

Hubbard Model in Mean Field Theory

Tyler C. Sterling

Department of Physics, University of Colorado Boulder, Boulder CO, 80309, USA

August 23, 2024

1 Introduction

Removing the chemical potential term from the Hamiltonian for now and calculating free energy later in grand canonical ensemble

The prototypical model for strong correlation in transition-metal oxide systems is the Hubbard model. The Hubbard model Hamiltonian is

$$\hat{H}_e = - \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} + U \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow} \quad (1)$$

In anticipation of adding in electron-phonon coupling below, we use the subscript e on \hat{H}_e to denote this as the electronic sector of a coupled electron-phonon system. The symbols i and α label the unitcells and basis-positions of the atoms¹. For example, $\hat{c}_{i\alpha\sigma}^\dagger$ and $\hat{c}_{i\alpha\sigma}$ create and annihilate electrons with spin σ on atom α in the i^{th} cell respectively. An arbitrary lattice vectors is $x_i = an_i$ with lattice parameter a and n_i an integer. The position of the basis atom is τ_α , the same in every unitcell. The generalization to higher dimensions is obvious. $t_{ij}^{\alpha\beta}$ is the “hopping” parameter; it is the amplitude for an electron to tunnel from the β^{th} atom in the j^{th} cell to the α^{th} atom in the i^{th} cell. $\hat{n}_{i\alpha\sigma} = \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{i\alpha\sigma}$ is the electron spin density operator; $\hat{n}_{i\alpha} = \hat{n}_{i\alpha\uparrow} + \hat{n}_{i\alpha\downarrow}$ is the electronic particle density. μ is the chemical potential, included to allow varying particle number [1, 2]. We assume that the on-site energies are the same for all sites, absorbing contribution to the energy into the chemical potential. The $\sim U$ term is the Hubbard interaction; we symbolize it by \hat{H}_U . The Hubbard interaction is valid for very localized electrons; it is a good approximation for the Cu-d electrons in cuprates (e.g. La_2CuO_4 , $\text{HgBa}_2\text{CuO}_4$), the Ni-d electrons in nickelates (e.g. La_2NiO_4), etc. The Hubbard Hamiltonian has been widely studied blah blah blah ...

¹ Usually a “single-site” model is studied and a single symbol is used to label the atom; however, we want to study charge and spin density wave ordering which, by necessity, requires multiple sites in the unitcell. We could leave the basis index implicit inside a single symbol, but it will be convenient later to distinguish the basis position from the unitcell.

Probably the most popular generalization of the Hubbard model that includes electron-phonon coupling is the Hubbard-Holstein model; it includes on-site coupling of the localized electrons to Einstein phonons. The Hubbard-Holstein Hamiltonian is

$$\begin{aligned}\hat{H} &= \hat{H}_e + \hat{H}_{ph} + \hat{H}_{eph} \\ \hat{H}_{ph} &= \omega_0 \sum_{i\alpha} \left(\hat{a}_{i\alpha}^\dagger \hat{a}_{i\alpha} + \frac{1}{2} \right) \\ \hat{H}_{eph}^H &= g \sum_{i\alpha\sigma} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{i\alpha\sigma} \left(\hat{a}_{i\alpha} + \hat{a}_{i\alpha}^\dagger \right)\end{aligned}\tag{2}$$

\hat{H}_e is the same as in eq. 1. \hat{H}_{ph} is the phonon Hamiltonian; $\hat{a}_{i\alpha}^\dagger$ and $\hat{a}_{i\alpha}$ create and annihilate optical phonons. Also define $\hat{m}_{i\alpha} \equiv \hat{a}_i^\dagger \hat{a}_i$ for the phonon number operator for later convenience. The last line is the electron-phonon interaction with g the coupling constant. The operator $\hat{X}_{i\alpha} \equiv \left(\hat{a}_{i\alpha} + \hat{a}_{i\alpha}^\dagger \right)$ is the phonon displacement.

Each phonon is a dispersionless optical mode that is localized to a single-site; this is a realistic approximation for e.g. zone-boundary full- and half-breathing phonons in layered perovskites like cuprates (La_2CuO_4 , $\text{HgBa}_2\text{CuO}_4$, etc.), nickelates (La_2NiO_4), and others. (We relax the assumption that the phonon is dispersionless later; formally this can be achieved by coupling neighboring Einstein oscillators², but I am lazy and just shoe-horn it in later.) The Hubbard-Holstein model has been studied blah blah blah ... list the short-comings, i.e. ways it fails to describe experiment.

In one of our papers [4], we used mean-field DFT+U calculations to show that the density fluctuations in La_2CuO_4 (LCO) depend strongly on the phonon amplitude; similarly, the phonon energy depends strongly on the magnitude of the U parameter. This could be a conventional electron-phonon coupling effect where the localized charge becomes “rigid”. The phonon that couples to the d orbitals hardens as it becomes more energetically unfavorable to pump charge onto/off the Cu atoms. Indeed, with the U parameter tuned to reproduce the magnetic moments and gap in LCO, the zone-boundary phonon energies are in excellent agreement with experiment, whereas in plain DFT (i.e. $U=0$) they are quite wrong (the electronic structure is non-magnetic/metallic with $U=0$ and the phonon energy is too soft).

Still, there are aspects of the ground state in LCO (and all other cuprates) that are not predicted by DFT+U: about half way to the zone-boundary, there is anomalous renormalization and broadening of the phonon energy that is completely absent in DFT and DFT+U calculations. The anomalous phonon dispersion has been attributed to coupling to dynamical charge and spin density ordering and indeed the momentum dependence of the anomalous dispersion is consistent this explanation. However, (to my knowledge) there has been no microscopic description of the phenomenon. It could be the case that the absence of dynamical charge and spin ordering in mean field calculations explains the absence of the anomalous phonon dispersion in the same. Maybe if the dynamical electronic ordering were correctly described by beyond-mean-field methods e.g. many body solutions of the Hubbard-Holstein model (eq. 2), then the anomalous phonon dispersion would appear there too. Unfortunately, I don’t think solutions of the Hubbard-Holstein model have predicted the correct dynamical charge and spin order or the anomalous renormalization of the phonons.

² For a wildly novel derivation, see ref. [3].

The situation is worse in La_2NiO_4 (LNO)! In analogy to the cuprates, there is dynamical charge and spin ordering, strong electron-phonon coupling, etc. but with doping, cuprates becomes superconducting and then metallic. LNO remains insulating even into the strongly over-doped regime! The electronic phase diagram has yet to be explained. Similarly, the relevant phonon branches are so strongly renormalized in LNO that they no longer appear as sharp quasiparticle peaks in inelastic neutron scattering measurements. In the absence of a Fermi surface (i.e. Fermi surface nesting) [5], I can think of no explanation for this phenomenon.

Based on these observations, and with the hope of describing unexplained (or even new) physics in cuprates, nickelates, etc. I propose an alternative model where the U parameter depends on phonon displacement $\hat{X}_{i\alpha}$. This is physically sensible because the optical phonons in layered perovskites strongly modulate the volume of the transition-metal/oxygen octahedra, compressing the density on the atoms where the U parameter is most important. When the volume gets smaller (larger) the U parameter should increase (decrease). Explicitly, the Hamiltonian I propose is

$$\begin{aligned}\hat{H} &= \hat{H}_e^{(0)} + \hat{H}_{ph} + \hat{H}_{eph} \\ \hat{H}_e^{(0)} &= - \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} \\ \hat{H}_{ph} &= \omega_0 \sum_{i\alpha} \left(\hat{a}_{i\alpha}^\dagger \hat{a}_{i\alpha} + \frac{1}{2} \right) \\ \hat{H}_{int} &= \sum_{i\alpha} U(\hat{X}_{i\alpha}) \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow}\end{aligned}\tag{3}$$

with $U(\hat{X}_{i\alpha}) = U_0[1 + g\hat{X}_{i\alpha}]$ an effective, environment dependent electron-electron interaction. The new notation, \hat{H}_{int} , is to symbolize that both electron-electron and electron-phonon interactions are contained in this term. Indeed,

$$\hat{H}_{int} = U_0 \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow} + gU_0 \sum_{i\alpha} \hat{X}_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow}\tag{4}$$

contains the usual Hubbard interaction, \hat{H}_U , plus the electron-phonon interaction, \hat{H}_{eph} . $\hat{H}_e^{(0)}$ is the free electron Hamiltonian; $\hat{H}_e = \hat{H}_e^{(0)} + \hat{H}_U$. All other symbols have the same meanings as above. The electron-phonon interaction in eq. 3 directly couples the *spin* densities, a feature that is absent in many models. Considering the non-trivial spin and charge ordering in layered perovskites, this coupling may lead to interesting physics!

The Hamiltonian in eq. 3 is reminiscent of the Su-Schrieffer-Heeger (SSH) model where the hopping $t \rightarrow t(\hat{X})$ depends on the phonon coordinates [6–11]. Recent quantum Monte Carlo (QMC) calculations of the SSH model in 2D [10, 11] have shown that the electron-phonon coupling drives the electronic system into either resonating valence-bond or antiferromagnetic ordered (in the absence of explicit exchange coupling!) ground states depending on the phonon energy scale and size of the coupling. The electron-phonon coupling proposed in eq. 4 is qualitatively different than phonon-dependent hopping, but hopefully can lead to new physics in analogy with refs. [10, 11]. Specifically, if the electron-electron interactions alone can't lead to the correct spin and charge ordering, maybe a novel electron-phonon interaction can!

2 Justification for Environment-dependent U

The usual argument for the Hubbard-U interaction starts with the assumption that the on-site potential for the localized electrons is atomic like; i.e. the electrons are so localized that they are agnostic about their environment. This assumption goes against the concept of an environment-dependent U parameter. However, experience (e.g. thousands of DFT+U calculations) has shown that the U value depends crucially on the environment; e.g. the “correct” U value for the Ni-d orbitals in NiO₂ is not the same as in La₂NiO₄. The U value *is* environment dependent. Whether or not this can be extended to depend dynamically on the phonon coordinates needs more work. Regardless, eq. 3 is probably a novel enough model to merit study (and publication!) regardless of the validity of environment dependent U.

3 Mean-Field Analysis

See ref. [12] for self-consistent mean-field theory. Also see refs. [1, 13–18]

A simple (approximate) way to solve this model is using mean-field theory (MFT). To do this, we separate the spin density into its *mean* value on each site, $n_{i\alpha\sigma}$, and its fluctuations around the mean value, $\delta\hat{n}_{i\alpha\sigma}$. The density is $\hat{n}_{i\alpha\sigma} = n_{i\alpha\sigma} + \delta\hat{n}_{i\alpha\sigma}$. In MFT, the density-density interaction in eqs. 2 and 3 become

$$\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} = n_{i\alpha\uparrow}n_{i\alpha\downarrow} + \delta\hat{n}_{i\alpha\uparrow}n_{i\alpha\downarrow} + \delta\hat{n}_{i\alpha\downarrow}n_{i\alpha\uparrow} + \delta\hat{n}_{i\alpha\uparrow}\delta\hat{n}_{i\alpha\downarrow}$$

This expression is exact; however, the last term is still quadratic in Fermion operators, rendering the model intractable. To make progress, we make the approximation that the fluctuations $\delta\hat{n}_{i\alpha\sigma}$ are small and drop the last term. Now notice that (somewhat tautologically...) $\delta\hat{n}_{i\alpha\sigma} = \hat{n}_{i\alpha\sigma} - n_{i\alpha\sigma}$. Then

$$\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} \approx \hat{n}_{i\alpha\uparrow}n_{i\alpha\downarrow} + \hat{n}_{i\alpha\downarrow}n_{i\alpha\uparrow} - n_{i\alpha\uparrow}n_{i\alpha\downarrow}$$

If we have an accurate model for the mean-field density, e.g. from DFT+U calculations, this might be a good approximation. Still, MFT totally neglects the effects of fluctuations (by coupling the fields only to the average density) and apparently breaks $SU(2)$ symmetry [19].

We can simplify things a little further by assuming that our system is homogeneous; i.e. $n_{i\alpha\sigma} \equiv n_{\alpha\sigma}$ doesn't depend on the unitcell index [13]. Then the Hubbard interaction in MFT is

$$\hat{H}_U = U_0 \sum_{i\alpha} (\hat{n}_{i\alpha\uparrow}n_{\alpha\downarrow} + \hat{n}_{i\alpha\downarrow}n_{\alpha\uparrow}) - U_0 N \sum_{\alpha} n_{\alpha\uparrow}n_{\alpha\downarrow}$$

The last term is a constant, but we have keep track of it since it affects the total energy; i.e. it plays a part in the phase stability. N is the number of unitcells in the crystal; in practice, it is equal to the number of k -points used to integrate the energy.

This is enough to study the electronic sector neglecting electron-phonon coupling or even to solve the Hubbard-Holstein model. Neglecting electron-phonon coupling, the Hubbard

model decouples into

$$\begin{aligned}
\hat{H} &= \hat{H}_\uparrow + \hat{H}_\downarrow + E_U \\
\hat{H}_\uparrow &= - \sum_{ij\alpha\beta} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\uparrow}^\dagger \hat{c}_{j\beta\uparrow} + U_0 \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} n_{\alpha\downarrow} \\
\hat{H}_\downarrow &= - \sum_{ij\alpha\beta} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\downarrow}^\dagger \hat{c}_{j\beta\downarrow} + U_0 \sum_{i\alpha} \hat{n}_{i\alpha\downarrow} n_{\alpha\uparrow} \\
E_U &= -U_0 N \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow}
\end{aligned} \tag{5}$$

Eq. 5 has to be solved self-consistently: given a suitable initial guess for $n_{\alpha\sigma}$, each spin-sector must be diagonalized and the average density recalculated. The resulting density is used to construct a new average density as input for eq. 5 and the equations are solved again; when the input and output densities are identical, the model is solved. Including coupling to a Holstein phonon, e.g. eq. 2, means the electronic sector can no longer be straightforwardly diagonalized. Still, the electronic action for eq. 5 is quadratic and the system can be studied using the standard methods of many-body theory, see below.

In the Hubbard-UX model, e.q. 3, the mean-field expression for the electron-phonon part of the Hamiltonian is

$$\begin{aligned}
\hat{H}_{eph} &= gU_0 \sum_{i\alpha} (\hat{n}_{i\alpha\uparrow} n_{\alpha\downarrow} + \hat{n}_{i\alpha\downarrow} n_{\alpha\uparrow}) \hat{X}_{i\alpha} - gU_0 \sum_{i\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} \hat{X}_{i\alpha} = \\
&gU_0 \sum_{i\alpha} (\hat{n}_{i\alpha\uparrow} n_{\alpha\downarrow} + \hat{n}_{i\alpha\downarrow} n_{\alpha\uparrow} - n_{\alpha\uparrow} n_{\alpha\downarrow}) \hat{X}_{i\alpha}
\end{aligned}$$

The first term couples the phonons directly to the Fermion fields, while the second couples the phonons only to the average spin-densities. The phonon sector of eqs. 2 and 3 is quadratic and can already be solved: \hat{H}_{ph} is unchanged in MFT.

3.1 Mean-Field Theory in Momentum Space

We now Fourier transform eq. 5 [13]. We define the Fourier transform of the operators $\hat{c}_{i\alpha\sigma}$ as

$$\begin{aligned}
\hat{c}_{k\alpha\sigma} &= N^{-1/2} \sum_i \exp(-ik(x_i + \tau_\alpha)) \hat{c}_{i\alpha\sigma} \\
\hat{c}_{k\alpha\sigma}^\dagger &= N^{-1/2} \sum_i \exp(ik(x_i + \tau_\alpha)) \hat{c}_{i\alpha\sigma}^\dagger
\end{aligned} \tag{6}$$

The inverse Fourier transforms can easily be deduced from eq. 6. With the momentum space spin density operator

$$\hat{n}_{i\alpha\sigma} = \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{i\alpha\sigma} = N^{-1} \sum_{kp} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{p\alpha\sigma} \exp(i(k-p)x_i) \exp(i(k-p)\tau_\alpha)$$

the chemical potential term is

$$\begin{aligned}
\mu \sum_{i\alpha} \hat{n}_{i\alpha\sigma} &= \frac{\mu}{N} \sum_{\alpha} \sum_{kp} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{p\alpha\sigma} \exp(i(k-p)\tau_\alpha) \sum_i \exp(i(k-p)x_i) = \\
&\frac{\mu}{N} \sum_{\alpha} \sum_{kp} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{p\alpha\sigma} \exp(i(k-p)\tau_\alpha) \delta_{kp} = \mu \sum_{\alpha} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{k\alpha\sigma}
\end{aligned}$$

The hopping term is

$$\hat{H}_{\sigma,t} = - \sum_{ij\alpha\beta} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} = -N^{-1} \sum_{\alpha\beta} \sum_{kp} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{p\beta\sigma} \exp(ik\tau_\alpha - ip\tau_\beta) \sum_{ij} t_{ij}^{\alpha\beta} \exp(ikx_i - ipx_j)$$

Using translational invariance and periodicity of the lattice,

$$\begin{aligned} \sum_{ij} t_{ij}^{\alpha\beta} \exp(ikx_i - ipx_j) &= \sum_R t_R^{\alpha\beta} \exp(ikR) \sum_j \exp(i(k-p)x_j) = \\ &= N \delta_{kp} \sum_R t_R^{\alpha\beta} \exp(ikR) \end{aligned}$$

with R a lattice vector; in general, the sum runs over all lattice vectors. However, we usually restrict the hopping to nearest-neighbors only and assume it to be the same for all atom types. Anyway, the hopping part of the Hamiltonian becomes³

$$\begin{aligned} \hat{H}_{\sigma,t} &= \sum_k \sum_{\alpha\beta} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{k\beta\sigma} \gamma_k^{\alpha\beta} \\ \gamma_k^{\alpha\beta} &= - \exp(ik(\tau_\alpha - \tau_\beta)) \sum_R t_R^{\alpha\beta} \exp(ikR) \end{aligned}$$

Similarly, the density-density terms become

$$\begin{aligned} \sum_{i\alpha} \hat{n}_{i\alpha\sigma} n_{\alpha(-\sigma)} &= N^{-1} \sum_{kp} \sum_{\alpha} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{p\alpha\sigma} n_{\alpha(-\sigma)} \exp(i(k-p)\tau_\alpha) \sum_i \exp(i(k-p)x_i) = \\ &= \sum_k \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{k\alpha\sigma} n_{\alpha(-\sigma)}. \end{aligned}$$

Then, for each spin-sector, we have

$$\begin{aligned} \hat{H}_\sigma &= \sum_k \sum_{\alpha\beta} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{k\beta\sigma} \left[\gamma_k^{\alpha\beta} + \delta_{\alpha\beta} U_0 n_{\alpha(-\sigma)} \right] \equiv \sum_k \hat{H}_{k\sigma} \\ \hat{H}_{k\sigma} &= \sum_{\alpha\beta} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{k\beta\sigma} h_{k\sigma}^{\alpha\beta} \\ h_{k\sigma}^{\alpha\beta} &= \gamma_k^{\alpha\beta} + \delta_{\alpha\beta} U_0 n_{\alpha(-\sigma)}. \end{aligned}$$

The Hamiltonian decouples into independent sub-spaces, called Bloch Hamiltonians $\hat{H}_{k\sigma}$, at each k -point. Moreover, it is quadratic and can be solved by diagonalization.

3.2 Solving by Diagonalization

Let us introduce the “vectors”

$$\begin{aligned} \hat{\Psi}_{k\sigma}^\dagger &= (\hat{c}_{k1\sigma}^\dagger, \hat{c}_{k2\sigma}^\dagger, \dots, \hat{c}_{kN\sigma}^\dagger) \\ \hat{\Psi}_{k\sigma} &= (\hat{c}_{k1\sigma}, \hat{c}_{k2\sigma}, \dots, \hat{c}_{kN\sigma})^T \end{aligned}$$

³ In general, the phase $\exp(ik(\tau_\alpha - \tau_\beta))$ is unobservable and can be removed by a unitary transformation. It won't matter in what follows if we keep it or not.

Then

$$\hat{H}_{k\sigma} = \hat{\Psi}_{k\sigma}^\dagger \hat{h}_{k\sigma} \hat{\Psi}_{k\sigma} = \begin{pmatrix} \hat{c}_{k1\sigma}^\dagger & \hat{c}_{k2\sigma}^\dagger & \cdots & \hat{c}_{kN\sigma}^\dagger \end{pmatrix} \begin{pmatrix} h_{k\sigma}^{11} & h_{k\sigma}^{12} & \cdots & h_{k\sigma}^{1N} \\ h_{k\sigma}^{21} & h_{k\sigma}^{22} & \cdots & h_{k\sigma}^{2N} \\ \vdots & \vdots & \ddots & \vdots \\ h_{k\sigma}^{N1} & h_{k\sigma}^{N2} & \cdots & h_{k\sigma}^{NN} \end{pmatrix} \begin{pmatrix} \hat{c}_{k1\sigma} \\ \hat{c}_{k2\sigma} \\ \vdots \\ \hat{c}_{kN\sigma} \end{pmatrix}$$

We proceed by diagonalizing $\hat{h}_{k\sigma}$ by unitary transformation. Let $\hat{U}_{k\sigma}$ be the unitary matrix that diagonalizes $\hat{h}_{k\sigma}$. Call $\hat{U}_{k\sigma}^\dagger \hat{h}_{k\sigma} \hat{U}_{k\sigma} \equiv \hat{D}_{k\sigma}$ the diagonal representation of $\hat{h}_{k\sigma}$. Then

$$\hat{H}_{k\sigma} = \hat{\Psi}_{k\sigma}^\dagger \hat{h}_{k\sigma} \hat{\Psi}_{k\sigma} = \hat{\Psi}_{k\sigma}^\dagger \hat{U}_{k\sigma} \hat{U}_{k\sigma}^\dagger \hat{h}_{k\sigma} \hat{U}_{k\sigma} \hat{U}_{k\sigma}^\dagger \hat{\Psi}_{k\sigma} = \hat{\Phi}_{k\sigma}^\dagger \hat{D}_{k\sigma} \hat{\Phi}_{k\sigma}$$

The new vectors are

$$\begin{aligned} \hat{\Phi}_{k\sigma}^\dagger &= \hat{\Psi}_{k\sigma}^\dagger \hat{U}_{k\sigma} = \left(\hat{d}_{k1\sigma}^\dagger, \hat{d}_{k2\sigma}^\dagger, \dots, \hat{d}_{kN\sigma}^\dagger \right) \\ \hat{d}_{k\alpha\sigma}^\dagger &= \sum_{\beta} \hat{c}_{k\beta\sigma}^\dagger U_{k\sigma}^{\beta\alpha} \\ \hat{\Phi}_{k\sigma} &= \hat{U}_{k\sigma}^\dagger \hat{\Psi}_{k\sigma} = \left(\hat{d}_{k1\sigma}, \hat{d}_{k2\sigma}, \dots, \hat{d}_{kN\sigma} \right)^T \\ \hat{d}_{k\alpha\sigma} &= \sum_{\beta} \hat{c}_{k\beta\sigma} [\hat{U}_{k\sigma}^\dagger]^{\alpha\beta} \end{aligned}$$

Let the diagonal elements of $\hat{D}_{k\sigma}$ be called $\hat{D}_{k\sigma} \equiv \epsilon_{kn\sigma}$ with n a “band” index; $\epsilon_{kn\sigma}$ are the band energies and μ is the chemical potential from before. Explicitly, they are given by

$$\begin{aligned} \xi_{kn\sigma} &= [\hat{D}_{k\sigma}]^n = \delta_{nm} [\hat{U}_{k\sigma}^\dagger \hat{h}_{k\sigma} \hat{U}_{k\sigma}]^{nm} = \sum_{\mu\nu} [\hat{U}_{k\sigma}^\dagger]^{n\mu} h_{k\sigma}^{\mu\nu} U_{k\sigma}^{\nu m} = \\ &= \sum_{\mu\nu} \bar{U}_{k\sigma}^{\mu n} U_{k\sigma}^{\nu n} h_{k\sigma}^{\mu\nu} \end{aligned} \quad (7)$$

Then

$$\hat{H}_{k\sigma} = \hat{\Phi}_{k\sigma}^\dagger \hat{D}_{k\sigma} \hat{\Phi}_{k\sigma} = \sum_n \hat{d}_{kn\sigma}^\dagger \hat{d}_{kn\sigma} \epsilon_{kn\sigma} = \sum_n \hat{n}_{kn\sigma}^{(d)} \epsilon_{kn\sigma}$$

where $\hat{n}_{kn\sigma}^{(d)} = \hat{d}_{kn\sigma}^\dagger \hat{d}_{kn\sigma}$ is the number operator in the basis of eigenstates of the Bloch Hamiltonian. We have solved the mean-field model! E.g. Taking the expectation value of this with respect to the groundstate determines the (band-structure) energy:

$$E_{bs} = \langle \hat{H} \rangle = \sum_{k\sigma} \langle \hat{H}_{k\sigma} \rangle = \sum_{kn\sigma} \epsilon_{kn\sigma} \langle \hat{n}_{kn\sigma}^{(d)} \rangle = \sum_{kn\sigma} n_{kn\sigma}^{(d)} \epsilon_{kn\sigma}$$

The symbol $\langle \cdot \rangle \equiv \langle \Omega | \cdot | \Omega \rangle$ means expectation value with respect to the thermal ground state. $n_{kn\sigma}^{(d)}$ is the “occupation” of the state with quantum numbers k, n, σ . For Fermions, it is the Fermi-Dirac function: $n_{kn\sigma}^{(d)} \equiv f(\xi_{kn\sigma})$ with $\xi_{kn\sigma} = \epsilon_{kn\sigma} - \mu$. The *total* electronic groundstate energy is

$$E_{tot} = E_{bs} + E_U.$$

3.3 Self-consistency

In the last section, we learned how to solve the Hamiltonian (e.g. by diagonalizing on a computer), but we still haven't really solved the model. The issue is in the mean field densities $n_{\alpha\sigma}$: an arbitrary configuration is unlikely to be physically relevant. To pick $n_{\alpha\sigma}$ that are physically meaningful, we need to apply the variational principle: namely, the energy, or at finite temperature, the *free* energy, should be minimized with respect to the site occupations $\{n_{\alpha\sigma}\}$.

We will work at finite temperature. The $T = 0$ groundstate properties can be obtained by replacing $T \rightarrow 0$ at the end of what follows. The partition function is

$$Z(T) = \int \mathcal{D}(\bar{d}, d) \exp(-S[\bar{d}, d])$$

with Euclidean action

$$S[\bar{d}, d] = \int_0^\beta d\tau \left[\sum_{kn\sigma} \bar{d}_{kn\sigma}(\tau) \partial_\tau d_{kn\sigma}(\tau) + H_{gc}(\bar{d}, d) \right] = \\ \sum_{kn\sigma} \int_0^\beta d\tau \bar{d}_{kn\sigma}(\tau) [\partial_\tau + (\epsilon_{kn\sigma} - \mu)] d_{kn\sigma}(\tau) - \beta U_0 N \sum_\alpha n_{\alpha\uparrow} n_{\alpha\downarrow}$$

The second term, which corresponds to the constant E_U term in eq. 5, is independent of the fields (\bar{d}, d) and τ and was integrated out without other consideration. Then

$$Z(T) = \exp \left(\beta U_0 N \sum_\alpha n_{\alpha\uparrow} n_{\alpha\downarrow} \right) \int \mathcal{D}(\bar{d}, d) \exp(-S[\bar{d}, d])$$

where we have redefined

$$S[\bar{d}, d] \equiv \sum_{kmn\sigma} \bar{d}_{kn\sigma}(i\omega_m) [-i\omega_m + \xi_{kn\sigma}] d_{kn\sigma}(i\omega_m).$$

ω_m are the Fermionic Matsubara frequencies (don't confuse m with band index n !). The (grand canonical) free energy is $G(T, \mu) = -T \ln Z(T)$. To determine the groundstate density, we minimize the free energy with respect to occupations, i.e. we need to solve

$$\frac{\partial G(T, \mu)}{\partial n_{\alpha\sigma}} = 0$$

So then let's calculate the partition function first.

3.3.1 The Partition Function

fix whats below here... since we put μ in the path integral, we calculate the GC free energy which is not $F=E-TS$. We want "canonical free energy"... its $F=E-TS-\mu N$

In the mean-field theory, the action is free and the partition function can be calculated exactly by Grassman Gaussian integration.

$$Z(T) = \exp \left(\beta U_0 N \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} \right) \times \left(\prod_{kmn} [-i\omega_m + \xi_{kn\uparrow}] \exp(i\omega_m 0^+) \right) \left(\prod_{plj} [-i\omega_l + \xi_{pj\downarrow}] \exp(i\omega_l 0^+) \right) = \exp \left(\beta U_0 N \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} \right) \left(\prod_{kmn} G_{n\uparrow}^{-1}(k, i\omega_m) \exp(i\omega_m 0^+) \right) \left(\prod_{plj} G_{j\downarrow}^{-1}(p, i\omega_l) \exp(i\omega_l 0^+) \right)$$

In general, we can't assume that $\xi_{kn\uparrow} = \xi_{kn\downarrow}$; if we did, we would miss ferromagnetic ground-states. The factors $\exp(i\omega 0^+)$ are included for convergence; physically, they appear because the functional integral is ill-defined at $\tau = 0^4$. The free energy becomes

$$-T \ln Z(T) = -T \sum_{kmn\sigma} \ln [G_{n\sigma}^{-1}(k, i\omega_m) \exp(i\omega_m 0^+)] - U_0 N \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow}.$$

The frequency summations can be performed (§1.F and eq. (1.F.14) in [20]):

$$G(T, \mu) = -T \sum_{kn\sigma} \ln [1 + \exp(-\beta \xi_{kn\sigma})] - U_0 N \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} = -T \sum_{kn\sigma} \ln [1 + \exp(-\beta \xi_{kn\sigma})] + E_U.$$

Note, we could have ignored the E_U term in the functional integral and recovered it here by simply adding it to the ground state energy E in the free energy $G(T, \mu) = E - TS - \mu N$.

3.3.2 Minimizing the Free Energy

Now that we have the free energy, we can calculate the derivative with respect to site occupation. It is important to note that both the E_U term and $\xi_{kn\sigma}$ depend *explicitly* on $n_{\alpha\sigma}$ (recall, the matrix element $h_{k\sigma}^{\alpha\beta}$ depends on $n_{\alpha\sigma}$). Then

$$0 = \frac{\partial G(T, \mu)}{\partial n_{\alpha\sigma'}} = -T \sum_{kn\sigma} \frac{\partial}{\partial n_{\alpha\sigma'}} \ln [1 + \exp(-\beta \xi_{kn\sigma})] + \frac{\partial E_U}{\partial n_{\alpha\sigma'}}$$

i.e.

$$T \sum_{kn\sigma} \frac{\partial}{\partial n_{\alpha\sigma'}} \ln [1 + \exp(-\beta \xi_{kn\sigma})] = \frac{\partial E_U}{\partial n_{\alpha\sigma'}}$$

In the first term,

$$T \sum_{kn\sigma} \frac{\partial}{\partial n_{\alpha\sigma'}} \ln [1 + \exp(-\beta \xi_{kn\sigma})] = - \sum_{kn\sigma} \frac{\exp(-\beta \xi_{kn\sigma})}{\exp(-\beta \xi_{kn\sigma}) + 1} \frac{\partial \xi_{kn\sigma}}{\partial n_{\alpha\sigma'}} = - \sum_{kn\sigma} f(\xi_{kn\sigma}) \frac{\partial \xi_{kn\sigma}}{\partial n_{\alpha\sigma'}}$$

⁴ Derive the functional integral expression for the partition function and note that only terms like $\tau_{i+1} - \tau_i$ appear; i.e. $\tau - \tau' \neq 0$.

we have

$$\frac{\partial \xi_{kn\sigma}}{\partial n_{\alpha\sigma'}} = \sum_{\mu\nu} \bar{U}_{k\sigma}^{\mu n} U_{k\sigma}^{\nu n} \frac{\partial h_{k\sigma}^{\mu\nu}}{\partial n_{\alpha\sigma'}}$$

and

$$\frac{\partial h_{k\sigma}^{\mu\nu}}{\partial n_{\alpha\sigma'}} = \frac{\partial}{\partial n_{\alpha\sigma'}} [\gamma_k^{\mu\nu} + \delta_{\mu\nu} U_0 n_{\mu(-\sigma)}] = \delta_{\mu\alpha} \delta_{\nu\sigma'} \delta_{\sigma'(-\sigma)} U_0.$$

Then

$$-\sum_{kn\sigma} f(\xi_{kn\sigma}) \frac{\partial \xi_{kn\sigma}}{\partial n_{\alpha\sigma'}} = -U_0 \sum_{kn} f(\xi_{kn(-\sigma')}) |U_{k(-\sigma')}^{\alpha n}|^2$$

and

$$-\sum_{kn} f(\xi_{kn\sigma}) |U_{k\sigma}^{\alpha n}|^2 U_0 = \frac{\partial E_U}{\partial n_{\alpha(-\sigma)}} = -U_0 N n_{\alpha\sigma}.$$

Finally, we find that

$$n_{\alpha\sigma} = N^{-1} \sum_{kn} f(\xi_{kn\sigma}) |U_{k\sigma}^{\alpha n}|^2.$$

The expression on the right is the thermal expectation value of the site density (see eq. 9):

$$N^{-1} \sum_i \langle \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{i\alpha\sigma} \rangle \equiv \langle n_{\alpha\sigma} \rangle.$$

Symbolically, $\partial G(T, \mu) / \partial n_{\alpha\sigma} = 0$ is solved if

$$n_{\alpha\sigma} = \langle n_{\alpha\sigma} \rangle. \quad (8)$$

We reiterate that the left hand side is a variational parameter while the right hand side is a thermal expectation value: i.e. we have a *self-consistency* condition. If satisfied, it determines the parameters $\{n_{\alpha\sigma}\}$ that minimize the free energy.

4 The Effective Electron-Electron Interaction

For non-interacting phonons, it is straightforward to “integrate out” the phonon variables [6], resulting in an effective electron-electron interaction. In conventional metals, the effective interaction can be attractive and lead to superconductivity. In the 2D SSH model, its an effective spin exchange interaction and leads to (anti-ferro)magnetic ordering [10, 11], ...

I mainly want to calculate the phonon spectral function; this is what we compare to neutron scattering experiments. However, to see if the electron-phonon interaction leads to novel effective electron-electron interactions, we actually do need to integrate out the phonons.

See [21] for effective interaction in this the UX model...

A Finite Temperature Site Occupations

The site occupations can be calculated as thermal expectation values of the site creation/annihilation operators $\hat{c}_{i\alpha\sigma}^\dagger$ and $\hat{c}_{i\alpha\sigma}$:

$$\begin{aligned}\langle n_{k\alpha\sigma} \rangle &\equiv n_{k\alpha\sigma} = \lim_{\tau \rightarrow 0^+} \langle T_\tau \{ \hat{c}_{k\alpha\sigma}^\dagger(\tau) \hat{c}_{k\alpha\sigma}(0) \} \rangle = - \lim_{\tau \rightarrow 0^+} \tilde{G}_{\alpha\sigma}(k, \tau) = \\ &= \beta^{-1} \sum_n \tilde{G}_{\alpha\sigma}(k, i\omega_n) \exp(i\omega_n 0^+) \\ \tilde{G}_{\alpha\sigma}(k, i\omega_n) &\equiv -\langle \hat{c}_{k\alpha\sigma}(i\omega_n) \hat{c}_{k\alpha\sigma}^\dagger(i\omega_n) \rangle\end{aligned}$$

The tilde on $\tilde{G}_{\alpha\sigma}(k, i\omega_n)$ is to distinguish it from the Green function for the operators $\hat{d}_{kn\sigma}$. We can express the site-dependent operators $\hat{c}_{k\alpha\sigma}^\dagger$ and $\hat{c}_{k\alpha\sigma}$ in terms of the operators $\hat{d}_{k\alpha\sigma}^\dagger$ and $\hat{d}_{k\alpha\sigma}$. They are

$$\begin{aligned}\hat{c}_{k\alpha\sigma}^\dagger &= \sum_\beta \hat{d}_{k\beta\sigma}^\dagger [\hat{U}_{k\sigma}^\dagger]^{\beta\alpha} \\ \hat{c}_{k\alpha\sigma} &= \sum_\beta \hat{d}_{k\beta\sigma} U_{k\sigma}^{\alpha\beta}\end{aligned}$$

Then

$$\begin{aligned}\tilde{G}_{\alpha\sigma}(k, i\omega_n) &= -\langle \hat{c}_{k\alpha\sigma}(i\omega_n) \hat{c}_{k\alpha\sigma}^\dagger(i\omega_n) \rangle = - \sum_{\mu\nu} [\hat{U}_{k\sigma}^\dagger]^{\mu\alpha} U_{k\sigma}^{\alpha\nu} \langle \hat{d}_{k\nu\sigma}(i\omega_n) \hat{d}_{k\mu\sigma}^\dagger(i\omega_n) \rangle = \\ &= \sum_{\mu\nu} [\hat{U}_{k\sigma}^\dagger]^{\mu\alpha} U_{k\sigma}^{\alpha\nu} G_{\mu\sigma}(k, i\omega_n) \delta_{\mu\nu}\end{aligned}$$

The δ -function appears since the propagator in the diagonal basis is diagonal. Then

$$n_{k\alpha\sigma} = \beta^{-1} \sum_n \tilde{G}_{\alpha\sigma}(k, i\omega_n) = \sum_\mu [\hat{U}_{k\sigma}^\dagger]^{\mu\alpha} U_{k\sigma}^{\alpha\mu} \left(\beta^{-1} \sum_n \frac{\exp(i\omega_n 0^+)}{i\omega_n - \xi_{k\mu\sigma}} \right)$$

The Matsubara sum in parenthesis can be performed (see eq. 1.F.7 in ref. [20]). The result is

$$n_{k\alpha\sigma} = \sum_n \frac{[\hat{U}_{k\sigma}^\dagger]^{\alpha\alpha} U_{k\sigma}^{\alpha\alpha}}{\exp(\beta \xi_{kn\sigma}) + 1} = \sum_n \frac{|U_{k\sigma}^{\alpha n}|^2}{\exp(\beta \xi_{kn\sigma}) + 1} = \sum_n |U_{k\sigma}^{\alpha n}|^2 f(\xi_{kn\sigma})$$

where $f(\xi_{kn\sigma})$ is the Fermi-Dirac function. The mean density per site is calculated by averaging the real space version, $n_{i\alpha\sigma}$, over all cells i . We assume that the density is homogeneous (i.e. the same in all cells) and the result is

$$\begin{aligned}n_{\alpha\sigma} &= N^{-1} \sum_i n_{i\alpha\sigma} = N^{-1} \sum_{kp} \langle \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{p\alpha\sigma} \rangle \exp(i(k-p)\tau_\alpha) \left(N^{-1} \sum_i \exp(i(k-p)x_i) \right) \\ &= N^{-1} \sum_k n_{k\alpha\sigma} = N^{-1} \sum_{kn} |U_{k\sigma}^{\alpha n}|^2 f(\xi_{kn\sigma}) \equiv \langle n_{\alpha\sigma} \rangle\end{aligned}\tag{9}$$

which agrees perfectly with eq. 16 in ref. [13].

Of course we could have more easily calculated this from

$$\langle \hat{c}_{k\alpha\sigma}(i\omega_n) \hat{c}_{k\alpha\sigma}^\dagger(i\omega_n) \rangle = \sum_{\mu\nu} [\hat{U}_{k\sigma}^\dagger]^{\mu\alpha} U_{k\sigma}^{\alpha\nu} \langle \hat{d}_{k\nu\sigma}(i\omega_n) \hat{d}_{k\mu\sigma}^\dagger(i\omega_n) \rangle = \sum_{\mu\nu} [\hat{U}_{k\sigma}^\dagger]^{\mu\alpha} U_{k\sigma}^{\alpha\nu} f(\xi_{k\mu\sigma}) \delta_{\mu\nu}$$

where we simply evaluate the thermal expectation value. However, the functional integral method above will remain valid when we turn electron-phonon interactions on, while this last equation will not.

B Free Phonon Propagator

We will need the free (i.e. ignoring electron-phonon coupling) phonon propagator, $D_0(q, \omega)$. We want to study dispersive phonons, so we generalize from the simple Einstein-Holstein phonons to the Hamiltonian $\hat{H}_{ph} = \sum_q \omega_q (\hat{a}_q^\dagger \hat{a}_q + \frac{1}{2})$. The free phonon propagator is

C Free Fermion Propagator

Assuming that we already know how to write down the free Fermion action, we want to calculate the propagator:

$$G(\alpha, \tau - \tau') = -\langle T_\tau \{ \hat{\psi}_\alpha(\tau) \hat{\psi}_\alpha^\dagger(\tau') \} \rangle = -Z^{-1} \int \mathcal{D}(\bar{\psi}, \psi) \psi_\alpha(\tau) \bar{\psi}_\alpha(\tau') \exp(-S[\bar{\psi}, \psi])$$

with action

$$S[\bar{\psi}, \psi] = \sum_\alpha \int_0^\beta d\tau \bar{\psi}_\alpha(\tau) [\partial_\tau + \xi_\alpha] \psi_\alpha(\tau).$$

We assume we already diagonalized the Hamiltonian; α is the “band” index and $\xi_\alpha = \epsilon_\alpha - \mu$ is the eigenvalue ϵ_α minus the chemical potential μ . The fields in Matsubara frequency space are

$$\begin{aligned} \psi_\alpha(\tau) &= \beta^{-1/2} \sum_n \exp(-i\omega_n \tau) \psi_\alpha(i\omega_n) \\ \psi_\alpha(i\omega_n) &= \beta^{-1/2} \int_0^\beta d\tau \exp(i\omega_n \tau) \psi_\alpha(\tau) \\ \omega_n &= \frac{\pi(2n+1)}{\beta} \end{aligned}$$

Then

$$S[\bar{\psi}, \psi] = \sum_{\alpha n} \bar{\psi}_\alpha(i\omega_n) [-i\omega_n + \xi_\alpha] \psi_\alpha(i\omega_n)$$

can be integrated. Using Grassman Gaussian integration rules, we find

$$G(\alpha, i\omega_n) = -\langle \hat{\psi}_\alpha(i\omega_n) \hat{\psi}_\alpha^\dagger(i\omega_n) \rangle = \frac{1}{i\omega_n - \xi_\alpha}. \quad (10)$$

If we are considering spinful particles, we simply have to put $\alpha \rightarrow \alpha\sigma$. The imaginary time version is recovered by inverse Matsubara transforming

$$G(\alpha, \tau) = \beta^{-1} \sum_n G(\alpha, i\omega_n) \exp(-i\omega_n \tau)$$

$$G(\alpha, i\omega_n) = \int_0^\beta d\tau G(\alpha, \tau) \exp(i\omega_n \tau)$$

Sometimes we need to calculate the particle number; we could naively guess that $n_\alpha = \langle \psi_\alpha^\dagger \psi_\alpha \rangle$ is the number of particles in the α^{th} single particle level. However, this is implicitly evaluated at equal-time and the functional integral is ill defined. What we really need to calculate is

$$n_\alpha = \lim_{\tau \rightarrow 0^+} \langle T_\tau \{ \hat{\psi}_\alpha^\dagger(\tau) \hat{\psi}_\alpha(0) \} \rangle = - \lim_{\tau \rightarrow 0^+} G(\alpha, \tau) =$$

$$= \beta^{-1} \sum_n G(\alpha, i\omega_n) \exp(i\omega_n 0^+).$$

D Bose-Hubbard Model

If instead of Fermions, our particles are spinless Bosons, then the Hubbard interaction is

$$\frac{U}{2} \sum_{i\alpha} \hat{n}_{i\alpha} (\hat{n}_{i\alpha} - 1) = \frac{U}{2} \sum_{i\alpha} (\hat{n}_{i\alpha}^2 - \hat{n}_{i\alpha}).$$

We won't consider spinless Fermions since the Pauli exclusion principle prohibits two Fermions with the same quantum numbers from occupying the same site: i.e. a Hubbard interaction between *spinless* Fermions would have no effect. Introduce a mean-field and fluctuation: $\hat{n}_{i\alpha} = n_\alpha + \delta\hat{n}_{i\alpha}$:

$$\frac{U}{2} \sum_{i\alpha} (\hat{n}_{i\alpha}^2 - \hat{n}_{i\alpha}) \approx \frac{U}{2} \sum_{i\alpha} (n_\alpha^2 + 2\delta\hat{n}_{i\alpha} n_\alpha - \hat{n}_{i\alpha})$$

not done ...

E Mixing

We are looking for the solution to the SCF problem derived above. In the SCF problem, we formulate the Kohn-Sham (KS) Hamiltonian as a functional of the density and look for the solution such that the density calculated by solving the KS equations is equal to the input density. Generally the input density is a *function* of position (i.e. a field) and the output density is a *functional* of the input density. In our tight binding approximation to the KS Hamiltonian, the density is a vector and the “KS functional” is just a function. The density is $\boldsymbol{\rho} = (\rho_0, \rho_1, \dots, \rho_n)$ where ρ_i is the density of electrons in the i^{th} orbital in the unitcell. We will use vector notation for convenience in what follows, but the formulation for continuous density is analogous.

We are looking for $\boldsymbol{\rho}^{(i)}$ such that $\boldsymbol{\rho}^{(o)}[\boldsymbol{\rho}^{(i)}] = \boldsymbol{\rho}^{(i)}$ where $\boldsymbol{\rho}^{(o)}$ is the output density calculated from the input density. Let us restate the problem: define the residual $\mathbf{R} = \boldsymbol{\rho}^{(o)} - \boldsymbol{\rho}^{(i)}$

and try to find $\rho^{(i)}$ such that $\mathbf{R} = 0$ is the null vector. In the SCF problem, we don't know the solution *a priori*. Instead we make an initial guess $\rho_0^{(i)}$, calculate $\rho_0^{(o)}$, and use some combination of these two (and possibly other iterations) to predict $\rho_1^{(i)}$. Let's call the input and output densities at the n^{th} step $\rho_n^{(i)}$ and $\rho_n^{(o)}$ and the residual $\mathbf{R}_n = \rho_n^{(o)} - \rho_n^{(i)}$. We iterate until $|\mathbf{R}_n| \approx 0$ to within some tolerance, where $|\mathbf{R}_n|$ is a suitable norm: e.g. $|\mathbf{R}_n| \equiv \langle \mathbf{R}_n | \mathbf{R}_n \rangle = \sum_i R_{n,i}^2$. i runs over all atoms in the unitcell, i.e. over all elements of the vector \mathbf{R}_n , with $R_{n,i} = \rho_{n,i}^{(o)} - \rho_{n,i}^{(i)}$ the residual at orbital i on the n^{th} step.

We want to find the solution in as few iterations as possible. To speed up convergence, we want to make a smart guess for each $\rho_n^{(i)}$. The Pulay method (also called “direct inversion in the iterative subspace” or DIIS for short; see below) is an example of an effective and popular method to make such a guess [22]. The idea is based on the assumption that, for some iteration n $\rho_n^{(i)}$, we are close to the exact solution ρ^* . Then the iterations in the vicinity of n are also close to the exact solution. For the input for the next iteration, we want to pick a linear combination of several $\rho_{n+1}^{(i)}$ near n , say s of them, and choose the coefficients so that $|\mathbf{R}_{n+1}| \approx 0$. In other words, we take the input density from the previous s steps as a basis and expand the next the input density in the basis with the coefficients chosen to be optimal. Experience shows that $s \sim 4$ is a good number.

Explicitly, we guess

$$\rho_{n+1}^{(i)} = \sum_{k=n}^{n-s} c_k \rho_k^{(i)} \quad (11)$$

with c_k the expansions coefficients that we determine subject to the condition $|\mathbf{R}_{n+1}| = 0$... ok. But unless we know $\rho_{n+1}^{(o)}$, we can't calculate \mathbf{R}_{n+1} ! To make progress, we assume that the function $\rho^{(o)}(\rho^{(i)})$ is linear⁵; i.e. $\rho^{(o)}(\rho_0^{(i)} + c\rho_1^{(i)}) = \rho_0^{(o)} + c\rho_1^{(o)}$.. Then we can calculate

$$\rho_{n+1}^{(o)} = \sum_{k=n}^{n-s} c_k \rho_k^{(o)} \quad (12)$$

where c_k are the same coefficients as in eq. 11. Finally we can calculate the residual

$$\mathbf{R}_{n+1} = \rho_{n+1}^{(o)} - \rho_{n+1}^{(i)} = \sum_k c_k [\rho_k^{(o)} - \rho_k^{(i)}] = \sum_k c_k \mathbf{R}_k \quad (13)$$

and determine c_k by minimizing

$$\langle \mathbf{R}_{n+1} | \mathbf{R}_{n+1} \rangle = \sum_k \sum_l c_k c_l \langle \mathbf{R}_k | \mathbf{R}_l \rangle \quad (14)$$

subject to the constraint $\sum_k c_k = 1$. Why do we need the constraint? Conceptually we don't want the output density to be “bigger” than the input so we expect some sort of normalization constraint. More formally, let's define the error vector $\mathbf{e}_n = \rho_n^{(i)} - \rho^*$ as the deviation from the exact solution. We can write

$$\rho_{n+1}^{(i)} = \sum_k c_k \rho_k^{(i)} = \sum_k c_k [\rho^* + \mathbf{e}_k] = \rho^* \sum_k c_k + \sum_k c_k \mathbf{e}_k. \quad (15)$$

⁵ This is valid in the limit that $\rho^{(i)} \approx \rho^*$ since then $\mathbf{R} \approx 0$ is near a minimum and higher orders in the Taylor series of \mathbf{R} are sub-dominant.

If we have solved the problem, then $\mathbf{e}_i \equiv 0$ and $\boldsymbol{\rho}_{n+1}^{(i)} = \boldsymbol{\rho}^*$ is the exact solution:

$$\boldsymbol{\rho}_{n+1}^{(i)} = \boldsymbol{\rho}^* \sum_k c_k = \boldsymbol{\rho}^* \quad (16)$$

and $\sum_k c_k \equiv 1$. We include the constraint using Lagrange multipliers. The Lagrangian we should minimize is⁶

$$L(\{c\}, \lambda) = \sum_l \sum_k c_l c_k \langle \mathbf{R}_l | \mathbf{R}_k \rangle - 2\lambda \left(\sum_k c_k - 1 \right). \quad (17)$$

So then we calculate

$$\begin{aligned} \frac{\partial}{\partial c_m} \left[\sum_l \sum_k c_l c_k \langle \mathbf{R}_l | \mathbf{R}_k \rangle - 2\lambda \left(\sum_k c_k - 1 \right) \right] &= 0 \\ &= \sum_k c_k [\langle \mathbf{R}_m | \mathbf{R}_k \rangle + \langle \mathbf{R}_k | \mathbf{R}_m \rangle] - 2\lambda \\ &= \sum_k c_k \langle \mathbf{R}_m | \mathbf{R}_k \rangle - \lambda = 0, \end{aligned} \quad (18)$$

where we used the fact that the \mathbf{R}_n are real, and

$$\begin{aligned} \frac{\partial}{\partial \lambda} \left[\sum_l \sum_k c_l c_k \langle \mathbf{R}_l | \mathbf{R}_k \rangle - 2\lambda \left(\sum_k c_k - 1 \right) \right] &= 0 \\ &= \sum_k c_k - 1 = 0. \end{aligned} \quad (19)$$

We find the system of equations

$$\begin{pmatrix} \langle \mathbf{R}_{n-s} | \mathbf{R}_{n-s} \rangle & \langle \mathbf{R}_{n-s} | \mathbf{R}_{n-s+1} \rangle & \cdots & \langle \mathbf{R}_{n-s} | \mathbf{R}_n \rangle & 1 \\ \langle \mathbf{R}_{n-s+1} | \mathbf{R}_{n-s} \rangle & \langle \mathbf{R}_{n-s+1} | \mathbf{R}_{n-s+1} \rangle & \cdots & \langle \mathbf{R}_{n-s+1} | \mathbf{R}_n \rangle & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \langle \mathbf{R}_n | \mathbf{R}_{n-s} \rangle & \langle \mathbf{R}_n | \mathbf{R}_{n-s+1} \rangle & \cdots & \langle \mathbf{R}_n | \mathbf{R}_n \rangle & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{pmatrix} \begin{pmatrix} c_{n-s} \\ c_{n-s+1} \\ \vdots \\ c_n \\ -\lambda \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}. \quad (20)$$

We can easily invert the matrix on the left (recall, it's only practical to keep 4 or 5 previous iterations in memory) to get the coefficients c_n . Then we can use them to construct our next guess $\boldsymbol{\rho}_{n+1}^{(i)}$ and repeat the process until desired convergence. The fact that we are inverting a matrix in only a “subspace” of all basis vectors \mathbf{R}_n leads to the popular name “DIIS”.

Since this method depends on already having several iterations in memory, we won't be able to use the Pulay scheme right away in a real calculation. We could guess several iterations from scratch, but a more reasonable procedure is to use simple mixing or some

⁶ The factor of 2 on the constraint 2λ is conventional.

other method for the first s iterations; once we have all of them available, we can begin using the Pulay procedure⁷.

It seems strange that the input in each step does not contain any of the output of each iteration, $\rho_n^{(o)}$; it's as if we are ignoring the information it provides⁸. Really, we are already including it in our earlier assumption that we are close to the true solution; in this regime $\rho_n^{(i)} \approx \rho_n^{(o)}$ anyway. This is actually a bad approximation in the beginning where we are far away from the true solution and, in fact, it is possible to get trapped into a subspace spanned by the earlier vectors. A simple solution to this problem is to mix in a little bit of the earlier residual; i.e. we mix in a little of $\rho_n^{(o)}$ early on and less of it as the residual gets smaller. Explicitly,

$$\begin{aligned}\rho_{n+1}^{(i)} &= \sum_k c_k \left[\rho_k^{(i)} + \beta \mathbf{R}_k \right] \\ &= \sum_k c_k \left[\rho_k^{(i)} + \beta \left(\rho_k^{(o)} - \rho_k^{(i)} \right) \right] = \sum_k c_k \left[\beta \rho_k^{(o)} + (1 - \beta) \rho_k^{(i)} \right].\end{aligned}\tag{21}$$

The input at each iteration is calculated from simple mixing! Note that in the limit that we only keep one iteration in history, this method reduces exactly to simple mixing. Obviously in the limit $\beta = 0$ we recover usual Pulay mixing.

See ref. [23] for more information and a neat review of DIIS.

F Additional Reading

Equation for Holstein model as phonon-dependent local chemical potential: [24]

Papers and notes related to stuff above... **Someone has already discovered this model :([21]. For other useful refs, see [25–27]**

A recent review of what is known about the Hubbard model by modelling: [28]. Probably good benchmark for my calculations.

Ref. [29] gives discussion of Hartree fock approximation and studies non-collinear spin ordering phase diagram.

Ref. Andy Millis paper about breathing mode effects on charge ordering in rare earth nickelates. Combines DFT+U for electronic energy and Landau mean field theory to study phase diagram I guess [30]

F.1 Physical Observables to Calculate

In ref. [31], they calculate optical conductivity and compressibility: they find no gap in the conductivity but a gap in the compressibility. They argue an intermediate “phase” between compressible Andersen insulator (where diffusion vanishes) and incompressible Mott insulator. Also see §17.4 and eq. 17.44 in Girvin and Yang: they give a formula for conductivity in terms of diffusivity and compressibility, the two quantities that determine insulating behavior.

⁷ In the original paper by Pulay [22], it is suggested to build the first several iterations by directly inverting the Hessian matrix.

⁸ See <https://prefetch.eu/know/concept/pulay-mixing/>

Some analysis of Strontium Manganate with a TB model and some many body stuff [32]
 See Ref. [33] for correlation functions that are interesting physical observables in 2d Hubbard model.

F.2 Stripe Order

For stripes in cuprates, look at fig. 1.7 in ref. [34]. For nickelates, look at fig. 2 in ref. [35].

Ref. [15] studies the 2D square lattice in mean-field just like me! Has good refs too. They show that diagonal and vertical stripes are stabilized away from half filling and, at fixed filling, there is a crossover with respect to U from the vertical to diagonal stripes. This implies a difference in U in cuprates vs. nickelates. They find that the “cross” stripes are never (globally) stable and are only a local minimum of the energy. They also find that uniform (checkerboard) AFM order is only the most stable at half filling. Importantly, they don’t study the model at finite temperature.

Ref. [36] is a more recent MFT stripe paper than Kato [15]. They claim the energy difference between diagonal and vertical stripes is small and thus competes with perturbations; e.g. Peirls eph coupling, next-nearest-neighbor hopping etc. They study the phase diagram with different couplings added in. Needs more reading.

Ref. [37] gives exp. results on incommensurate vs. commensurate stripe crossover for T vs doping. For $x > 1/3$, incommensurate order dominates at all T. At lower doping, there is a crossover.

Ref. [38] studies doped Hubbard model using more advanced methods than MFT; they find phase transition wrt to temp. from AFM to stripe phase and study thermodynamical properties of the transition.

Ref. [39] imposes incommensurability in MFT by assuming inhomogeneity of the mean density... but this will couple Bloch functions at different k ... since translational invariance is lost.

Ref. [40] uses DMFT to study crossover from vertical to diagonal stripes in LSCO. They say the critical doping concentration is quantitatively accurate and study thermodynamics of the stripe phase.

Ref. [41] has very thorough phase diagrams wrt to doping and nearest/next-to-nearest hopping.

F.3 Relevant Many-Body Calcs

Ref. [42] calculates phonon self-energy assuming RPA electron-electron interactions. They use a model dispersion and calculate renormalization of the dispersion. Similar work: [43].

Ref. [44] predicts phonon-polarons in Peirls-Hubbard model for doped nickelate. **Re-read**

Ref. [33] provides an absolutely excellent study of the phase diagram and correlation functions at finite temperature. Interacting tight binding model solved by some sort of Monte Carlo. Importantly, the sample perturbative diagrams around the Hartree renormalized chemical potential (i.e. around Hartree mean field solutions I think...). They study large supercell and finite finite size effects. They also enumerate they interesting physical correlation functions and discuss how to calculate. **this is a good ref.**

Ref. [45] studies $t - t'$ model in DMFT and compares to $t - j$ model. They calculate spin correlation functions and hole dispersions and other interesting things.

Ref. [46] derives some sum rules for stuff in the Holstein model. not super relevant, but there are good details on what propagators are supposed to look like

Ref. [47] solves a similar 1d model and calculates spectral functions etc

F.4 Finite Temperature Mean-Field Theory

Ref. [48]

F.5 Symmetries of the Hubbard Model

See ref. [49].

F.6 misc

Ref. [50] shows a way to “decouple” the interaction in a “rotationally invariant” way. They say this is the only way that leads to the correct Hartree-Fock equations...? Their method does lead to a nice expression when decoupled using Hubbard–Stratonovich (auxiliary field) transformation.

Ref. [51] derives mean field equations with vector magnetization

F.7 Path-Integral Hubbard Model

See ref. [52]. At finite temperature, see ref. [53].

F.8 Solving the Many-Body Model

Probably use auxiliary-field quantum Monte Carlo (AFQMC). See ref. [54, 55]; I think this is what the 2D SSH model papers [10, 11] use. Other options are diagrammatic Monte Carlo (DMC) [56] and continuous-time quantum Monte Carlo (CTQMC) [57].

References

- [1] *NOTES: "Elementary-Introduction-to-the-Hubbard-Model"*.
- [2] Victor Gurarie. *Lecture Notes: Many-Body Physics*. 2022.
- [3] RD Mattuck. “Phonons from a many-body viewpoint”. In: *Annals of Physics* 27.2 (1964), pp. 216–226.
- [4] Tyler C Sterling and Dmitry Reznik. “Effect of the electronic charge gap on LO bond-stretching phonons in undoped La₂CuO₄ calculated using LDA+ U”. In: *Physical Review B* 104.13 (2021), p. 134311.
- [5] OV Dolgov, OK Andersen, and II Mazin. “Self-consistent theory of phonon renormalization and electron-phonon coupling near a two-dimensional Kohn singularity”. In: *Physical Review B* 77.1 (2008), p. 014517.

- [6] Enzhi Li. “Schwinger-Dyson Equation Method to Calculate Total Energy in Periodic Anderson Model with Electron-Phonon Interactions”. In: *arXiv preprint arXiv:1904.09881* (2019).
- [7] Arne Schobert et al. “Downfolding the Su-Schrieffer-Heeger model”. In: *SciPost Phys.* 11 (4 2021), p. 79. DOI: 10.21468/SciPostPhys.11.4.079. URL: <https://scipost.org/10.21468/SciPostPhys.11.4.079>.
- [8] Shaozhi Li and Steven Johnston. “Quantum Monte Carlo study of lattice polarons in the two-dimensional three-orbital Su-Schrieffer-Heeger model”. In: *npj Quantum Materials* 5.1 (2020), pp. 1–10.
- [9] Chao Zhang, Nikolay V Prokof’ev, and Boris V Svistunov. “Peierls/Su-Schrieffer-Heeger polarons in two dimensions”. In: *Physical Review B* 104.3 (2021), p. 035143.
- [10] Xun Cai, Zi-Xiang Li, and Hong Yao. “Antiferromagnetism Induced by Bond Su-Schrieffer-Heeger Electron-Phonon Coupling: A Quantum Monte Carlo Study”. In: *Physical review letters* 127.24 (2021), p. 247203.
- [11] Anika Götz et al. “Valence-bond solid to antiferromagnet transition in the two-dimensional Su-Schrieffer-Heeger model by Langevin dynamics”. In: *Physical Review B* 105.8 (2022), p. 085151.
- [12] Hélène Feldner et al. “Magnetism of finite graphene samples: Mean-field theory compared with exact diagonalization and quantum Monte Carlo simulations”. In: *Physical Review B* 81.11 (2010), p. 115416.
- [13] Yann Claveau, Brice Arnaud, and Sergio Di Matteo. “Mean-field solution of the Hubbard model: the magnetic phase diagram”. In: *European Journal of Physics* 35.3 (2014), p. 035023.
- [14] Keiichiro Nasu. “Extended Peierls-Hubbard model for one-dimensional N-sites N-electrons system. I. Phase diagram by mean field theory”. In: *Journal of the Physical Society of Japan* 52.11 (1983), pp. 3865–3873.
- [15] Masaru Kato et al. “Soliton lattice modulation of incommensurate spin density wave in two dimensional Hubbard model-a mean field study”. In: *Journal of the Physical Society of Japan* 59.3 (1990), pp. 1047–1058.
- [16] Marcin Raczkowski et al. “Hubbard model on the honeycomb lattice: From static and dynamical mean-field theories to lattice quantum Monte Carlo simulations”. In: *Physical Review B* 101.12 (2020), p. 125103.
- [17] Anders B Eriksson, Torbjörn Einarsson, and Stellan Östlund. “Symmetries and mean-field phases of the extended Hubbard model”. In: *Physical Review B* 52.5 (1995), p. 3662.
- [18] Seva Nimkar et al. “Mean-field results of the multiple-band extended Hubbard model for the square-planar CuO 2 lattice”. In: *Physical Review B* 48.10 (1993), p. 7355.
- [19] Harald Jeschke. *Computational Methods in Solid State Theory, Chp 4*.
- [20] Nicolas Dupuis. *NOTES: "Functional Integration"*.

- [21] Alexander E Lukyanov et al. “Strength of the Hubbard potential and its modification by breathing distortion in BaBiO 3”. In: *Physical Review B* 105.4 (2022), p. 045131.
- [22] Péter Pulay. “Convergence acceleration of iterative sequences. The case of SCF iteration”. In: *Chemical Physics Letters* 73.2 (1980), pp. 393–398.
- [23] Ron Shepard and Michael Minkoff. “Some comments on the DIIS method”. In: *Molecular Physics* 105.19-22 (2007), pp. 2839–2848.
- [24] JK Freericks, M Jarrell, and DJ Scalapino. “Holstein model in infinite dimensions”. In: *Physical Review B* 48.9 (1993), p. 6302.
- [25] Natanael C Costa et al. “Phase diagram of the two-dimensional Hubbard-Holstein model”. In: *Communications Physics* 3.1 (2020), pp. 1–6.
- [26] E Berger, P Valášek, and W Von Der Linden. “Two-dimensional Hubbard-Holstein model”. In: *Physical Review B* 52.7 (1995), p. 4806.
- [27] W Von der Linden, E Berger, and P Valášek. “The hubbard-holstein model”. In: *Journal of low temperature physics* 99.3 (1995), pp. 517–525.
- [28] Mingpu Qin et al. “The Hubbard model: A computational perspective”. In: *Annual Review of Condensed Matter Physics* 13 (2022), pp. 275–302.
- [29] M Inui and PB Littlewood. “Hartree-Fock study of the magnetism in the single-band Hubbard model”. In: *Physical Review B* 44.9 (1991), p. 4415.
- [30] Zhuoran He and Andrew J Millis. “Strain control of electronic phase in rare-earth nickelates”. In: *Physical Review B* 91.19 (2015), p. 195138.
- [31] Young Woo Choi and Hyoung Joon Choi. “Strong electron-phonon coupling, electron-hole asymmetry, and nonadiabaticity in magic-angle twisted bilayer graphene”. In: *Physical Review B* 98.24 (2018), p. 241412.
- [32] Xu-jing Li et al. “Octahedral rotations trigger electronic and magnetic transitions in strontium manganate under volume expansion”. In: *Journal of Physics: Condensed Matter* 33.36 (2021), p. 365501.
- [33] Fedor Šimkovic IV, Riccardo Rossi, and Michel Ferrero. “Two-dimensional Hubbard model at finite temperature: Weak, strong, and long correlation regimes”. In: *Physical Review Research* 4.4 (2022), p. 043201.
- [34] Igor A Zaliznyak and John M Tranquada. “Neutron scattering and its application to strongly correlated systems”. In: *Strongly Correlated Systems*. Springer, 2015, pp. 205–235.
- [35] S Anissimova et al. “Direct observation of dynamic charge stripes in La_{2-x}Sr_xNiO₄”. In: *Nature Communications* 5.1 (2014), pp. 1–10.
- [36] Marcin Raczkowski, Andrzej M Oleś, and Raymond Frésard. “Stripe phases—possible ground state of the high-T_c superconductors”. In: *Low Temperature Physics* 32.4 (2006), pp. 305–319.
- [37] Kyoko Ishizaka et al. “Commensurate-Incommensurate Crossover of Charge Stripe in La_{2-x}Sr_xNiO₄ (x = 1/3)”. In: *Physical review letters* 92.19 (2004), p. 196404.

- [38] Alexander Wietek et al. “Stripes, antiferromagnetism, and the pseudogap in the doped Hubbard model at finite temperature”. In: *Physical Review X* 11.3 (2021), p. 031007.
- [39] Masanori Ichioka and Kazushige Machida. “Electronic structure of stripes in two-dimensional Hubbard model”. In: *Journal of the Physical Society of Japan* 68.12 (1999), pp. 4020–4031.
- [40] Marcus Fleck et al. “One-dimensional metallic behavior of the stripe phase in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ”. In: *Physical Review Letters* 84.21 (2000), p. 4962.
- [41] PA Igoshev et al. “Incommensurate magnetic order and phase separation in the two-dimensional Hubbard model with nearest-and next-nearest-neighbor hopping”. In: *Physical Review B* 81.9 (2010), p. 094407.
- [42] Eiji Kaneshita, Masanori Ichioka, and Kazushige Machida. “Phonon anomalies due to collective stripe modes in high T_c cuprates”. In: *Physical review letters* 88.11 (2002), p. 115501.
- [43] Kwon Park and Subir Sachdev. “Bond-operator theory of doped antiferromagnets: From Mott insulators with bond-centered charge order to superconductors with nodal fermions”. In: *Physical Review B* 64.18 (2001), p. 184510.
- [44] J Zaanen and PB Littlewood. “Freezing electronic correlations by polaronic instabilities in doped La_2NiO_4 ”. In: *Physical Review B* 50.10 (1994), p. 7222.
- [45] IA Goremykin and AA Katanin. “Commensurate and incommensurate magnetic order in the doped two-dimensional Hubbard model: dynamical mean-field theory analysis”. In: *arXiv preprint arXiv:2212.14656* (2022).
- [46] JK Freericks et al. “Nonequilibrium sum rules for the Holstein model”. In: *arXiv preprint arXiv:1403.5604* (2014).
- [47] Cyrill Slezak et al. “Spectral properties of Holstein and breathing polarons”. In: *Physical Review B* 73.20 (2006), p. 205122.
- [48] Ramesh V Pai, K Sheshadri, and Rahul Pandit. “Phases and transitions in the spin-1 Bose-Hubbard model: Systematics of a mean-field theory”. In: *Physical Review B* 77.1 (2008), p. 014503.
- [49] David Grabovsky. *NOTES: “Limits of the Hubbard Model”*.
- [50] Anamitra Mukherjee et al. “Testing the Monte Carlo–mean field approximation in the one-band Hubbard model”. In: *Physical Review B* 90.20 (2014), p. 205133.
- [51] Edwin Langmann and Mats Wallin. “Mean Field Magnetic Phase Diagrams for the Two Dimensional t – t' – U Hubbard Model”. In: *Journal of statistical physics* 127 (2007), pp. 825–840.
- [52] ZY Weng, CS Ting, and TK Lee. “Path-integral approach to the Hubbard model”. In: *Physical Review B* 43.4 (1991), p. 3790.
- [53] Liang He and Su Yi. “Finite temperature mean-field theory with intrinsic non-Hermitian structures for Bose gases in optical lattices”. In: *New Journal of Physics* 24.2 (2022), p. 023035.

- [54] FF Assaad et al. “The ALF (Algorithms for Lattice Fermions) project release 2.0. Documentation for the auxiliary-field quantum Monte Carlo code”. In: *arXiv preprint arXiv:2012.11914* (2020).
- [55] Fakher F Assaad. “Quantum Monte Carlo methods on lattices: The determinantal approach”. In: *Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms* 10 (2002), pp. 99–147.
- [56] Kris Van Houcke et al. “Diagrammatic monte carlo”. In: *Physics Procedia* 6 (2010), pp. 95–105.
- [57] Emanuel Gull et al. “Continuous-time auxiliary-field Monte Carlo for quantum impurity models”. In: *EPL (Europhysics Letters)* 82.5 (2008), p. 57003.