# Electron-phonon coupling in infinite-layer nickelates

Hanghui Chen

December 26, 2020

Here we provide some simple modelling of electron-phonon coupling in the normal and superconducting states of infinite-layer nickelates. Throughout the notes, we use:

$$k = (\mathbf{k}, i\omega_n) \tag{1}$$

$$q = (\mathbf{q}, i\Omega_m) \tag{2}$$

where the Matsubara frequencies are:

$$\omega_n = \frac{(2n+1)\pi}{\beta} = (2n+1)\pi T \tag{3}$$

$$\Omega_m = \frac{2m\pi}{\beta} = 2m\pi T \tag{4}$$

where $T$ is the temperature and $\beta$ is the inverse temperature.

# 1 Single-orbital case

## 1.1 Normal state

In the normal state, the electron-phonon self-energy

$$\Sigma_{\text{ep}}(k) = \Sigma_{\text{ep}}(\mathbf{k}, i\omega_n) = -\frac{1}{\beta}\sum_{k',\nu} |g_\nu(\mathbf{k}, \mathbf{k}')|^2 D_\nu(k-k') G_0(k') \tag{5}$$

where $\nu$ is the phonon branch. Introduce the phonon momentum $q$:

$$q = k' - k \tag{6}$$

Therefore we get:

$$\Sigma_{\text{ep}}(k) = \Sigma_{\text{ep}}(\mathbf{k}, i\omega_n) = -\frac{1}{\beta}\sum_{q,\nu} |g_\nu(\mathbf{k},\mathbf{q})|^2 D_\nu(-q) G_0(k+q) \tag{7}$$

Because

$$D_\nu(-q) = D_\nu(q) \tag{8}$$

we get:

$$\Sigma_{\text{ep}}(k) = \Sigma_{\text{ep}}(\mathbf{k}, i\omega_n) = -\frac{1}{\beta}\sum_{q,\nu} |g_\nu(\mathbf{k},\mathbf{q})|^2 D_\nu(q) G_0(k+q) \tag{9}$$

The phonon Green function is:

$$D_\nu(q) = \frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_m)^2 - \omega_{\mathbf{q}\nu}^2} \tag{10}$$

The electron Green function is:

$$G_0(k) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} \tag{11}$$

Therefore we have:

$$\Sigma_{\text{ep}}(\mathbf{k}, i\omega_n) = -\frac{1}{\beta}\sum_{\Omega_m,\nu} \int \frac{d\mathbf{q}}{V_{\text{BZ}}} |g_\nu(\mathbf{k},\mathbf{q})|^2 \frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_m)^2 - \omega_{\mathbf{q}\nu}^2} \frac{1}{i\omega_n + i\Omega_m - \epsilon_{\mathbf{k}+\mathbf{q}}} \tag{12}$$

where $V_{\text{BZ}}$ is the volume of the phonon Brillouin zone.

The sum over the phonon Matsubara frequencies can be carried out analytically:

$$-\frac{1}{\beta}\sum_{\Omega_m}\frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_m)^2-\omega_{\mathbf{q}\nu}^2}\frac{1}{i\omega_n+i\Omega_m-\epsilon_{\mathbf{k}+\mathbf{q}}}= \tag{13}$$
$$\frac{n_B(\omega_{\mathbf{q}\nu})+n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}+\omega_{\mathbf{q}\nu}}+\frac{n_B(\omega_{\mathbf{q}\nu})+1-n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}-\omega_{\mathbf{q}\nu}}$$

where

$$n_B(\omega_{\mathbf{q}\nu})=\frac{1}{e^{\beta\omega_{\mathbf{q}\nu}}-1} \tag{14}$$

$$n_F(\epsilon_{\mathbf{k}})=\frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)}+1} \tag{15}$$

The electron-phonon self-energy is recast into:

$$\Sigma_{\mathrm{ep}}(\mathbf{k},i\omega_n)=\sum_{\nu}\int\frac{d\mathbf{q}}{V_{\mathrm{BZ}}}|g_\nu(\mathbf{k},\mathbf{q})|^2\left[\frac{n_B(\omega_{\mathbf{q}\nu})+n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}+\omega_{\mathbf{q}\nu}}+\frac{n_B(\omega_{\mathbf{q}\nu})+1-n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}-\omega_{\mathbf{q}\nu}}\right] \tag{16}$$

In a discrete version, we have:

$$\Sigma_{\mathrm{ep}}(\mathbf{k},i\omega_n)=\sum_{\mathbf{q}\nu}w_{\mathbf{q}}|g_\nu(\mathbf{k},\mathbf{q})|^2\left[\frac{n_B(\omega_{\mathbf{q}\nu})+n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}+\omega_{\mathbf{q}\nu}}+\frac{n_B(\omega_{\mathbf{q}\nu})+1-n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}-\omega_{\mathbf{q}\nu}}\right] \tag{17}$$

where $w_{\mathbf{q}}$ is the weight of $\mathbf{q}$.

The interacting Green function $G(k)$ is obtained via Dyson equation:

$$G^{-1}(k)=G_0^{-1}(k)-\Sigma(k) \tag{18}$$

In our case, $G(k)$ is:

$$G(k)=G(\mathbf{k},i\omega_n)= \tag{19}$$
$$\left\{i\omega_n-\epsilon_{\mathbf{k}}-\sum_{\mathbf{q}\nu}w_{\mathbf{q}}|g_\nu(\mathbf{k},\mathbf{q})|^2\left[\frac{n_B(\omega_{\mathbf{q}\nu})+n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}+\omega_{\mathbf{q}\nu}}+\frac{n_B(\omega_{\mathbf{q}\nu})+1-n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}-\omega_{\mathbf{q}\nu}}\right]\right\}^{-1}$$

Doing analytical continuation $i\omega_n\to\omega+i\delta$:

$$G(\mathbf{k},\omega+i\delta) = \left\{\omega+i\delta-\epsilon_{\mathbf{k}}-\sum_{\mathbf{q}\nu} w_{\mathbf{q}}|g_\nu(\mathbf{k},\mathbf{q})|^2\left[\frac{n_B(\omega_{\mathbf{q}\nu})+n_F(\epsilon_{\mathbf{k+q}})}{\omega+i\delta-\epsilon_{\mathbf{k+q}}+\omega_{\mathbf{q}\nu}}+\frac{n_B(\omega_{\mathbf{q}\nu})+1-n_F(\epsilon_{\mathbf{k+q}})}{\omega+i\delta-\epsilon_{\mathbf{k+q}}-\omega_{\mathbf{q}\nu}}\right]\right\}^{-1} \tag{20}$$

where $\delta$ is infinitesimal. Numerically we set $\delta$ to be a small number.

Finally we calculate the spectral function:

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega+i\delta) \tag{21}$$

We note that there is another way to express the self-energy that arises from the electron-phonon coupling. Eq. (17) on the real-axis is:

$$\Sigma_{\mathrm{ep}}(\mathbf{k},\omega) = \sum_{\mathbf{q}\nu} w_{\mathbf{q}}|g_\nu(\mathbf{k},\mathbf{q})|^2\left[\frac{n_B(\omega_{\mathbf{q}\nu})+n_F(\epsilon_{\mathbf{k+q}})}{\omega+i\delta-\epsilon_{\mathbf{k+q}}+\omega_{\mathbf{q}\nu}}+\frac{n_B(\omega_{\mathbf{q}\nu})+1-n_F(\epsilon_{\mathbf{k+q}})}{\omega+i\delta-\epsilon_{\mathbf{k+q}}-\omega_{\mathbf{q}\nu}}\right] \tag{22}$$

in which we replace $\omega$ by $\epsilon_{\mathbf{k}}$. This leads to:

$$\Sigma_{\mathrm{ep}}(\mathbf{k}) = \sum_{\mathbf{q}\nu} w_{\mathbf{q}}|g_\nu(\mathbf{k},\mathbf{q})|^2\left[\frac{n_B(\omega_{\mathbf{q}\nu})+n_F(\epsilon_{\mathbf{k+q}})}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k+q}}+\omega_{\mathbf{q}\nu}+i\delta}+\frac{n_B(\omega_{\mathbf{q}\nu})+1-n_F(\epsilon_{\mathbf{k+q}})}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k+q}}-\omega_{\mathbf{q}\nu}+i\delta}\right] \tag{23}$$

## 1.2 Superconducting state

In the superconducting state, we introduce Nambu-Eliashberg formalism. The Pauli matrices are:

$$\hat{\tau}_0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \quad \hat{\tau}_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \quad \hat{\tau}_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \quad \hat{\tau}_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{24}$$

We use $\hat{A}$ on the symbol $A$ to refer to a matrix.

A general self-energy $\Sigma(k)$ can be parameterized as:

$$\hat{\Sigma}(k) = i\omega_n\left(1-Z(k)\right)\hat{\tau}_0+\chi(k)\hat{\tau}_3+\phi(k)\hat{\tau}_1+\overline{\phi}(k)\hat{\tau}_2 \tag{25}$$

We can choose a gauge so that $\overline{\phi}(k) = 0$.

In the superconducting state with a weak coupling, we may set:

$$Z(k) \to 1 \quad \chi(k) \to 0 \quad \Delta(k) = \frac{\phi(k)}{Z(k)} \to \phi(k) = \Delta(k) \tag{26}$$

Therefore we have:

$$\hat{\Sigma}_{\rm sc}(k) = \Delta(k)\hat{\tau}_1 \tag{27}$$

For a $d$-wave superconductivity in two-dimension, we have:

$$\Delta(k) = \Delta_{\mathbf{k}} = \Delta_0 \left[\cos(k_x a) - \cos(k_y a)\right]/2 \tag{28}$$

where $\Delta_0$ and $a$ are constants. We note that the frequency dependence in $\Delta(k)$ disappears.

With the above approximation, the superconducting Green function is:

$$\hat{G}_{\rm sc}^{-1}(k) = \hat{G}_0^{-1}(k) - \Sigma_{\rm sc}(k) \tag{29}$$

In the superconducting state, the non-interacting Green function is:

$$\hat{G}_0^{-1}(k) = i\omega_n\hat{\tau}_0 - \epsilon_{\mathbf{k}}\hat{\tau}_3 \tag{30}$$

Therefore we have:

$$\hat{G}_{\rm sc}^{-1}(k) = i\omega_n\hat{\tau}_0 - \epsilon_{\mathbf{k}}\hat{\tau}_3 - \Delta_{\mathbf{k}}\hat{\tau}_1 \tag{31}$$

Or more explicitly:

$$\hat{G}_{\rm sc}(k) = \frac{i\omega_n\hat{\tau}_0 + \epsilon_{\mathbf{k}}\hat{\tau}_3 + \Delta_{\mathbf{k}}\hat{\tau}_1}{(i\omega_n)^2 - E_{\mathbf{k}}^2} \tag{32}$$

where $E_{\mathbf{k}}$ is:

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} \tag{33}$$

Next the electron-phonon self-energy in the superconducting state is (in a matrix form):

$$\hat{\Sigma}_{\rm ep}(k) = \hat{\Sigma}_{\rm ep}(\mathbf{k}, i\omega_n) = -\frac{1}{\beta}\sum_{q\nu}|g_\nu(\mathbf{k},\mathbf{q})|^2 D_\nu(q)\hat{\tau}_3\hat{G}_{\rm sc}(k+q)\hat{\tau}_3 \tag{34}$$

Since we have:

$$\hat{\tau}_3\hat{\tau}_0\hat{\tau}_3 = \hat{\tau}_0 \quad \hat{\tau}_3\hat{\tau}_3\hat{\tau}_3 = \hat{\tau}_3 \quad \hat{\tau}_3\hat{\tau}_1\hat{\tau}_3 = -\hat{\tau}_1 \tag{35}$$

then explicitly we have:

$$\hat{\Sigma}_{\rm ep}(\mathbf{k}, i\omega_n) = -\frac{1}{\beta}\sum_{\nu}\sum_{\mathbf{q},\Omega_m} w_{\mathbf{q}}|g_\nu(\mathbf{k},\mathbf{q})|^2 \frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_m)^2-\omega_{\mathbf{q}\nu}^2}\frac{(i\omega_n+i\Omega_m)\hat{\tau}_0+\epsilon_{\mathbf{k+q}}\hat{\tau}_3-\Delta_{\mathbf{k+q}}\hat{\tau}_1}{(i\omega_n+i\Omega_m)^2-E_{\mathbf{k+q}}^2} \tag{36}$$

where $w_{\mathbf{q}}$ is the weight of $\mathbf{q}$ in the numerical implementation.

The full interacting Green function is obtained via Dyson equation:

$$\hat{G}^{-1}(k) = \hat{G}_0^{-1}(k) - \hat{\Sigma}_{\rm ep}(k) \tag{37}$$

$$\hat{G}(k) = \hat{G}(\mathbf{k}, i\omega_n) = \left\{ i\omega_n\hat{\tau}_0 - \epsilon_{\mathbf{k}}\hat{\tau}_3 - \frac{1}{\beta}\sum_{\nu}\sum_{\mathbf{q},\Omega_m}|g_\nu(\mathbf{k},\mathbf{q})|^2\frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_m)^2-\omega_{\mathbf{q}\nu}^2}\frac{(i\omega_n+i\Omega_m)\hat{\tau}_0+\epsilon_{\mathbf{k+q}}\hat{\tau}_3-\Delta_{\mathbf{k+q}}\hat{\tau}_1}{(i\omega_n+i\Omega_m)^2-E_{\mathbf{k+q}}^2}\right\}^{-1} \tag{38}$$

Why not use the superconducting Green function in the Dyson equation

$$\hat{G}^{-1}(k) = \hat{G}_{\rm sc}^{-1}(k) - \hat{\Sigma}_{\rm ep}(k) \tag{39}$$

$$\hat{G}(k) = \hat{G}(\mathbf{k}, i\omega_n) = \left\{ i\omega_n\hat{\tau}_0 - \epsilon_{\mathbf{k}}\hat{\tau}_3 - \Delta_{\mathbf{k}}\hat{\tau}_1 - \frac{1}{\beta}\sum_{\nu}\sum_{\mathbf{q},\Omega_m}|g_\nu(\mathbf{k},\mathbf{q})|^2\frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_m)^2-\omega_{\mathbf{q}\nu}^2}\frac{(i\omega_n+i\Omega_m)\hat{\tau}_0+\epsilon_{\mathbf{k+q}}\hat{\tau}_3-\Delta_{\mathbf{k+q}}\hat{\tau}_1}{(i\omega_n+i\Omega_m)^2-E_{\mathbf{k+q}}^2}\right\}^{-1} \tag{40}$$

Here we have to use numerical method to do the 'analytical continuation'. Finally we calculate the spectral function:

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}{\rm Im}G_{11}(\mathbf{k}, i\omega_n \to \omega + i\delta) \tag{41}$$

# 2 Multi-orbital case

## 2.1 Normal state

The extension to multi-orbital case is straightforward because both the non-interacting Green function and the electron-phonon self-energy are diagonal in the Bloch state basis $|n\mathbf{k}\rangle$.

We first calculate the band-resolved electron-phonon self-energy. In the normal state, we can directly calculate the self-energy on the real-axis:

$$\Sigma_n^{\mathrm{ep}}(\mathbf{k},\omega) = \sum_{m\mathbf{q}\nu} w_{\mathbf{q}} |g_{mn}^{\nu}(\mathbf{k},\mathbf{q})|^2 \left[ \frac{n_B(\omega_{\mathbf{q}\nu}) + n_F(\epsilon_{m\mathbf{k}+\mathbf{q}})}{\omega - \epsilon_{m\mathbf{k}+\mathbf{q}} + \omega_{\mathbf{q}\nu} + i\delta} + \frac{n_B(\omega_{\mathbf{q}\nu}) + 1 - n_F(\epsilon_{m\mathbf{k}+\mathbf{q}})}{\omega - \epsilon_{m\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{q}\nu} + i\delta} \right] \tag{42}$$

where $m$ and $n$ are band indices.

The non-interacting Green function is:

$$G_n^0(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{n\mathbf{k}} + i\delta} \tag{43}$$

Therefore the full Green function is also diagonal in the Bloch state basis:

$$G_n(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{n\mathbf{k}} - \Sigma_n^{\mathrm{ep}}(\mathbf{k},\omega) + i\delta} \tag{44}$$

The spectral function is also diagonal in the Bloch state basis:

$$A_n(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G_n(\mathbf{k},\omega) \tag{45}$$

Similar to the single-orbital case, instead of calculating spectral function, we can also express the electron-phonon self-energy in another way:

$$\Sigma_{n\mathbf{k}}^{\mathrm{ep}} = \sum_{m\mathbf{q}\nu} w_{\mathbf{q}} |g_{mn}^{\nu}(\mathbf{k},\mathbf{q})|^2 \left[ \frac{n_B(\omega_{\mathbf{q}\nu}) + n_F(\epsilon_{m\mathbf{k}+\mathbf{q}})}{\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}+\mathbf{q}} + \omega_{\mathbf{q}\nu} + i\delta} + \frac{n_B(\omega_{\mathbf{q}\nu}) + 1 - n_F(\epsilon_{m\mathbf{k}+\mathbf{q}})}{\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{q}\nu} + i\delta} \right] \tag{46}$$

That is the electron-phonon self-energy for each Bloch state $|n\mathbf{k}\rangle$.

## 2.2 Superconducting case

For the superconducting case, we can still use this band-by-band method. However, each digonal element in the electron-phonon self-energy and Green function needs to be expanded into a $2 \times 2$ matrix (which is not diagonal).

For each $2\times 2$ matrix block, we can label it with a band index $a$ (we reserve $n$ for $i\omega_n$). Therefore, in the superconducting state with a weak-coupling:

$$\hat{\Sigma}_a^{\mathrm{sc}}(k) = \Delta_a(k)\hat{\tau}_1 \tag{47}$$

where $\Delta_a(k)$ is the superconducting order parameter for band $a$. If we ignore retardation effect, we can replace $k$ by $\mathbf{k}$ (neglect frequency dependence). That is:

$$\hat{\Sigma}_a^{\mathrm{sc}}(k) = \Delta_{a\mathbf{k}}\hat{\tau}_1 \tag{48}$$

The superconducting Green function is:

$$\hat{G}_a^{\mathrm{sc}}(k) = \frac{i\omega_n\hat{\tau}_0 + \epsilon_{a\mathbf{k}}\hat{\tau}_3 + \Delta_{a\mathbf{k}}\hat{\tau}_1}{(i\omega_n)^2 - E_{a\mathbf{k}}^2} \tag{49}$$

where $E_{a\mathbf{k}}$ is:

$$E_{a\mathbf{k}} = \sqrt{\epsilon_{a\mathbf{k}}^2 + \Delta_{a\mathbf{k}}^2} \tag{50}$$

Next the electron-phonon self-energy in the superconducting state is (in a matrix form):

$$\hat{\Sigma}_a^{\mathrm{ep}}(\mathbf{k}, i\omega_n) = -\frac{1}{\beta}\sum_{\nu}\sum_{a,\mathbf{q},\Omega_m} w_{\mathbf{q}}|g_{ab}^{\nu}(\mathbf{k},\mathbf{q})|^2 \frac{2\omega_{\mathbf{q}\nu}}{(i\Omega_m)^2 - \omega_{\mathbf{q}\nu}^2} \frac{(i\omega_n + i\Omega_m)\hat{\tau}_0 + \epsilon_{a\mathbf{k}+\mathbf{q}}\hat{\tau}_3 - \Delta_{a\mathbf{k}+\mathbf{q}}\hat{\tau}_1}{(i\omega_n + i\Omega_m)^2 - E_{a\mathbf{k}+\mathbf{q}}^2} \tag{51}$$

Finally the full interacting Green function is:

$$\hat{G}_a(k) = \hat{G}_a(\mathbf{k}, i\omega_n) = \left[i\omega_n\hat{\tau}_0 - \epsilon_{a\mathbf{k}}\hat{\tau}_3 - \hat{\Sigma}_a^{\mathrm{ep}}(\mathbf{k}, i\omega_n)\right]^{-1} \tag{52}$$

The spectral function is:

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi}\mathrm{Im}\left[\hat{G}_a(\mathbf{k}, i\omega_n \to \omega + i\delta)\right]_{11} \tag{53}$$