

# Electron Phonon Coupling in a Modified Hubbard-Holstein Model

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## 1 Introduction

In this document, I introduce a model for a coupled 2d perovskite-like electron-phonon system. The model consists of transition metal (TM) sites surrounded by a square of “oxygen” atoms. Each TM site holds one orbital, similar to the situation in cuprates where only a single  $d$  band crosses the Fermi level. I include an electron-electron Hubbard interaction between the orbitals that is treated in mean-field theory to find the self-consistent spin and charge densities. The electronic densities are coupled to Holstein-like optical phonons through a phenomenological model interaction: interaction strength is proportional to the relative “volume” modulation of the octahedra around the TM sites by the phonon displacements. The motivation for the form of the interaction is that phonon-induced fluctuation of the octahedra dynamically modulates the “volume” around the TM atom at the center. Since the orbitals are localized around the TM sites, the volume modulation modifies the local, on-site potential leading to an effective site dependent chemical potential. In other words, the phonons “pump” charge onto/off the TM atoms, which effectively modulates the local chemical potential.

## 2 Model

The Hamiltonian for the full interacting electron-phonon system is

$$\hat{H} = \hat{H}_e + \hat{H}_{ph} + \hat{H}_{eph}. \quad (1)$$

The Hamiltonian for the electronic system is

$$\hat{H}_e = - \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} - \mu_0 \sum_{i\alpha} \hat{n}_{i\alpha} + U \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow} \quad (2)$$

The indices  $i$  and  $\alpha$  label unit cell and orbitals respectively. There is only one orbital per site (actually, only one orbital per TM site; no orbitals are placed on the octahedra vertices).  $\sigma$  labels spin. The operators  $\hat{c}_{i\alpha\sigma}^\dagger$  and  $\hat{c}_{i\alpha\sigma}$  create and annihilate electrons respectively.  $\hat{n}_{i\alpha\sigma} = \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{i\alpha\sigma}$  is a spin-density operator.  $\hat{n}_{i\alpha} = \hat{n}_{i\alpha\uparrow} + \hat{n}_{i\alpha\downarrow}$  is an electron-density operator.  $U$  is the (bare) Hubbard energy and  $\mu_0$  is the (bare) chemical potential.

For the phonons

$$\hat{H}_{ph} = \sum_{ia} \frac{\hat{\mathbf{p}}_{ia}^2}{2m_a} + \frac{1}{2} \sum_{ijab} \hat{\mathbf{x}}_{ia} \Phi_{ij}^{ab} \hat{\mathbf{x}}_{jb} = \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu} \left( \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} + \frac{1}{2} \right) \quad (3)$$

$\hat{\mathbf{p}}_{ia}$  and  $\hat{\mathbf{x}}_{ia}$  are the momentum and displacement operators for the atoms.  $m_a$  is the mass of the  $a^{th}$  atom in the unit cell. Latin symbols e.g.  $a, b$  label atoms while Greek symbols e.g.  $\alpha, \beta$  label orbitals.  $\Phi_{ij}^{ab}$  is the force-constant matrix between atoms  $(ia)$  and  $(jb)$ .  $\hat{a}_{\mathbf{q}\nu}^\dagger$  and  $\hat{a}_{\mathbf{q}\nu}$  are phonon creation and annihilation operators;  $\hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu}$  is the phonon number operator.  $\mathbf{q}$  labels crystal momentum and  $\nu$  labels the phonon branch.  $\omega_{\mathbf{q}\nu}$  is the phonon frequency.

The electron-phonon interaction Hamiltonian is

$$\hat{H}_{eph} = g \sum_{i\alpha} \xi_{i\alpha}(\hat{\mathbf{x}}) \hat{n}_{i\alpha}. \quad (4)$$

$g$  is the coupling constant that sets the energy scale of the interaction.  $\xi_{i\alpha}(\hat{\mathbf{x}})$  is the “relative volume change” of the octahedra centered at site  $(i\alpha)$  by the phonon displacement; i.e. by displacement of the atoms on the vertices around the octahedra. The sum only runs over TM sites (there may be more than one per cell). Really, in 2d, relative “volume” change is relative area change, but I will use the words “volume” and “area” interchangeably. The relative volume change is a function of the displacement operators. It is

$$\xi_{i\alpha}(\hat{\mathbf{x}}) = \frac{\Delta A_{i\alpha}(\hat{\mathbf{x}})}{A_{i\alpha}^{(0)}} = \frac{A_{i\alpha}(\hat{\mathbf{x}}) - A_{i\alpha}^{(0)}}{A_{i\alpha}^{(0)}} = \frac{1}{2A_{i\alpha}^{(0)}} \left( \sum_{j(i\alpha)} \boldsymbol{\delta}_j^{(0)} \times (\hat{\mathbf{x}}_{j+1} - \hat{\mathbf{x}}_{j-1}) \right) \cdot \mathbf{z}. \quad (5)$$

The sum runs over all of the neighbors,  $j$ , around the the site  $i\alpha$ . Note that  $j$  is a composite index for unit cell and basis atom. The sum runs in the *counter-clockwise* direction and is cyclic: i.e. if there are  $n$  neighbors,  $n+1=1$ .  $\boldsymbol{\delta}_j^{(0)}$  is the equilibrium bond vector from the TM atom holding orbital  $(i\alpha)$  to  $j$ .  $A_{i\alpha}^{(0)}$  is the equilibrium area of the “octahedra” around the  $\alpha^{th}$  site (the same in all unit cells).

Putting everything together, we have

$$\begin{aligned} \hat{H} = & - \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} - \sum_{i\alpha} (\mu_0 - g\xi_{i\alpha}(\hat{\mathbf{x}})) \hat{n}_{i\alpha} + U \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow} + \\ & \sum_{ia} \frac{\hat{\mathbf{p}}_{ia}^2}{2m_a} + \frac{1}{2} \sum_{ijab} \hat{\mathbf{x}}_{ia} \Phi_{ij}^{ab} \hat{\mathbf{x}}_{jb}. \end{aligned} \quad (6)$$

Consider the term

$$\mu_0 - g\xi_{i\alpha}(\hat{\mathbf{x}}) = \mu_0 \left( 1 - \frac{g}{\mu_0} \xi_{i\alpha}(\hat{\mathbf{x}}) \right) \equiv \mu_{i\alpha}(\hat{\mathbf{x}}). \quad (7)$$

We generally assume  $g/\mu_0 \geq 0$ . Then if  $\xi_{i\alpha}(\hat{\mathbf{x}}) > 0$ , the octahedra is dilated (the volume is larger) and  $\mu_{i\alpha}(\hat{\mathbf{x}}) < \mu_0$ . The dilated octahedra lowers the local chemical potential, allowing more density on a site. Conversely, if  $\xi_{i\alpha}(\hat{\mathbf{x}}) < 0$ , the octahedra is contracted (the volume is smaller) and  $\mu_{i\alpha}(\hat{\mathbf{x}}) > \mu_0$ . The chemical potential is increased, the density decreases, etc. so this interactions make sense. In this notation,

$$\begin{aligned} \hat{H} = & - \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} - \sum_{i\alpha} \mu_{i\alpha}(\hat{\mathbf{x}}) \hat{n}_{i\alpha} + U \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow} + \\ & \sum_{ia} \frac{\hat{p}_{ia}^2}{2m_a} + \frac{1}{2} \sum_{ijab} \hat{\mathbf{x}}_{ia} \Phi_{ij}^{ab} \hat{\mathbf{x}}_{jb}. \end{aligned} \quad (8)$$

Now we work on solving the model.

## 2.1 Volume modulation

We will work in reciprocal space and in terms of second quantized phonon operators. So let us rewrite the volume modulation in this basis. We can rewrite the atom displacement operator in reciprocal space and in terms of creation/annihilation operators as

$$\hat{\mathbf{x}}_{ia} = \sum_{\mathbf{q}\nu} \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^a}{\sqrt{2m_a\omega_{\mathbf{q}\nu}N}} (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \exp(i\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)}). \quad (9)$$

$\boldsymbol{\epsilon}_{\mathbf{q}\nu}^a$  is the  $a^{th}$  component of the  $\nu^{th}$  eigenvector of the dynamical matrix.  $\mathbf{r}_{ia}^{(0)} = \mathbf{R}_i + \boldsymbol{\tau}_a$  is the equilibrium position of the  $a^{th}$  atom in the  $i^{th}$  unit cell.  $\mathbf{R}_i$  is the coordinate of the origin of the  $i^{th}$  unit cell;  $\boldsymbol{\tau}_a$  is the equilibrium position of the  $a^{th}$  atom in the unit cell. Then the reciprocal space representation of the volume modulation is

$$\begin{aligned} \xi_{i\alpha}(\hat{\mathbf{x}}) = & \sum_{\mathbf{q}\nu j(i\alpha)} \frac{(\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu})}{2A_\alpha^{(0)} \sqrt{2\omega_{\mathbf{q}\nu}N}} \left( \boldsymbol{\delta}_j^{(0)} \times \left( \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^{j+1} \exp(i\mathbf{q} \cdot \mathbf{r}_{j+1}^{(0)})}{\sqrt{m_{j+1}}} - \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^{j-1} \exp(i\mathbf{q} \cdot \mathbf{r}_{j-1}^{(0)})}{\sqrt{m_{j-1}}} \right) \right) \cdot \mathbf{z} \\ = & \sum_{\mathbf{q}\nu} \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}) (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \times \\ & \left[ \frac{1}{2A_\alpha^{(0)} \sqrt{2\omega_{\mathbf{q}\nu}N}} \sum_{j(\alpha)} \left( \boldsymbol{\delta}_j^{(0)} \times \left( \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^{j+1} \exp(i\mathbf{q} \cdot \boldsymbol{\delta}_{j+1}^{(0)})}{\sqrt{m_{j+1}}} - \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^{j-1} \exp(i\mathbf{q} \cdot \boldsymbol{\delta}_{j-1}^{(0)})}{\sqrt{m_{j-1}}} \right) \right) \cdot \mathbf{z} \right] \end{aligned} \quad (10)$$

with  $\boldsymbol{\delta}_j^{(0)} = \mathbf{r}_j^{(0)} - \mathbf{r}_{i\alpha}^{(0)}$  (recall  $j$  is composite index for unit cell and basis atom index). Everything inside the square bracket is unit cell periodic (i.e. doesn't depend on  $i$ ). We define<sup>1</sup>

$$\Xi_{\mathbf{q}\nu}^\alpha = \frac{1}{2A_\alpha^{(0)} \sqrt{2\omega_{\mathbf{q}\nu}N}} \sum_{j(\alpha)} \left( \boldsymbol{\delta}_j^{(0)} \times \left( \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^{j+1} \exp(i\mathbf{q} \cdot \boldsymbol{\delta}_{j+1}^{(0)})}{\sqrt{m_{j+1}}} - \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^{j-1} \exp(i\mathbf{q} \cdot \boldsymbol{\delta}_{j-1}^{(0)})}{\sqrt{m_{j-1}}} \right) \right) \cdot \mathbf{z}. \quad (11)$$

<sup>1</sup> This is notationally convenient, but it is easier to work with intensive quantities in my code so I actually use  $\Xi_{\mathbf{q}\nu}^\alpha = N^{-1/2} \tilde{\Xi}_{\mathbf{q}\nu}^\alpha$  with  $\tilde{\Xi}_{\mathbf{q}\nu}^\alpha$  equal to  $\Xi_{\mathbf{q}\nu}^\alpha$  without the  $N^{-1/2}$ .

This is a phonon-symmetry dependent factor that is large for modes that significantly modulate the volume of the octahedra and small for ones that don't. Then

$$\xi_{i\alpha}(\hat{\mathbf{x}}) = \sum_{\mathbf{q}\nu} \Xi_{\mathbf{q}\nu}^{\alpha} (\hat{a}_{-\mathbf{q}\nu}^{\dagger} + \hat{a}_{\mathbf{q}\nu}) \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}) \quad (12)$$

is the relative volume modulation in the basis of the phonon creation and annihilation operators.

### 3 Interactions

We can't directly solve this model; the electron-electron interaction and the electron-phonon (eph) interactions are not free. In principle, we can study the model as-is using many-body perturbation theory (MBPT). However, the convergence with respect to orders of perturbation theory is not necessarily fast or guaranteed at all and we want to study phase transitions and other non-perturbative effects. So instead of jumping into MBPT, we use self-consistent, variational mean-field-theory to find the best single-particle approximation to the exact ground-state. *Then* we can treat the interactions that we neglect in perturbation theory.

#### 3.1 Mean field theory for the electrons

Define the electronic (spin) density as a mean-density plus fluctuations:

$$\hat{n}_{i\alpha\sigma} = n_{\alpha\sigma} + \delta\hat{n}_{i\alpha\sigma}. \quad (13)$$

$n_{\alpha\sigma} \equiv \langle n_{i\alpha\sigma} \rangle$  is the mean density and  $\delta\hat{n}_{i\alpha\sigma}$  are the fluctuations (the fluctuation is now the operator). We used translational symmetry to remove the unit cell dependence (i.e. dependence on index  $i$ ) of the mean-density. Somewhat tautologically,  $\delta\hat{n}_{i\alpha\sigma} = \hat{n}_{i\alpha\sigma} - n_{\alpha\sigma}$ . This is exact; the approximation we make is that  $\delta\hat{n}_{i\alpha\sigma}$  is small and terms second order in density fluctuations can be neglected. Then the density-density interactions become

$$\begin{aligned} \hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} &= (n_{\alpha\uparrow} + \delta\hat{n}_{i\alpha\uparrow})(n_{\alpha\downarrow} + \delta\hat{n}_{i\alpha\downarrow}) = \\ &= n_{\alpha\uparrow}n_{\alpha\downarrow} + n_{\alpha\uparrow}\delta\hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow}\delta\hat{n}_{i\alpha\uparrow} + \delta\hat{n}_{i\alpha\uparrow}\delta\hat{n}_{i\alpha\downarrow}. \end{aligned} \quad (14)$$

So far, this is exact. We make the approximation that fluctuations are small and disregard the term  $\delta\hat{n}_{i\alpha\uparrow}\delta\hat{n}_{i\alpha\downarrow}$ . Then

$$\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} \approx n_{\alpha\uparrow}n_{\alpha\downarrow} + n_{\alpha\uparrow}\delta\hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow}\delta\hat{n}_{i\alpha\uparrow} = n_{\alpha\uparrow}\hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow}\hat{n}_{i\alpha\uparrow} - n_{\alpha\uparrow}n_{\alpha\downarrow}. \quad (15)$$

This term is now free (quadratic) and can be solved. Let us use this approximation to simplify the interactions.

### 3.2 Hubbard interaction

For Hubbard e-e interaction:

$$U\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} \approx U(n_{\alpha\uparrow}\hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow}\hat{n}_{i\alpha\uparrow}) - Un_{\alpha\uparrow}n_{\alpha\downarrow}. \quad (16)$$

We define

$$\begin{aligned} \hat{H}_U \approx \hat{H}_U^{MFT} &= U \sum_{i\alpha} (n_{\alpha\uparrow}\hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow}\hat{n}_{i\alpha\uparrow} - n_{\alpha\uparrow}n_{\alpha\downarrow}) = \\ &U \sum_{i\alpha} (n_{\alpha\uparrow}\hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow}\hat{n}_{i\alpha\uparrow}) - NU \sum_{\alpha} n_{\alpha\uparrow}n_{\alpha\downarrow} \end{aligned} \quad (17)$$

with  $E_U = -NU \sum_{\alpha} n_{\alpha\uparrow}n_{\alpha\downarrow}$  the classical electrostatic Hubbard energy.

### 3.3 Electron-phonon interaction

The electron-phonon interaction is still problematic: they depend on both electron and phonon operators so can't be solved exactly. We need some more simplifications.

There are two ways to proceed here and we will consider both separately. (i) We can treat the interaction as a perturbation and drop terms  $\sim g\delta\hat{n}_{i\alpha\sigma}$ . This is a good first approximation that will produce some interesting results. (ii) We can treat the phonon operators in mean-field theory too. This will recover the terms we find in perturbation theory but, as we will see, will also provide us with some more interesting physics that the perturbation approximation does not.

## 4 Electron-phonon interaction as a perturbation

First, we treat the electron phonon interaction as a perturbation (i.e. small) and drop terms containing both electron-phonon interactions and quantum fluctuations. The electron-phonon interaction is

$$\hat{H}_{eph} = g \sum_{i\alpha} \xi_{i\alpha}(\hat{\mathbf{x}}) \hat{n}_{i\alpha}. \quad (18)$$

We use MFT to rewrite each term as

$$g\xi_{i\alpha}(\hat{\mathbf{x}})\hat{n}_{i\alpha} = g\xi_{i\alpha}(\hat{\mathbf{x}})(n_{\alpha} + \delta\hat{n}_{i\alpha}). \quad (19)$$

Treat the second term with the product  $g\delta\hat{n}_{i\alpha}$  as small. The mean-field electron-phonon interaction simplified in perturbation theory is

$$\hat{H}_{eph}^{(0)} = g \sum_{i\alpha} \xi_{i\alpha}(\hat{\mathbf{x}}) n_{\alpha}. \quad (20)$$

This only depends on phonon operators; the electrons only enter as a mean-field. We can solve the phonon sector with this term included as we see below.

With these simplifications, the model is

$$\hat{H}^{MFT} = \hat{H}_e^{MFT} + \hat{H}_{ph}^{MFT} \quad (21)$$

The electronic sector is

$$\begin{aligned} \hat{H}_e^{MFT} &= \hat{H}_e^{(0)} + E_U^{MFT} = \\ &- \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} - \mu_0 \sum_{i\alpha} \hat{n}_{i\alpha} + U \sum_{i\alpha} (n_{\alpha\uparrow} \hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow} \hat{n}_{i\alpha\uparrow}) - NU \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow}. \end{aligned} \quad (22)$$

The last term,  $E_U^{MFT} = -NU \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow}$ , is a mean-field Hubbard interaction energy. It is a constant (in the sense of not a quantum operator). The phonon sector is

$$\hat{H}_{ph}^{MFT} = \hat{H}_{ph}^{(0)} + \hat{H}_{eph}^{(0)} = \sum_{ia} \frac{\hat{\mathbf{p}}_{ia}^2}{2m_a} + \frac{1}{2} \sum_{ijab} \hat{\mathbf{x}}_{ia} \Phi_{ij}^{ab} \hat{\mathbf{x}}_{jb} + g \sum_{i\alpha} \xi_{i\alpha}(\hat{\mathbf{x}}) n_{\alpha}. \quad (23)$$

Let us work on each of these in turn.

## 4.1 Electrons

The electronic sector can be solved by diagonalization. I do this in another set of notes. The results are quoted here. Define  $\varepsilon_{\mathbf{k}n\sigma}$  as the eigenvalue of state with momentum  $\mathbf{k}$  and spin  $\sigma$  in the  $n^{th}$  band. The diagonal electron creation and annihilation operators are  $\hat{d}_{\mathbf{k}n\sigma}^\dagger$  and  $\hat{d}_{\mathbf{k}n\sigma}$  respectively. The diagonal electron Hamiltonian is

$$\hat{H}_e^{(0)} = \sum_{\mathbf{k}n\sigma} (\varepsilon_{\mathbf{k}n\sigma} - \mu_0) \hat{d}_{\mathbf{k}n\sigma}^\dagger \hat{d}_{\mathbf{k}n\sigma} \equiv \sum_{\mathbf{k}n\sigma} \zeta_{\mathbf{k}n\sigma} \hat{d}_{\mathbf{k}n\sigma}^\dagger \hat{d}_{\mathbf{k}n\sigma} \quad (24)$$

with  $\hat{n}_{\mathbf{k}n\sigma}^{(d)} \equiv \hat{d}_{\mathbf{k}n\sigma}^\dagger \hat{d}_{\mathbf{k}n\sigma}$  the electron number operator.  $\zeta_{\mathbf{k}n\sigma} = \varepsilon_{\mathbf{k}n\sigma} - \mu_0$  is the energy relative to the chemical potential (Fermi level).

## 4.2 Phonons

Let's go to second quantization. The solution of the phonon dynamical equations is done in another set of notes; I quote the results here

$$\begin{aligned} \hat{H}_{ph}^{MFT} &= \sum_{ia} \frac{\hat{\mathbf{p}}_{ia}^2}{2m_a} + \frac{1}{2} \sum_{ijab} \hat{\mathbf{x}}_{ia} \Phi_{ij}^{ab} \hat{\mathbf{x}}_{jb} + g \sum_{i\alpha} \xi_{i\alpha}(\hat{\mathbf{x}}) n_{\alpha} = \\ &\sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu} \left( \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} + \frac{1}{2} \right) + g \sum_{\mathbf{q}\nu} \sum_{i\alpha} \Xi_{\mathbf{q}\nu}^\alpha n_{\alpha} (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}). \end{aligned} \quad (25)$$

The second term can be simplified:

$$\begin{aligned} g \sum_{\mathbf{q}\nu} \sum_{\alpha} \Xi_{\mathbf{q}\nu}^\alpha n_{\alpha} (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \sum_i \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}) &= \sum_{\mathbf{q}\nu} \left( Ng \sum_{\alpha} \Xi_{\mathbf{q}\nu}^\alpha n_{\alpha} \right) (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \delta_{\mathbf{q}} \\ &= \sum_{\nu} \Gamma_{\nu}^{MFT} (\hat{a}_{\nu}^\dagger + \hat{a}_{\nu}) \end{aligned} \quad (26)$$

where we defined

$$\hat{a}_{\mathbf{0}\nu}^\dagger = \hat{a}_\nu^\dagger \quad \hat{a}_{\mathbf{0}\nu} = \hat{a}_\nu \quad (27)$$

and

$$\Gamma_\nu^{MFT} = Ng \sum_\alpha \Xi_\nu^\alpha n_\alpha. \quad (28)$$

$\mathbf{q}$ -dependent symbols without a label  $\mathbf{q}$  are to be evaluated at  $\mathbf{q} = \mathbf{0}$ . The phonon Hamiltonian is

$$\hat{H}_{ph}^{MFT} = \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu} \left( \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} + \frac{1}{2} \right) + \sum_\nu \Gamma_\nu^{MFT} (\hat{a}_\nu^\dagger + \hat{a}_\nu). \quad (29)$$

For  $\mathbf{q} \neq 0$ , this is the usual phonon Hamiltonian. For  $\mathbf{q} = 0$ , it is in the form of a charged harmonic oscillator in an electric field. Specifically,

$$\hat{H}_{ph,\mathbf{q}=0}^{MFT} = \sum_\nu \left[ \omega_\nu \left( \hat{a}_\nu^\dagger \hat{a}_\nu + \frac{1}{2} \right) + \Gamma_\nu^{MFT} (\hat{a}_\nu^\dagger + \hat{a}_\nu) \right]. \quad (30)$$

The coupling constant  $\Gamma_\nu^{MFT}$  depends on both the phonon mode symmetry and the symmetry of the charge ordering within the unit cell. The fact that it couples at  $\mathbf{q} = 0$  only is consistent with translational invariance: the density doesn't vary from unit cell to unit cell, so neither does the coupling.

It seems like this is useless: how could this interaction ever renormalize the zone-boundary breathing phonons (which we know to couple most strongly)? The answer comes from the fact that we *must* use a supercell model to capture the charge and spin density wave ordering. For example, in a single-site model, the only possible spin ordering is non-magnetic or ferromagnetic. In either case, the wavelength of the electronic order is infinite, i.e.  $\mathbf{q} = 0$ . To capture shorter wavelength spin ordering, e.g. antiferromagnetism (AFM), we have to use a supercell. The short-wavelength nature of the commensurate spin ordering within a unit cell is then given by Fourier components that are unit cell periodic, i.e.  $\sim \exp(i\mathbf{G} \cdot \boldsymbol{\tau})$ . The same argument follows for charge order.

In a supercell, the phonons are “folded” so that, even with a simple two-atom AFM unit cell, the breathing phonons are already folded to  $\mathbf{q} = 0$  and should be renormalized by the coupling to the AFM order. With more and more unit cells in the supercell, more and more primitive  $\mathbf{q}$  points are shifted to  $\mathbf{q} = 0$  in the supercell Brillouin zone.

Anyway, let us solve the Hamiltonian. We will leave things general to simplify the notation down the road. Define the “stretched” phonon operators

$$\hat{b}_{-\mathbf{q}\nu}^\dagger = \hat{a}_{-\mathbf{q}\nu}^\dagger + \delta_{\mathbf{q}} \frac{\Gamma_\nu^{MFT}}{\omega_\nu} \quad \hat{b}_{\mathbf{q}\nu} = \hat{a}_{\mathbf{q}\nu} + \delta_{\mathbf{q}} \frac{\Gamma_\nu^{MFT}}{\omega_\nu}. \quad (31)$$

For  $\mathbf{q} = 0$ , these are the stretched operators. For  $\mathbf{q} \neq 0$ , these are identical to the original phonon operators. The original operators are

$$\hat{a}_{-\mathbf{q}\nu}^\dagger = \hat{b}_{-\mathbf{q}\nu}^\dagger - \delta_{\mathbf{q}} \frac{\Gamma_\nu^{MFT}}{\omega_\nu} \quad \hat{a}_{\mathbf{q}\nu} = \hat{b}_{\mathbf{q}\nu} - \delta_{\mathbf{q}} \frac{\Gamma_\nu^{MFT}}{\omega_\nu}. \quad (32)$$

With these, the Hamiltonian becomes

$$\begin{aligned}\hat{H}_{ph}^{MFT} &= \sum_{q\nu} \left[ \omega_{q\nu} \left( \hat{b}_{q\nu}^\dagger \hat{b}_{q\nu} + \frac{1}{2} \right) - \delta_q \frac{(\Gamma_\nu^{MFT})^2}{\omega_\nu} \right] = \\ &= \sum_{q\nu} \omega_{q\nu} \left( \hat{b}_{q\nu}^\dagger \hat{b}_{q\nu} + \frac{1}{2} \right) + E_{polaron}^{MFT}.\end{aligned}\quad (33)$$

The last term is a type of “relaxation” energy. It is the energy gained stretching the bonds around the charge modulation on the TM site. In terms of phonons, the coupled phonons are displaced to a new equilibrium amplitude. Define  $E_{polaron}^{MFT} = -\sum_\nu (\Gamma_\nu^{MFT})^2 / \omega_\nu$  where the subscript “polaron” is used because this is basically the energy of a *polaron*; the charge ordering stretches the lattice around the charge rich/poor regions in a combined electron-phonon effect<sup>2</sup>. Importantly, the mean-field coupling does not renormalize the phonon eigenvalues or eigenvectors: the atoms simply vibrate around new equilibrium positions.

### 4.3 Polaron lattice distortion

The real-space displacement of the atoms, in terms of the stretched operators, is

$$\begin{aligned}\hat{x}_{ia} &= \sum_{q\nu} \frac{\epsilon_{q\nu}^a}{\sqrt{2m_a\omega_{q\nu}N}} (\hat{a}_{-q\nu}^\dagger + \hat{a}_{q\nu}) \exp(i\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)}) = \\ &= \sum_{q\nu} \frac{\epsilon_{q\nu}^a}{\sqrt{2m_a\omega_{q\nu}N}} \left( \hat{b}_{-q\nu}^\dagger + \hat{b}_{q\nu} - 2\delta_q \frac{\Gamma_\nu^{MFT}}{\omega_\nu} \right) \exp(i\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)}) \\ &= \sum_{q\nu} \frac{\epsilon_{q\nu}^a}{\sqrt{2m_a\omega_{q\nu}N}} \left( \hat{b}_{-q\nu}^\dagger + \hat{b}_{q\nu} \right) \exp(i\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)}) - 2 \sum_\nu \frac{\epsilon_\nu^a}{\sqrt{2m_a\omega_\nu N}} \frac{\Gamma_\nu^{MFT}}{\omega_\nu}.\end{aligned}\quad (34)$$

Let  $\eta_{q\nu}^a \equiv \epsilon_{q\nu}^a / \sqrt{2m_a\omega_{q\nu}N}$  and define

$$\begin{aligned}\hat{x}_{ia} &= \hat{u}_{ia} + \delta\tau_a \\ \hat{u}_{ia} &= \sum_{q\nu} \eta_{q\nu}^a \left( \hat{b}_{-q\nu}^\dagger + \hat{b}_{q\nu} \right) \exp(i\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)}) \\ \delta\tau_a &= -2 \sum_\nu \eta_\nu^a \frac{\Gamma_\nu^{MFT}}{\omega_\nu}\end{aligned}\quad (35)$$

The coupled phonons are “stretched” and oscillate around a new equilibrium position but at the original frequency.  $\hat{u}_{ia}$  is the displacement operator around the new stretched position;  $\delta\tau_a$  is the displacement from  $\tau_a$  due to the polaron lattice distortion. Note that the stretched position  $\delta\tau_a$  doesn’t depend on the unit cell since, in MFT, the electronic ordering is long

<sup>2</sup> See §1.3.2 in Mahan [1]. He writes a similar expression and discusses the result in terms of polarons; however, in his version, the matrix elements are still  $\mathbf{q}$  dependent (see eqs. 1.237-1.239). The problem is, his matrix elements are  $M_{\mathbf{q}} \sim \sum_i \exp(i\mathbf{q} \cdot \mathbf{R}_i) = N\delta_{\mathbf{q}}$  so that the  $\mathbf{q}$ -dependence vanishes and only the  $\Gamma$  point contributes... I have no idea why he doesn’t drop the  $\mathbf{q}$ -dependence.



wave-length. The new relaxed position is  $\boldsymbol{\tau}'_a = \boldsymbol{\tau}_a + \delta\boldsymbol{\tau}_a$ . The time evolution of the stretched operators is the same as the un-stretched ones. The time dependent displacement operator is

$$\hat{\mathbf{u}}_{ia}(t) = \sum_{\mathbf{q}\nu} \boldsymbol{\eta}_{\mathbf{q}\nu}^a \left[ \hat{b}_{\mathbf{q}\nu}^\dagger \exp(-i(\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)} - \omega_{\mathbf{q}\nu}t)) + \hat{b}_{\mathbf{q}\nu} \exp(i(\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)} - \omega_{\mathbf{q}\nu}t)) \right] \quad (36)$$

To renormalize the phonon frequencies, we need to allow frequency dependence of the electronic order. We do that later by putting the charge and spin fluctuations back into the model in perturbation theory.

The displacement of each atom due the polaron lattice relaxation is

$$\begin{aligned} \delta\boldsymbol{\tau}_a = & -2 \sum_{\nu} \boldsymbol{\eta}_{\nu}^a \frac{\Gamma_{\nu}^{MFT}}{\omega_{\nu}} = -2Ng \sum_{\alpha\nu} \boldsymbol{\epsilon}_{\nu}^a \frac{n_{\alpha} \Xi_{\nu}^a}{\omega_{\nu} \sqrt{2m_a \omega_{\nu} N}} = \\ & -g \sum_{\alpha\nu} \sum_{j(\alpha)} \frac{n_{\alpha} \boldsymbol{\epsilon}_{\nu}^a}{2A_{\alpha}^{(0)} \omega_{\nu}^{3/2}} \left( \boldsymbol{\delta}_j^{(0)} \times \left( \frac{\boldsymbol{\epsilon}_{\nu}^{j+1}}{\sqrt{m_a m_{j+1}}} - \frac{\boldsymbol{\epsilon}_{\nu}^{j-1}}{\sqrt{m_a m_{j-1}}} \right) \right) \cdot \mathbf{z}. \end{aligned} \quad (37)$$

This is a mess, but for a given set of occupations  $\{n_{\alpha\sigma}\}$  and phonons  $\{\omega_{\nu}, \boldsymbol{\epsilon}_{\nu}^a\}$ , we can calculate it.

#### 4.4 The solved model

To summarize, the mean-field Hamiltonian for the electron-phonon system is

$$\begin{aligned} \hat{H}^{MFT} = & \hat{H}_e^{(0)} + \hat{H}_{ph}^{MFT} + E_U^{MFT} = \\ & \sum_{\mathbf{k}n\sigma} \zeta_{\mathbf{k}n\sigma} \hat{d}_{\mathbf{k}n\sigma}^\dagger \hat{d}_{\mathbf{k}n\sigma} + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu} \left( \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} + \frac{1}{2} \right) + \sum_{\nu} \Gamma_{\nu}^{MFT} (\hat{a}_{\nu}^\dagger + \hat{a}_{\nu}) + E_U^{MFT} = \\ & \sum_{\mathbf{k}n\sigma} \zeta_{\mathbf{k}n\sigma} \hat{d}_{\mathbf{k}n\sigma}^\dagger \hat{d}_{\mathbf{k}n\sigma} + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu} \left( \hat{b}_{\mathbf{q}\nu}^\dagger \hat{b}_{\mathbf{q}\nu} + \frac{1}{2} \right) + E_{polaron}^{MFT} + E_U^{MFT} \end{aligned} \quad (38)$$

where the last line is diagonal in both phonons and electrons.

### 5 Electron-phonon interaction in the Hartree approximation

Rather than treating the coupling strength as small, we can do a different type of mean field approximation: we can make a Hartree approximation for the atom displacements. Let

$$\xi_{i\alpha}(\hat{\mathbf{x}}) = \langle \xi_{i\alpha}(\mathbf{x}) \rangle + \delta\xi_{i\alpha}(\hat{\mathbf{x}}) \quad (39)$$

with

$$\begin{aligned}\langle \xi_\alpha(\hat{\mathbf{x}}) \rangle &\equiv \xi_\alpha(\mathbf{x}) = \frac{1}{2A_\alpha^{(0)}} \left( \sum_{j(\alpha)} \boldsymbol{\delta}_j^{(0)} \times (\langle \hat{\mathbf{x}}_{j+1} \rangle - \langle \hat{\mathbf{x}}_{j-1} \rangle) \right) \cdot \mathbf{z} \\ &= \frac{1}{2A_\alpha^{(0)}} \left( \sum_{j(\alpha)} \boldsymbol{\delta}_j^{(0)} \times (\mathbf{x}_{j+1} - \mathbf{x}_{j-1}) \right) \cdot \mathbf{z}\end{aligned}\quad (40)$$

and

$$\delta \xi_{i\alpha}(\hat{\mathbf{x}}) = \frac{1}{2A_\alpha^{(0)}} \left( \sum_{j(i\alpha)} \boldsymbol{\delta}_j^{(0)} \times (\delta \hat{\mathbf{x}}_{j+1} - \delta \hat{\mathbf{x}}_{j-1}) \right) \cdot \mathbf{z}. \quad (41)$$

$\xi_{i\alpha}(\mathbf{x})$  is the classical volume modulation due to static distortion of the lattice and  $\delta \xi_{i\alpha}(\hat{\mathbf{x}})$  is the modulation due to quantum fluctuations. We treat  $\delta \xi_{i\alpha}(\hat{\mathbf{x}})$  as small.

Note that these equations will be very unwieldy... especially if we take derivatives of them with respect to  $\mathbf{x}_a$  to minimize the free energy. To that end, it is probably better to work in the phonon basis. Define  $\hat{A}_{\mathbf{q}\nu} \equiv \hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}$  as the mode amplitude. Then

$$\xi_\alpha(\mathbf{x}) = \sum_{\mathbf{q}\nu} \Xi_{\mathbf{q}\nu}^\alpha \langle \hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu} \rangle \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}) = \sum_{\mathbf{q}\nu} \Xi_{\mathbf{q}\nu}^\alpha \hat{A}_{\mathbf{q}\nu} \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}) \quad (42)$$

with  $\langle \hat{A}_{\mathbf{q}\nu} \rangle = \hat{A}_{\mathbf{q}\nu}$  and

$$\delta \xi_{i\alpha}(\hat{\mathbf{x}}) = \sum_{\mathbf{q}\nu} \Xi_{\mathbf{q}\nu}^\alpha (\delta \hat{a}_{-\mathbf{q}\nu}^\dagger + \delta \hat{a}_{\mathbf{q}\nu}) \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}) = \sum_{\mathbf{q}\nu} \Xi_{\mathbf{q}\nu}^\alpha \delta \hat{A}_{\mathbf{q}\nu} \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}). \quad (43)$$

We can simplify the expectation value a little by summing over unit cells:

$$\sum_i \xi_\alpha(\mathbf{x}) = N \xi_\alpha(\mathbf{x}) = \sum_{\mathbf{q}\nu} \Xi_{\mathbf{q}\nu}^\alpha A_{\mathbf{q}\nu} \sum_i \exp(i\mathbf{q} \cdot \mathbf{r}_{i\alpha}^{(0)}) = N \sum_{\mathbf{q}\nu} \delta_{\mathbf{q}0} \Xi_{\mathbf{q}\nu}^\alpha A_{\mathbf{q}\nu} \quad (44)$$

i.e.

$$\xi_\alpha(\mathbf{x}) = \sum_\nu \Xi_\nu^\alpha A_\nu \quad (45)$$

where  $A_\nu$  are the mean phonon amplitudes. Recall that momentum dependent quantities with no momentum subscript are to be evaluated at  $\mathbf{q} = 0$ . Using eq. 9, we can calculate the mean phonon amplitude from

$$\langle \hat{\mathbf{x}}_{ia} \rangle = \mathbf{x}_a = \sum_{\mathbf{q}\nu} \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^a}{\sqrt{2m_a \omega_{\mathbf{q}\nu} N}} A_{\mathbf{q}\nu} \exp(i\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)}) \quad (46)$$

where we assumed homogeneity, i.e. the mean displacement is the same from unit cell to unit cell. We can simplify this too by summing over unit cells:

$$\sum_i \mathbf{x}_a = N \mathbf{x}_a = \sum_{\mathbf{q}\nu} \frac{\boldsymbol{\epsilon}_{\mathbf{q}\nu}^a}{\sqrt{2m_a \omega_{\mathbf{q}\nu} N}} A_{\mathbf{q}\nu} \sum_i \exp(i\mathbf{q} \cdot \mathbf{r}_{ia}^{(0)}) = N \sum_\nu \frac{\boldsymbol{\epsilon}_\nu^a}{\sqrt{2m_a \omega_\nu N}} A_\nu \quad (47)$$

i.e.

$$\sqrt{2m_a N} \mathbf{x}_a = \sum_{\nu} \epsilon_{\nu}^a \frac{A_{\nu}}{\sqrt{\omega_{\nu}}}. \quad (48)$$

We can use orthogonality of the eigenvectors,  $\sum_a \epsilon_{\mathbf{q}\mu}^{\dagger a} \cdot \epsilon_{\mathbf{q}\nu}^a = \delta_{\mu\nu}$ . Then<sup>3</sup>

$$A_{\nu} = \sum_a \sqrt{2m_a \omega_{\nu} N} \epsilon_{\nu}^a \cdot \mathbf{x}_a. \quad (49)$$

In the volume modulation,

$$\xi_{\alpha}(\mathbf{x}) = \sum_{a\nu} \Xi_{\nu}^{\alpha} \sqrt{2m_a \omega_{\nu} N} \epsilon_{\nu}^a \cdot \mathbf{x}_a. \quad (50)$$

$\Xi_{\nu}^{\alpha} \sim N^{-1/2}$ , so this is intensive as it should be. Importantly, this thing will be easy to take derivatives of with respect to coordinates  $\mathbf{x}_a$  and we will already have calculated  $\Xi_{\nu}^{\alpha}$  in the perturbation approximation above.

If we allow the atoms to stretch to new equilibrium positions, with displacements  $\delta\boldsymbol{\tau}_a$ , we can write  $\hat{\mathbf{x}}_{ia} = \hat{\mathbf{u}}_{ia} + \delta\boldsymbol{\tau}_a$  with  $\hat{\mathbf{u}}_{ia}$  the operator for displacement around the new equilibrium position. Then  $\langle \hat{\mathbf{x}}_{ia} \rangle \equiv \mathbf{x}_a = \langle \hat{\mathbf{u}}_{ia} \rangle + \delta\boldsymbol{\tau}_a = \delta\boldsymbol{\tau}_a \dots$   $\delta\boldsymbol{\tau}_a$  could be the polaron displacements from above :)

## 5.1 Electron-phonon interaction

Now let us use this to decouple the electron-phonon interaction:

$$\begin{aligned} \xi_{i\alpha}(\hat{\mathbf{x}}) \hat{n}_{i\alpha} &= (\xi_{\alpha}(\mathbf{x}) + \delta\xi_{i\alpha}(\hat{\mathbf{x}}))(n_{\alpha} + \delta\hat{n}_{i\alpha}) \approx \xi_{\alpha}(\mathbf{x})n_{\alpha} + \delta\xi_{i\alpha}(\hat{\mathbf{x}})n_{\alpha} + \xi_{\alpha}(\mathbf{x})\delta\hat{n}_{i\alpha} \\ &= \xi_{i\alpha}(\hat{\mathbf{x}})n_{\alpha} + \xi_{\alpha}(\mathbf{x})\hat{n}_{i\alpha} - \xi_{\alpha}(\mathbf{x})n_{\alpha}. \end{aligned} \quad (51)$$

We dropped terms  $O(\delta^2)$ . Then

$$\hat{H}_{eph}^{MFT} = g \sum_{i\alpha} (\xi_{i\alpha}(\hat{\mathbf{x}})n_{\alpha} + \xi_{\alpha}(\mathbf{x})\hat{n}_{i\alpha}) - Ng \sum_{\alpha} \xi_{\alpha}(\mathbf{x})n_{\alpha}. \quad (52)$$

Note that the Hartree approximation to the electron-phonon interaction recovers the term we found above by treating the interaction as a perturbation, but also provides two more terms we missed before!

Decoupling the electron and phonon operators in mean-field theory is apparently a better approximation than lowest order perturbation theory. However, there is a new complication: we have to minimize the free energy with respect to occupations  $n_{\alpha\sigma}$  and displacements  $\mathbf{x}_a$ , since we are looking for the minimum with respect to both charge order and lattice distortions. There will be self-consistency conditions for both charge and displacements. A good approach is probably to solve the equations in the simple perturbation approximation first to find the polaron displacements and then use the displacements as an initial guess for the coupled self-consistent equations.

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<sup>3</sup> Note that at  $\mathbf{q} = 0$ , the eigenvectors are real so that  $\epsilon_{\mathbf{q}\nu}^{\dagger a} = \epsilon_{\mathbf{q}\nu}^a$

Anyway, these equations are free (quadratic in operators) and can be solved by diagonalization. This is cool because the mean phonon coordinates show up in the electronic Hamiltonian, i.e. they will change the electron eigenvalues!

## 5.2 The model

Let us separate the mean field Hamiltonian into electron, phonon, and classical parts. The electronic part is

$$\begin{aligned}\hat{H}_e^{MFT} &= - \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} - \sum_{i\alpha} (\mu_0 - g\xi_\alpha(\mathbf{x})) \hat{n}_{i\alpha} + U \sum_{i\alpha} (n_{\alpha\uparrow} \hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow} \hat{n}_{i\alpha\uparrow}) \\ &= - \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} - \sum_{i\alpha} \mu_\alpha(\mathbf{x}) \hat{n}_{i\alpha} + U \sum_{i\alpha} (n_{\alpha\uparrow} \hat{n}_{i\alpha\downarrow} + n_{\alpha\downarrow} \hat{n}_{i\alpha\uparrow}).\end{aligned}\quad (53)$$

Given a guess for the initial displacements, we can calculate the site dependent chemical potentials and simply diagonalize the Hamiltonian.

The phonon Hamiltonian is

$$\hat{H}_{ph}^{MFT} = \sum_{ia} \frac{\hat{\mathbf{p}}_{ia}^2}{2m_a} + \frac{1}{2} \sum_{ijab} \hat{\mathbf{x}}_{ia} \Phi_{ij}^{ab} \hat{\mathbf{x}}_{jb} + g \sum_{i\alpha} \xi_{i\alpha}(\hat{\mathbf{x}}) n_{i\alpha}.\quad (54)$$

Note that this is the same as we found in perturbation theory above: i.e. the solution will be the same eigenvectors and frequencies oscillating around stretched positions.

The classical energy is

$$\begin{aligned}E_{cl}^{MFT} &= -NU \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} - Ng \sum_{\alpha} \xi_{\alpha}(\mathbf{x}) n_{\alpha} \\ &= -N \sum_{\alpha} (U n_{\alpha\downarrow} n_{\alpha\uparrow} + g n_{\alpha}).\end{aligned}\quad (55)$$

## 6 Many body theory

Now we plug back in interactions that we neglected above in mean-field theory. We assumed that operators could be separated into a mean part and a fluctuation and that the fluctuations were small. We then found the mean part that minimized the energy. We can use the Hamiltonian with these mean parts in it as the unperturbed Hamiltonian and reintroduce the fluctuations as a perturbation.

We will use the diagonal electron and phonon Hamiltonians as the unperturbed Hamiltonian: FORGOT POLARON ENERGY HERE AND ABOVE

$$\begin{aligned}\hat{H}_{(0)} &= \hat{H}_e^{MFT} + \hat{H}_{ph}^{MFT} = \\ &= \sum_{\mathbf{k}n\sigma} \zeta_{\mathbf{k}n\sigma} \hat{d}_{\mathbf{k}n\sigma}^\dagger \hat{d}_{\mathbf{k}n\sigma} + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu} \left( \hat{b}_{\mathbf{q}\nu}^\dagger \hat{b}_{\mathbf{q}\nu} + \frac{1}{2} \right) + E_{cl}^{MFT}.\end{aligned}\quad (56)$$

## 6.1 Electron-electron interaction

The electron-electron interaction we ignored was

$$\hat{H}_{ee} = U \sum_{i\alpha} \delta \hat{n}_{i\alpha\uparrow} \delta \hat{n}_{i\alpha\downarrow} = U \sum_{i\alpha} (\hat{n}_{i\alpha\uparrow} - n_{\alpha\uparrow})(\hat{n}_{i\alpha\downarrow} - n_{\alpha\downarrow}) \quad (57)$$

## 6.2 Electron-phonon interaction

The electron-electron interaction is

$$\hat{H}_{eph} = g \sum_{i\alpha} \xi_{i\alpha}(\hat{\mathbf{x}}) \hat{n}_{i\alpha} \quad (58)$$

which is basically a local electronic potential that depends dynamically on the atomic displacements. It couples the electron and phonon operators. In this form, we can't do that much with it so we rewrite it in momentum space. Using eq. 12 and the Fourier transform of the electron operators

$$\begin{aligned} \hat{c}_{i\alpha\sigma} &= N^{-1/2} \sum_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{r}_{i\alpha}^{(0)}) \hat{c}_{\mathbf{k}\alpha\sigma} \\ \hat{c}_{i\alpha\sigma}^\dagger &= N^{-1/2} \sum_{\mathbf{k}} \exp(-i\mathbf{k} \cdot \mathbf{r}_{i\alpha}^{(0)}) \hat{c}_{\mathbf{k}\alpha\sigma}^\dagger \end{aligned} \quad (59)$$

we can rewrite the interaction as

$$\hat{H}_{eph} = g \sum_{\mathbf{k}\alpha\sigma} \sum_{\mathbf{q}\nu} \Xi_{\mathbf{q}\nu}^\alpha (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \hat{c}_{\mathbf{k}+\mathbf{q}\alpha\sigma}^\dagger \hat{c}_{\mathbf{k}\alpha\sigma}. \quad (60)$$

This is better, but we want to use the diagonal electron operators. They are related to the local ones by

$$\hat{c}_{\mathbf{k}\alpha\sigma}^\dagger = \sum_n \hat{d}_{\mathbf{k}n\sigma}^\dagger [\hat{U}_{\mathbf{k}\sigma}^\dagger]^{n\alpha} \quad \hat{c}_{\mathbf{k}\alpha\sigma} = \sum_n \hat{d}_{\mathbf{k}n\sigma} [\hat{U}_{\mathbf{k}\sigma}]^{\alpha n} \quad (61)$$

with  $\hat{U}_{\mathbf{k}\sigma}$  the unitary matrix that diagonalizes the Bloch Hamiltonian for electrons with spin  $\sigma$  and momentum  $\mathbf{k}$ . Then

$$\begin{aligned} \hat{H}_{eph} &= \sum_{\mathbf{k}n\sigma} \sum_{\mathbf{q}\nu} \left( g \sum_{\alpha} \Xi_{\mathbf{q}\nu}^\alpha [\hat{U}_{\mathbf{k}+\mathbf{q}\sigma}^\dagger]^{n\alpha} [\hat{U}_{\mathbf{k}\sigma}]^{\alpha n} \right) (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \hat{d}_{\mathbf{k}+\mathbf{q}n\sigma}^\dagger \hat{d}_{\mathbf{k}m\sigma} \\ &= \sum_{\mathbf{k}n\sigma} \sum_{\mathbf{q}\nu} \Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu} (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \hat{d}_{\mathbf{k}+\mathbf{q}n\sigma}^\dagger \hat{d}_{\mathbf{k}m\sigma} \end{aligned} \quad (62)$$

where we defined the matrix element

$$\Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu} = g \sum_{\alpha} \Xi_{\mathbf{q}\nu}^\alpha [\hat{U}_{\mathbf{k}+\mathbf{q}\sigma}^\dagger]^{n\alpha} [\hat{U}_{\mathbf{k}\sigma}]^{\alpha m}. \quad (63)$$

This depends on the symmetry of both the phonon modes and the electrons, on the phonon and electron momenta, and on the electron spin through the eigenvectors.

Finally, we can go to the basis of the stretched phonon operators, eq. 32

$$\begin{aligned}
 \hat{H}_{eph} &= \sum_{\mathbf{k}n\mathbf{m}\sigma} \sum_{\mathbf{q}\nu} \Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu} (\hat{a}_{-\mathbf{q}\nu}^\dagger + \hat{a}_{\mathbf{q}\nu}) \hat{d}_{\mathbf{k}+\mathbf{q}n\sigma}^\dagger \hat{d}_{\mathbf{k}\mathbf{m}\sigma} \\
 &= \sum_{\mathbf{k}n\mathbf{m}\sigma} \sum_{\mathbf{q}\nu} \Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu} (\hat{b}_{-\mathbf{q}\nu}^\dagger + \hat{b}_{\mathbf{q}\nu}) \hat{d}_{\mathbf{k}+\mathbf{q}n\sigma}^\dagger \hat{d}_{\mathbf{k}\mathbf{m}\sigma} - 2 \sum_{\mathbf{k}n\mathbf{m}\sigma} \sum_{\nu} \frac{\Gamma_{\nu}^{MFT}}{\omega_{\nu}} \Gamma_{\mathbf{k}\mathbf{0}\sigma}^{mn\nu} \hat{d}_{\mathbf{k}n\sigma}^\dagger \hat{d}_{\mathbf{k}\mathbf{m}\sigma}
 \end{aligned} \tag{64}$$

## A Equations from literature

The full phonon propagator at finite temperature is given by

$$D(\mathbf{q}\nu, i\Omega_n) = \frac{1}{D_0^{-1}(\mathbf{q}\nu, i\Omega_n) - \Pi(\mathbf{q}\nu, i\Omega_n)} \quad (65)$$

with

$$D_0(\mathbf{q}\nu, i\Omega_n) = \frac{1}{i\Omega_n - \omega_{\mathbf{q}\nu}} - \frac{1}{i\Omega_n + \omega_{\mathbf{q}\nu}} = \frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_n)^2 - \omega_{\mathbf{q}\nu}^2} \quad (66)$$

the free (adiabatically screened) phonon propagator (eqs. 3.75-3.76 in [1]).  $i\Omega_n$  is Bosonic Matsubara frequency and  $\omega_{\mathbf{q}\nu}$  is the adiabatic phonon frequency. Non-adiabatic contributions to the full phonon propagator are given by the phonon self-energy, which in the lowest order Migdal approximation is [2, 3]:

$$\Pi(\mathbf{q}\nu, i\Omega_n) = N^{-1} \sum_{\mathbf{k}n m \sigma} |\Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu}|^2 \frac{f(\epsilon_{\mathbf{k}m\sigma}) - f(\epsilon_{\mathbf{k}+\mathbf{q}n\sigma})}{i\Omega_n + \epsilon_{\mathbf{k}m\sigma} - \epsilon_{\mathbf{k}+\mathbf{q}n\sigma}}. \quad (67)$$

Explicitly

$$D(\mathbf{q}\nu, i\Omega_n) = \frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_n)^2 - \omega_{\mathbf{q}\nu}^2 - 2\omega_{\mathbf{q}\nu}\Pi(\mathbf{q}\nu, i\Omega_n)} \quad (68)$$

Analytic continuation of these functions to the infinitesimally shifted positive real axis,  $i\Omega_n \rightarrow \omega + i0^+$ , yields the real-time retarded propagator (pg. 328 in [4], eqs. 3.111-3.112 in [1]):

$$D^R(\mathbf{q}\nu, \omega) = \frac{1}{[D_0^R(\mathbf{q}\nu, \omega)]^{-1} - \Pi^R(\mathbf{q}\nu, \omega)}. \quad (69)$$

The retarded free propagator is (pg. 155 in [5] but note the “-” sign in front of  $i0^+$ . My independent result rather agrees with eq. 8.76 in [6].)

$$D_0^R(\mathbf{q}\nu, \omega) = \frac{2\omega_{\mathbf{q}\nu}}{\omega^2 - \omega_{\mathbf{q}\nu}^2 + 2i\omega 0^+} = \frac{2\omega_{\mathbf{q}\nu}}{\omega^2 - \omega_{\mathbf{q}\nu}^2 + i0^+ \text{sgn}(\omega)} \quad (70)$$

and the full propagator is

$$D^R(\mathbf{q}\nu, \omega) = \frac{2\omega_{\mathbf{q}\nu}}{\omega^2 - \omega_{\mathbf{q}\nu}^2 + 2i\omega 0^+ - 2\omega_{\mathbf{q}\nu}\Pi^R(\mathbf{q}\nu, \omega)} = \frac{1}{(\omega^2 - \omega_{\mathbf{q}\nu}^2)/2\omega_{\mathbf{q}\nu} + 2i\omega 0^+ - \Pi^R(\mathbf{q}\nu, \omega)} \quad (71)$$

Fourier transforming to the time domain,

$$D^R(\mathbf{q}\nu, t) = \int \frac{dt}{2\pi} D^R(\mathbf{q}\nu, \omega) \exp(-i\omega t). \quad (72)$$

...

The phonon spectral function is (the definition is not unique but this form is given in eq.

7.29 in [4] and in eq. 3.114 in [1]):

$$\begin{aligned} B(\mathbf{q}, \omega) &= \sum_{\nu} B(\mathbf{q}\nu, \omega) \\ B(\mathbf{q}\nu, \omega) &= -2\text{Im}[D^R(\mathbf{q}\nu, \omega)]. \end{aligned} \quad (73)$$

Using the identity

$$\frac{1}{x - iy} = \frac{x + iy}{(x - iy)(x + iy)} = \frac{x}{x^2 + y^2} + i\frac{y}{x^2 + y^2}, \quad (74)$$

we can identify  $x = (\omega^2 - \omega_{\mathbf{q}\nu}^2 - 2\omega_{\mathbf{q}\nu}\text{Re}[\Pi^R(\mathbf{q}\nu, \omega)])/2\omega_{\mathbf{q}\nu}$  and  $y = 2\omega_{\mathbf{q}\nu}\text{Im}[\Pi^R(\mathbf{q}\nu, \omega)] - 2\omega 0^+$  where we drop the infinitesimal  $0^+$  in favor of  $\text{Im}[\Pi^R(\mathbf{q}\nu, \omega)]$ . Then the spectral function is

$$B(\mathbf{q}\nu, \omega) = -\frac{2\omega_{\mathbf{q}\nu}(2\omega_{\mathbf{q}\nu}\text{Im}[\Pi^R(\mathbf{q}\nu, \omega)] - 2\omega 0^+)}{(\omega^2 - \omega_{\mathbf{q}\nu}^2 - 2\omega_{\mathbf{q}\nu}\text{Re}[\Pi^R(\mathbf{q}\nu, \omega)])^2 + (2\omega_{\mathbf{q}\nu}\text{Im}[\Pi^R(\mathbf{q}\nu, \omega)] - 2\omega 0^+)^2}. \quad (75)$$

We need the analytic continuation of the retarded self-energy (<https://docs.epw-code.org/doc/Electron-phononCoupling.html> and eq. 145 in [2]):

$$\Pi^R(\mathbf{q}\nu, \omega) = N^{-1} \sum_{\mathbf{k}n\mathbf{m}\sigma} |\Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu}|^2 \left[ \frac{f(\epsilon_{\mathbf{k}+\mathbf{q}n\sigma}) - f(\epsilon_{\mathbf{k}\mathbf{m}\sigma})}{\epsilon_{\mathbf{k}+\mathbf{q}n\sigma} - \epsilon_{\mathbf{k}\mathbf{m}\sigma} - \omega - i0^+} - \frac{f(\epsilon_{\mathbf{k}+\mathbf{q}n\sigma}) - f(\epsilon_{\mathbf{k}\mathbf{m}\sigma})}{\epsilon_{\mathbf{k}+\mathbf{q}n\sigma} - \epsilon_{\mathbf{k}\mathbf{m}\sigma}} \right]. \quad (76)$$

The infinitesimal poses a problem here. Fortunately we can calculate the imaginary part using the identity  $1/(x + i0^+) = \mathcal{P}[1/x] - i\pi\delta(x)$ . Then

$$\text{Im}[\Pi^R(\mathbf{q}\nu, \omega)] = -\frac{\pi}{N} \sum_{\mathbf{k}n\mathbf{m}\sigma} |\Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu}|^2 [f(\epsilon_{\mathbf{k}\mathbf{m}\sigma}) - f(\epsilon_{\mathbf{k}+\mathbf{q}n\sigma})]\delta(\omega + \epsilon_{\mathbf{k}\mathbf{m}\sigma} - \epsilon_{\mathbf{k}+\mathbf{q}n\sigma}) \quad (77)$$

and we can calculate the real part from the Kramers-Kronig relation:

$$\begin{aligned} \text{Re}[\Pi^R(\mathbf{q}\nu, \omega)] &= \frac{1}{\pi} \mathcal{P} \int d\omega' \text{Im}[\Pi^R(\mathbf{q}\nu, \omega')] \frac{1}{\omega' - \omega} = \\ &= -\frac{1}{N} \sum_{\mathbf{k}n\mathbf{m}\sigma} |\Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu}|^2 [f(\epsilon_{\mathbf{k}\mathbf{m}\sigma}) - f(\epsilon_{\mathbf{k}+\mathbf{q}n\sigma})] \mathcal{P} \int d\omega' \delta(\omega' + \epsilon_{\mathbf{k}\mathbf{m}\sigma} - \epsilon_{\mathbf{k}+\mathbf{q}n\sigma}) \frac{1}{\omega' - \omega}. \end{aligned} \quad (78)$$

If we naively calculate the integral, the real part is

$$\begin{aligned} \text{Re}[\Pi^R(\mathbf{q}\nu, \omega)] &= \\ &= -\frac{1}{N} \sum_{\mathbf{k}n\mathbf{m}\sigma} |\Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu}|^2 [f(\epsilon_{\mathbf{k}\mathbf{m}\sigma}) - f(\epsilon_{\mathbf{k}+\mathbf{q}n\sigma})] \mathcal{P} \int d\omega' \delta(\omega' + \epsilon_{\mathbf{k}\mathbf{m}\sigma} - \epsilon_{\mathbf{k}+\mathbf{q}n\sigma}) \frac{1}{\omega' - \omega} = \\ &= \frac{1}{N} \sum_{\mathbf{k}n\mathbf{m}\sigma} |\Gamma_{\mathbf{k}\mathbf{q}\sigma}^{mn\nu}|^2 [f(\epsilon_{\mathbf{k}\mathbf{m}\sigma}) - f(\epsilon_{\mathbf{k}+\mathbf{q}n\sigma})] \frac{1}{\epsilon_{\mathbf{k}\mathbf{m}\sigma} - \epsilon_{\mathbf{k}+\mathbf{q}n\sigma} + \omega}. \end{aligned} \quad (79)$$



## B Additional reading

Exp. IXS paper [7] mentions/cites that in cuprates, softening only happens along 100 and only big dip at single  $q$ . In other materials (La<sub>2</sub>NiO<sub>4</sub> and perovskites) softening is along 110 and 100. Comments that could be due to CDW. Note, in La<sub>2</sub>NiO<sub>4</sub>, CDW vector is along diagonal, while in cuprates is along edge.

Wang [8] gives good discussion of approximations and bare vs screened stuff. Copy them lol

For phonon linewidth equations etc. see Giustino [2]

Giustino paper says optimal and overdoped are well described by mean field, but not underdoped [9].

ref. [10] gives doping,  $U$ , and energetics of different magnetic configurations for doped LSCO. They also use HTT (I4/mmm) structure, same as [9]. This makes sense since doped LSCO is HTT.

refs. [11, 12] give LTT structure... but the order is not tetragonal?

Giustino gives good discussion of bare vs screened vertex in self energy as well as an explanation of adiabatic vs nonadiabatic frequencies etc. instead of bare vs screened ones. my dispersions are adiabatic, the renormalization is non adiabatic [13]. Also see Wang and Berges [8, 14] and [15] for calculation separated into adiabatic/non adiabatic

Expression for phonon spectral function is general, self energy depends on model/approximation. For spectral function, see <https://phonopy.github.io/phonopy/command-options.html#self-energy-options> and <https://ollehellman.github.io/program/lineshape.html>

Analytic continuation: [16, 17]

for approximation to  $\delta f_n$  with smearing, see eq. 79 in ref. [14]

Numerical Kramers-Kronig [18]. See <https://www.physicsforums.com/threads/kramers-kronig-parity-and-delta-function.1046594/> for analytical result?

DFT paper on LSCO showing gap and magnons vs structural phase for many DFT functionals [19].

Exp. papers for Fermi surface vs doping in LSCO [20, 21]

Frozen phonon elph coupling: [22] and eq. 41 in [2].

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