), just as it happens for a pure Hubbard model. We have indeed verified that starting instead with negative values for  $\Delta$  (without touching  $a$ ) and  $m$  would lead to selfconsistent solutions where the former is again positive and the latter negative. Clarified this, all the results we will present in the following are obtained for positive starting values.
- In the actual selfconsistency routine (Listing 2) we update the two rotated parameters  $x$  and  $y$  (cf. previous section for notations) at the same time in the code. This will exclude any bias toward one of the two in the iterative procedure.
- To numerically determine whether selfconsistency is achieved or not we have defined two independent tunable bounds for both the  $x$  and  $y$ . After each step the condition that is checked is if *both* parameters deviation from old values is smaller than respective bound (cf. line 25 of Listing 2). As you can see the check for the two conditions is done at the same moment in the code. Any deviation from this approach would lead to wrong results whenever one of the parameters converges to selfconsistency faster than the other.
- Finally we shall notice that the actual iterative move is not a pure update: we mix each pair of values computed from expression (47) with their respective “old” values, by means of a linear combination (cf. lines 9-10 and 28-29 of Listing 2). This *simple mixing* approach

allows to fine-tune the speed of the routine (a.k.a. the number of required iterations) by balancing the *step-length* at each iteration and the *stability* of the procedure (too large steps may lead to undamped oscillations around the target value). More sophisticated mixing procedures are available<sup>4</sup> but a simple linear combination appeared to be sufficient within our scope.

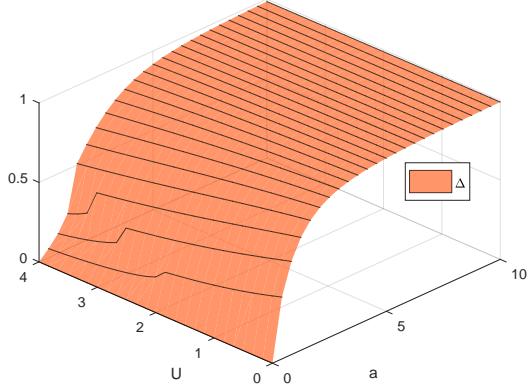
### 5.2 LANDSCAPE RESULTS

We proceed to analyze our results for a wide range of Hamiltonian values, namely a coarse-grained grid in the set  $\{a \in [0, 10] \text{ & } U \in [0, 4]\}$ . Let’s note that from now on the hopping term  $t$  will be always set to 1, as the *energy scale* of the underlying tight binding model. Hence is evident that we have restricted the interaction strength to never exceed  $4t$ , i.e. the minimal value for the total band-width of the noninteracting model (cf. eq. (13) and fig. 2). This amounts to a “relaxed” weak-coupling limit, for which we assume the single-determinant description to be still reliable (cf. the discussion on Hartree Fock theory in the introductory section).

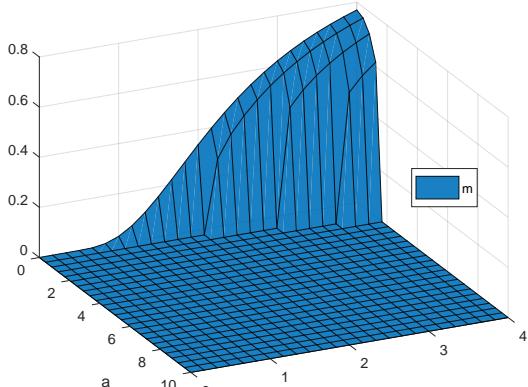
In figs. 6a and 6b is reported the resulting behaviour of polarization  $\Delta$  and magnetization  $m$ . We shall notice that:

- Overall polarization dependence on  $a$  is very little affected by switching on the interaction. The convergence speed of the  $a \gg t$  limit is hardly slowed by any of the sampled  $U$  values and only in the  $a \lesssim t$  regime we notice some steep jumps at certain values of  $U$ . The chain is ferroelectric (FE) for each nonzero value of  $a$ .
- Magnetization  $m$  appears to be strictly suppressed for the main portion of parameter-space, with a sharp peak emerging again in a very tight “large  $U$ ” and “small  $a$ ” region. The border of this magnetized phase region coincide exactly with the “jump-line” in the polarization defining it as the critical line marking the phase transition from a FE to an AFM+FE *multiferroic* phase.
- A finer sampling across a constant- $U$  line (fig. 7) reveals the transition to be of the 1<sup>st</sup> order, in the sense that the values of both the order parameters jump discontinuously at the critical point.<sup>6</sup>
- To carefully assure that the the transition is indeed of 1<sup>st</sup> order we have looked for finite-size effects (figs. 8a and 8b) and actually found that for very short chains the smoothing behaviour is indeed the one characterizing 1<sup>st</sup> order transitions.<sup>5</sup>

<sup>6</sup>Being it a *quantum phase transition* no temperature is involved, so that the usual formal classification in terms of *latent heat* is not appropriate here.



(a) Polarization



(b) Magnetization

Figure 6: Landscape behaviour of the two order parameters introduced in the variational ansatz (eq. 33).

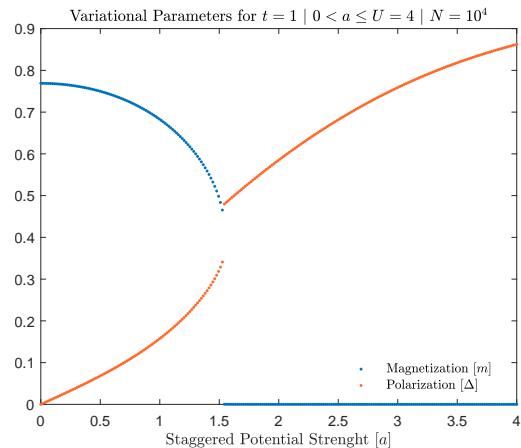
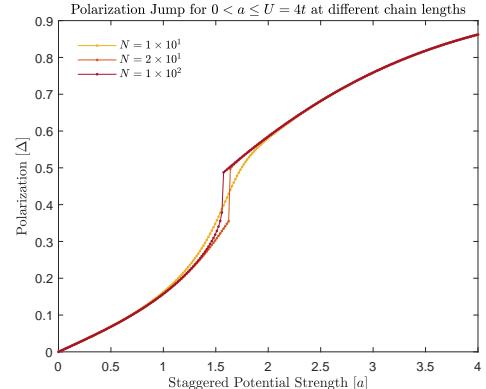
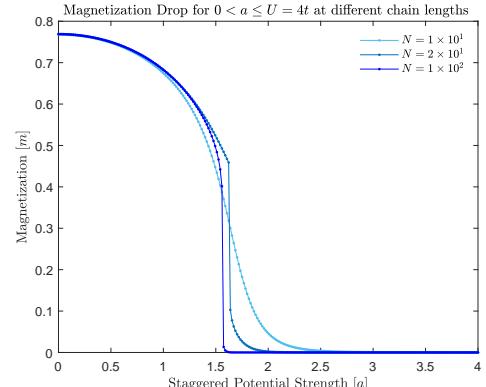


Figure 7: Behaviour of the two order parameters for fixed interaction strength and increasing staggered potential. A first order phase transition takes place at  $a \simeq 1.5t$ .



(a) Polarization



(b) Magnetization

Figure 8: Finite-size effects on the transition between the FE and the FE+AFM phases for a fixed value of the interaction:  $U = 4t$ . For lower values of  $U$  the transition is sharper until being discontinuous already for  $N \simeq 10$ . The opposite happens increasing  $U$ , so that the thermodynamic limit discontinuity is more and more difficult to achieve, until it becomes (for  $U > 10t$ ) quite difficult to actually classify the transition as first order. This might suggest that the critical line at some point ends in a critical point, where as usual the transition becomes of second order. Nevertheless for such large values of  $U$  the mean-field picture should not be taken as a reliable description of the system so that we shall not discuss any further the issue.

Finally we shall briefly discuss the *quantum* character of the phase transition. The basic tenet of quantum phase transitions (QPTs) theory is that at a critical point the relevant excitation gap of the system has to vanish in the thermodynamic limit<sup>6;7</sup>. This ensures the infamous result that at any arbitrary small but finite temperature the critical behaviour of the system can be studied within classical statistical mechanics:  $k_B T$  will be always greater than  $\hbar\omega_g$ , if  $\omega_g \rightarrow 0$ .

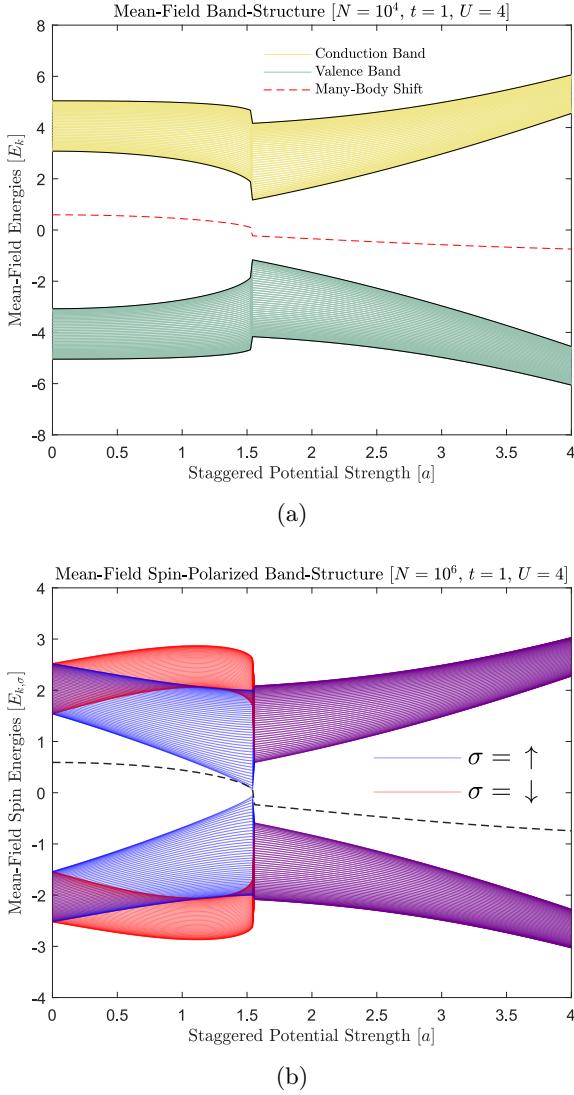


Figure 9: Mean-field bands at selfconsistency after (a) and before (b) summing over spin variable. For clarity purposes in both graphs only 200 lines per band are shown, despite  $N$  being much larger. See Listing 1 for details.

The result surely applies for the trivial  $a$ -driven phase transition that characterizes the noninteracting ground state: if one considers to extend the lower panel of fig. 2, to include negative values of  $a$  (which amounts to a mirror-symmetry, since the band-structure (eq. 13) depends only on  $a^2$ ), it readily follows that the  $a = 0$  point marks a second order quantum phase transition, separating two opposite-polarization ferroelectric phases. So there the closing of the band-gap identifies exactly the position of the critical point.

For the interacting case the same result is not so straightforward to show, for two main reasons: we are solving numerically the selfconsistent problem, so the thermodynamic limit can only be extrapolated; we have many different contributions to the energy per particle and interpretation can become knotty. In fact looking at fig. 9a one would argue that the mean-field gap never closes, even accounting for the many-body shift (eq. 35). But when one recognizes that the two spin-polarized bands are nondegenerate whenever there is AFM ordering (cf. eq. 39) is readily found that the gap indeed closes (fig. 9b), even if it happens for just one of the spin-polarizations.<sup>7</sup> The fact that the Hamiltonian does not contain any spin-flip terms is not relevant, for the two touching bands have same spin-polarization. Hence at the critical point the system has indeed a zero-energy excitation channel, satisfying the quantum phase transition condition. We shall notice that the separation of the two spin-bands is not an effect of the sole AFM ordering, but a combined product of both the magnetization and polarization of the chain: indeed at  $a = 0$  we have again spin-degeneration. The physical interpretation is straightforward: in fig. 9b we see that for  $0 < a < a_c$  the lowest energy levels correspond to  $\sigma = \downarrow$  states. The positive magnetization AFM ordering ensures the down-spins to be mainly located at odd sites and odd sites have enhanced population due to the positive polarization. Hence we expect those states to experience a larger overlap than the others (up-spins located mainly in even, depleted, states) and their energy consequently go down, exactly as we see in the computed band-structure.<sup>8</sup>

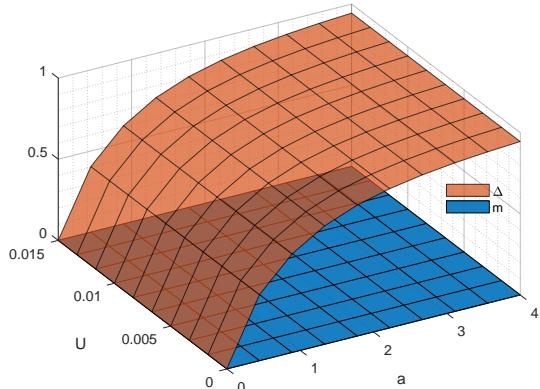
### 5.3 ASYMPTOTICS OF “small $U$ ” AND “small $a$ ” LIMITS

Here we will conclude our numerical analysis by addressing two interesting limits, namely:

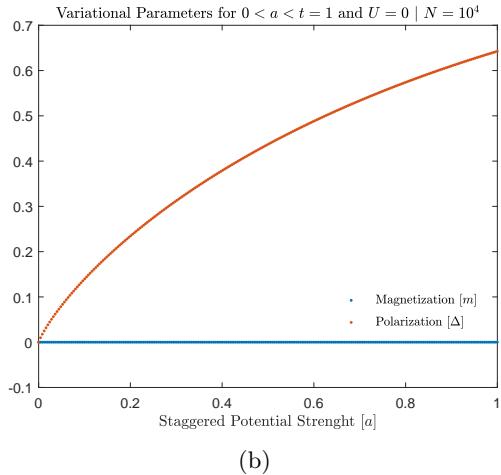
- $U \ll a \lesssim t$ , which tells us how the interacting model connects to the noninteracting ionic chain.
- $a \ll U \lesssim t$ , which in turn tells us how standard Hubbard theory is recovered and furthermore gives as the opportunity to inspect the phase transition in a safer weak-coupling regime, being  $U$  smaller than not only the noninteracting band-width but the hopping term itself. So that kinetic energy would surely dominate the energetics of the system, as it should be for any mean-field treatment.

<sup>7</sup>The other spin-family will close the gap at the opposite-sign value of the staggered potential  $a$ , since  $\mu$  and  $\delta$  will naturally exchange their roles and so will do the resulting mean-field bands.

<sup>8</sup>An analogue discussion applies for the negative  $a$  states, that interchange the roles of odd and even sites or even for reversed magnetization, that would just interchange up- and down- spin roles.



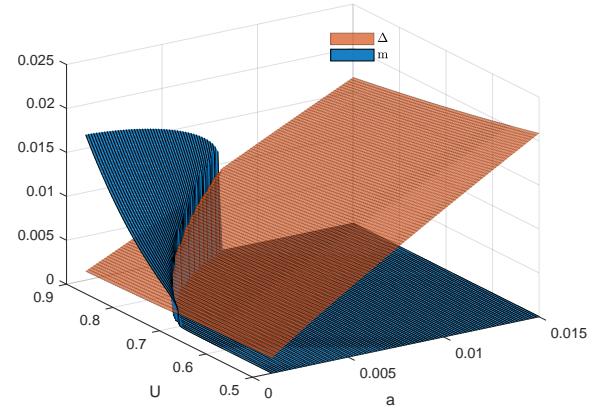
(a)



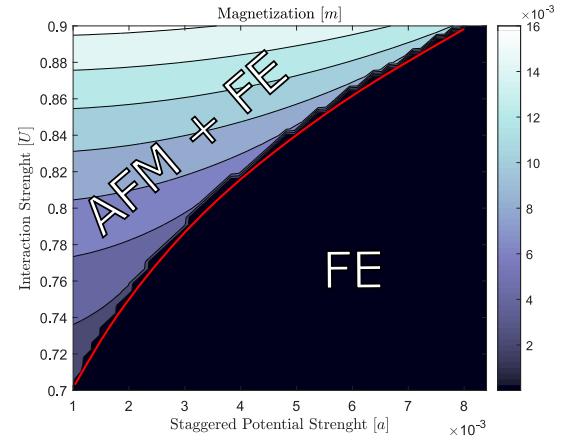
(b)

Figure 10: Behaviour of the two order parameters for (a) a coarse-grained small interaction landscape and (b) a fine mesh of the  $U = 0$  limit. We notice that the magnetization is totally absent.

So let's start with the small interaction case by inspecting the restricted landscape reported in fig. 10a. Is immediately evident that the physics is essentially that of the noninteracting ionic chain: the polarization saturates very quickly to its maximum value for increasing  $a$  values and the variation with the small  $U$  is totally negligible. This is not surprise since we already know that for most of the complete landscape there is no finite magnetization and in particular there is not for any  $U$  smaller than some relevant fraction of  $t$ . We can also verify that, as far as there is no finite magnetization, a second order quantum phase transition is driven by a change in sign of  $a$ . In particular in fig. 10b we see, in a finer mesh, how for the  $U = 0$  case the polarization reproduces exactly the typical behaviour of an order parameter characterizing a second order phase transition.



(a) Landscape behaviour of the two order parameters in the small staggering case.

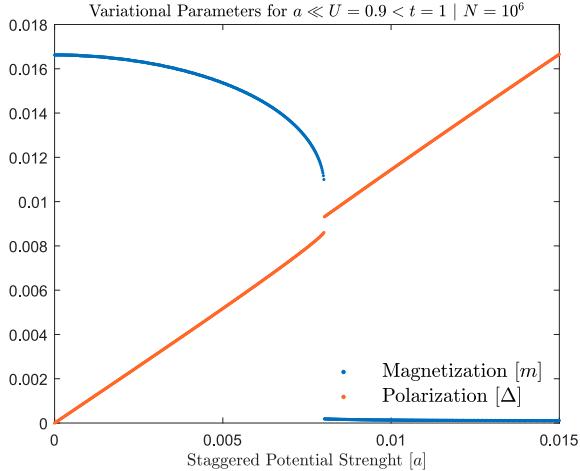


(b) Contour-plot of the magnetization profile shown in the panel above. The red line highlights the *critical curve* separating the ferroelectric (FE) and multiferroic (AFM+FE) phases in the  $aU$  plane.

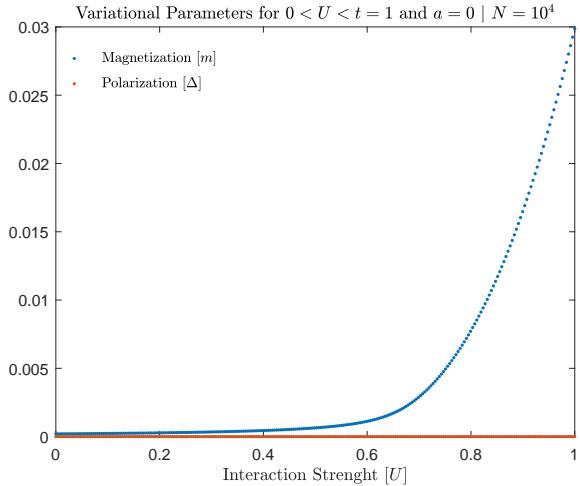
Figure 11

By the same token we inspect the small staggering landscape (fig. 11a) to find that the critical curve (put in evidence in fig. 11b) is thankfully comprised in our safer  $U$ -range, with just some slight modifications on how the order parameters behave around the transition. In particular the polarization increases linearly on  $a$ , with just a very small jump at the phase transition (cf. fig. 12a), while the magnetization profile appears unchanged.

Finally we reconnect to standard Hubbard theory by inspecting the dependence of magnetization on  $U \in [0, 1]$ , for  $a = 0$ . As reported in fig. 12b our calculation recovers the exponential behaviour found in literature.<sup>1</sup>



(a) Small staggering strength dependence of variational parameters for a fixed interaction strength value.



(b) Interaction strength dependence of variational parameters for the non ionic ( $a = 0$ ) Hubbard chain. Well-known exponential behaviour of magnetization is successfully predicted.

Figure 12

## 6 EXTENDING THE MODEL

Before concluding our analysis we will briefly discuss a relevant extension of the model, namely adding a staggered interaction term:

$$\hat{H}_{\text{u}'} := U' \sum_j j(-1)^j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}. \quad (48)$$

If  $|U'| < U$  and  $\text{sgn}(U') = \text{sgn}(a)$  this term can be interpreted as a *screening* effect due to the polarization of the chain. More explicitly we know that the staggered

potential term controlled by a positive  $a$  produces a charge accumulation on *odd-site* ions in the chain, so that, according to e.g. Thomas-Fermi theory<sup>8</sup>, we can expect that around that family of ions the screening of Coulomb static repulsion is increased proportionally to the square root of the charge density therein: the term in eq. (48) indeed adds  $U'$  to  $U$  on even lattice sites and subtracts on odd ones.

Before doing any calculation one could wonder if this term will just make the model more accurate on quantitative predictions or if it will actually disclose some brand new physics (a totally different shape of the phase space or even some new order parameter). Being the role of Hubbard interaction that of disfavouring double occupancy on a given site, we could argue that the role of  $U'$  is somewhat similar to that of the staggered potential, for it favours (by depleting  $U$ ) double occupancy on the same sites where  $a$  favours higher density (which, for a half-filled model, means favouring double occupancy again). Hence at first glance we will not explicitly look for new physics and proceed to analyze the problem according to our “old” ansatz, given in eq. (33).

Within mean-field theory we can partition again the summation in three terms:

$$\hat{H}_{\text{u}'} \simeq E_{\text{u}'} + \hat{H}_{\text{u}'}^{\downarrow} + \hat{H}_{\text{u}'}^{\uparrow}$$

$$\begin{aligned} E_{\text{u}'} &:= -U' \sum_j (-1)^j \langle \hat{n}_{j,\uparrow} \rangle \langle \hat{n}_{j,\downarrow} \rangle, \\ \hat{H}_{\text{u}'}^{\downarrow} &:= U' \sum_j (-1)^j \langle \hat{n}_{j,\uparrow} \rangle \hat{n}_{j,\downarrow}, \\ \hat{H}_{\text{u}'}^{\uparrow} &:= U' \sum_j (-1)^j \langle \hat{n}_{j,\downarrow} \rangle \hat{n}_{j,\uparrow}, \end{aligned}$$

where this time a crucial staggering factor  $(-1)^j$  is present.

For the first nonoperatorial term we have (cf. eq. 34)

$$\begin{aligned} E_{\text{u}'} &= -U' \sum_j \left[ \frac{(-1)^j}{4} - \frac{(-1)^{2j}\Delta}{2} + (-1)^j \frac{\Delta^2 - m^2}{4} \right] \\ &= \frac{U'}{2} \sum_j [\Delta] = \frac{NU'}{2} \Delta, \end{aligned} \quad (49)$$

namely an *interaction price* to polarize the system. So we expect a *kinetic gain* to polarize from the mean-field hamiltonians, in perfect analogy with the staggered potential role.

We have

$$\begin{aligned}\hat{H}_{\text{v}'}^{\sigma} &= \frac{U'}{2} \sum_j (-1)^j [1 - (-1)^j \diamond_{\sigma}] \hat{n}_{j,\sigma} \\ &= \frac{U'}{2} \sum_j (-1)^j \hat{n}_{j,\sigma} - \frac{U'}{2} \sum_j \diamond_{\sigma} \hat{n}_{j,\sigma}.\end{aligned}\quad (50)$$

Indeed the first term is formally identical to the staggered potential, so that we can define an effective staggering strength as

$$a' := a + \frac{U'}{2}.\quad (51)$$

The second term is instead proportional to the identity matrix in the Hilbert space, so that can be summed, at half-filling, to

$$-\sum_j \frac{U'}{2} \diamond_{\sigma} \hat{n}_{j,\sigma} = -\frac{NU'}{2} \diamond_{\sigma},\quad (52)$$

a many-body interaction term coupled with a *spin-dependent* variational parameter. Thus the chemical potentials of the two spin-polarized bands will be shifted by an amount proportional to the screening strength  $U'$ .

One might think this could in principle lead to new physics, namely a macroscopic magnetization of the chain should arise if the shift of the two chemical potentials is so large to make the valence band of one of the two spin-polarizations cross the conduction band of the other. This is not possible by construction of the ansatz: an inspection of eq. (33) easily reveals that the assumed form for the mean-field averages does not allow a net magnetic dipole in the unit-cell. Hence whatever selfconsistent solution of the problem will be so that the band edges do not cross.<sup>9</sup>

So the relevant matrix to diagonalize is again of the form

$$\begin{pmatrix} t_k & a + \frac{U'}{2} - U \diamond_{\sigma} \\ a + \frac{U'}{2} - U \diamond_{\sigma} & t_{k+Q} \end{pmatrix} =: \begin{pmatrix} t_k & a'_{\sigma} \\ a'_{\sigma} & -t_k \end{pmatrix},\quad (53)$$

with eigenvalues

$$\lambda_{k,\sigma} = \pm \sqrt{t_k^2 + (a'_{\sigma})^2}.\quad (54)$$

Putting together eqs. (52) and (54) we can thus write the mean-field energies as:

$$E_{k,\sigma} = -\frac{NU'}{2} \diamond_{\sigma} \pm \sqrt{t_k^2 + \left(a + \frac{U'}{2} - U \diamond_{\sigma}\right)^2}.\quad (55)$$

<sup>9</sup>It is actually possible to prove that for whatever value of the variational parameters within their range  $[-1, 1]$  the gaps do not actually cross. But we have chosen to not discuss the issue as it's not really necessary, for the variational ansatz cannot contradict itself.

The ground state to optimize is then (cf. previous notations)

$$\begin{aligned}E_{\text{GS}} &= \frac{NU'}{2} (\Delta - \mu - \delta) - \frac{NU}{2} \mu \delta - \sum_{\sigma} \sum_{\text{QBZ}} \lambda_{k,\sigma} \\ &= \frac{N}{2} \frac{U'}{U} (x + y - x - y) - \frac{N}{U} xy - \sum_{\sigma} \sum_{\text{QBZ}} \lambda_{k,\sigma} \\ &= -\frac{N}{U} xy - \sum_{\text{QBZ}} \left[ \sqrt{t_k^2 + (a' - x)^2} + \sqrt{t_k^2 + (a' - y)^2} \right],\end{aligned}$$

an expression formally identical to (45), provided the substitution  $a \mapsto a'$ . Hence the minimization on the variational space will lead to the very same selfconsistency conditions expressed in eq. (47): within the ansatz (33) the screening term  $U'$  has definitely the sole role of enhancing the staggered potential term  $a$ , since the only two terms exiting this picture (49, 52) cancel out exactly.

\* \* \*

At this point an interesting question may arise: our mean-field treatment somehow tried to open a channel for a macroscopic magnetization, but eventually failed due to an inherent impossibility for the unit-cell to be magnetized in the ansatz itself. This may suggest that such a channel could be actually favoured by the new interaction term, so that we will try to modify the ansatz to allow for this new order parameter. Thus we'll modify the equation for AFM ordering (30), inserting a nonstaggered additive term:

$$\langle \hat{n}_{j,\uparrow} \rangle - \langle \hat{n}_{j,\downarrow} \rangle = (-1)^j m + \mathcal{M}, \quad \text{with } \mathcal{M} \in [-1, 1].\quad (56)$$

Then, combining with the polarization condition, eq. (32), we obtain the “new” variational ansatz, namely

$$\begin{cases} \langle \hat{n}_{j,\uparrow} \rangle = \frac{1 + (-1)^{1+j} (\Delta - m) + \mathcal{M}}{2} \\ \langle \hat{n}_{j,\downarrow} \rangle = \frac{1 + (-1)^{1+j} (\Delta + m) - \mathcal{M}}{2} \end{cases}.\quad (57)$$

Let's notice before everything that this new ansatz does preserve the half-filling condition. Then we proceed at evaluating the effects of the new term  $\mathcal{M}$  on

- The product of mean-field averages:

$$\begin{aligned}\langle \hat{n}_{j,\uparrow} \rangle \langle \hat{n}_{j,\downarrow} \rangle &= \frac{1}{4} - \frac{(-1)^j \Delta}{2} - \frac{(-1)^j m \mathcal{M}}{2} + \frac{\Delta^2 - m^2}{4} \\ &= \frac{1}{4} - \frac{(-1)^j (\Delta + m \mathcal{M})}{2} + \frac{\Delta^2 - m^2}{4}\end{aligned}\quad (58)$$

The term of interest will vanish when summed on  $j$  to evaluate  $E_u$ , but will give a finite result when evaluated

on the “staggered sum” defining  $E_{U'}$ . So we’ll have to just substitute:

$$\frac{NU'}{2}\Delta \mapsto \frac{NU'}{2}(\Delta + m\mathcal{M}). \quad (59)$$

- The  $U$  mean-field diagonal terms:

$$\frac{NU}{2} \mapsto \frac{NU}{2}(1 \mp \mathcal{M}). \quad (60)$$

Being dependent on an order parameter this term cannot be neglected anymore, so contributing to the chemical potential shift between the two spin-bands (sign minus is for  $\sigma = \uparrow$  and sign plus for  $\sigma = \downarrow$ ).

- The  $U'$  mean-field effective staggered terms:

$$a' \mapsto a'_{\mathcal{M}} := a + \frac{U'}{2} \left( 1 \mp \frac{\mathcal{M}}{2} \right) \quad (61)$$

The new mean-field energies are then:

$$E_{k,\sigma} = \frac{U\mathcal{M}}{2}(\delta_{\sigma,\downarrow} - \delta_{\sigma,\uparrow}) - \frac{U'\diamondsuit_{\sigma}}{2} + \pm \sqrt{t_k^2 + a + \frac{U'}{2} \left[ 1 + \frac{\mathcal{M}}{2} (\delta_{\sigma,\downarrow} - \delta_{\sigma,\uparrow}) \right]^2}. \quad (62)$$

The ground state is now not straightforward to define, for the two spin-gaps are totally free to cross, so we don’t know before actually solving the problem how to order and fill the states. The approach might then be a brute-force-numerics one: we could in principle span the whole variational space  $(m, \Delta, \mathcal{M})$  with a fine grid covering the range  $[-1, 1] \times [-1, 1] \times [-1, 1]$ , and for each triplet of values compute all the eigenvalues (62). Then sorting them and start to fill the first lower  $N$ . The sum of these energies, plus the many-body contributes depending only on the variational triplet will then be the true ground state energy, sampled on the numerical grid. Fitting with a paraboloid near the numerical minimum of the sampled grid will then give a good estimate of the selfconsistent variational triplet. Of course such a numerical recipe will imply a huge workload, making the mean-field approach’s inherent simplicity just disappear in practice. A partial cure might be found implementing an advanced minimization routine, like Nelder-Mead’s *Amoeba Method*<sup>10</sup>, which once initialized with a starting triplet  $(m_0, \Delta_0, \mathcal{M}_0)$ , looks for the minimum with an iterative procedure requiring just evaluations of the optimization target (no derivatives!). The method is very reliable and stable, but might be still quite slow if the initial triplet is not wisely chosen. We will not attack the problem here.

<sup>10</sup>[https://en.wikipedia.org/wiki/Nelder-Mead\\_method](https://en.wikipedia.org/wiki/Nelder-Mead_method)

## REFERENCES

- [1] M. Fabrizio, *Lecture Notes on Many-Body Theory*, Cond. Mat. Th. PhD Program, SISSA
- [2] F. Lechermann, *Model Hamiltonians and Basic Techniques* in “The LDA+DMFT approach to strongly correlated materials”, Chapter 3, Forschungszentrum Jülich, 2011
- [3] R. Resta & D. Vanderbilt, *Theory of Polarization: A Modern Approach*. in “Physics of Ferroelectrics. Topics in Applied Physics”, Volume 105, Springer, 2007
- [4] V. Eyert, *A Comparative Study on Methods for Convergence Acceleration of Iterative Vector Sequences*, J. C. Phys. **124**, 271–285, 1996
- [5] K. Binder, *Finite Size Effects on Phase Transitions*, Ferroelectrics **73**:1, 43–67, 2011
- [6] M. Vojta, *Quantum Phase Transitions*, Rep. Prog. Phys. **66**, 2069, 2003
- [7] S. Sachdev, *Quantum Phase Transitions*, Cambridge University Press, 2011
- [8] N. W. Ashcroft & N. D. Mermin, *Solid State Physics*, Saunders College (1976)

## APPENDIX: MATLAB SCRIPTS

Listing 1: Main Script

```

1 % Imperturbed Band-Structure
2 t = 1;
3 ell = 1;
4 N = 10^6;
5 dk = 2*pi/N;
6 k = linspace(dk,pi/ell,N/2);
7 tk = -2*t*cos(k.*ell);
8 % Perturbative Physical Scales
9 U = < a List of Values >
10 a = < a List of Values >
11
12 % Cycle
13 D = zeros(length(U),length(a));
14 M = zeros(length(U),length(a));
15 Emb = zeros(length(U),length(a));
16 Ek = zeros(length(U),length(a),N/2);
17 Eku = zeros(length(U),length(a),N/2);
18 Ekd = zeros(length(U),length(a),N/2);
19 for i = 1:length(U)
20     for j = 1:length(a)
21         % INIT VALUES for mean-field parameters
22         Delta = rand;
23         Magn = rand;
24         x = U(i)*(Delta+Magn)/2;
25         y = U(i)*(Delta-Magn)/2;
26         % Looking for Self-Consistency
27         [X,Y] = selfconsistence(x,y,U(i),a(j),N,tk);
28         D(i,j) = (X+Y)/U(i);
29         M(i,j) = (X-Y)/U(i);
30         Emb(i,j) = -X*Y/U(i);
31         Eku(i,j,:) = sqrt(tk.^2 + (a(j)-X)^2);
32         Ekd(i,j,:) = sqrt(tk.^2 + (a(j)-Y)^2);
33         Ek(i,j,:)= Eku(i,j,:)+ Ekd(i,j,:);
34     end
35 end
36
37 figure("Name",'Whole Parameter Space')
38 surf(a,U,D); hold on
39 surf(a,U,M);
40 xlabel('a');
41 ylabel('U');
42
43 figure("Name",sprintf('Mean-Field Parameters Vs U [a fixed to %f]',a(10)));
44 plot(U,D(:,10),'Color',[0.8500, 0.3250, 0.0980],'MarkerSize',6); hold on
45 plot(U,M(:,10),'Color',[0, 0.4470, 0.7410], 'MarkerSize',6);
46
47 figure("Name",sprintf('Mean-Field Parameters Vs a [U fixed to %f]',U(1)));
48 plot(a,D(1,:),'Color',[0.8500, 0.3250, 0.0980], 'MarkerSize',6); hold on
49 plot(a,M(1,:),'Color',[0, 0.4470, 0.7410]);
50
51 figure("Name",'Mean-Field Single Particle Energies')
52 for ik = 1:ceil(N/200):N/2
53     plot(a,-Ek(1:length(U),1:length(a),ik),'Color',[155/255, 194/255, 177/255]); hold on
54     plot(a,Emb(1:length(U),1:length(a)), '--r')
55 end
56
57 figure("Name",'Mean-Field Single Particle Energies [spin-polarized]')
58 for ik = 1:ceil(N/200):N/2
59     plot(a,-Ekd(1:length(U),1:length(a),ik),'Color',[1 0 0 0.3]); hold on
60     plot(a,-Eku(1:length(U),1:length(a),ik),'Color',[0 0 1 0.3]);
61 end

```

Listing 2: Iterative Routine for Self-Consistency

```

1 %% SELF CONSISTENCY ROUTINE %%
2 function [x,y] = selfconsistence(x,y,U,a,N,tk)
3
4 % Self-Consistency definition parameters
5 SELFx = 0.00001;
6 SELFy = 0.00001;
7
8 % Mixing Parameter -> Tunable Speed (vs Stability!)
9 SELFmix = 0.9;
10 PRODmix = 1-SELFmix;
11
12 stepCOUNTER = 0;
13 exitFLAG = false;
14 while exitFLAG ~= true
15
16     % Computing new parameters
17     X = U/N*sum((a-y)./sqrt(tk.^2 + (a-y).^2));
18     Y = U/N*sum((a-x)./sqrt(tk.^2 + (a-x).^2));
19
20     % Computing relative distances from self-consistency
21     Dx = abs(x-X); dx = norm(Dx/x);
22     Dy = abs(y-Y); dy = norm(Dy/y);
23
24     % ~Comparison and Move~
25     if (dx < SELFx && dy < SELFy) || stepCOUNTER > 10*N
26         exitFLAG = true;
27     else
28         x = SELFmix * x + PRODmix * X;
29         y = SELFmix * y + PRODmix * Y;
30         clc
31         fprintf('nUPDATE of MEAN-FIELD Parameters!\n');
32         fprintf('*****\n');
33         fprintf('Delta = %f\n', x+y/U);
34         fprintf('Magn = %f\n', x-y/U);
35     end
36     stepCOUNTER = stepCOUNTER + 1;
37 end
38
39 % Returned Values
40 Delta = (x+y)/U;
41 Magn = (x-y)/U;
42
43 % Final Output
44 fprintf('*****\n');
45 fprintf('nConvergence achieved in %d steps\n', stepCOUNTER);
46 fprintf('*****\n');
47 fprintf('Accuracy on Delta+Magn: %f\n', dx);
48 fprintf('Accuracy on Delta-Magn: %f\n', dy);
49 fprintf('*****\n');
50 fprintf('*****\n');
51
52 end

```