Iterative analytic continuation of the phonon self-energy to the real axis

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Abstract

- probably never been done before
- lowest order perturbation theory can be important
- provides an computationally efficient way to calculate renormalized ME theory on the real axis
- self-consistent el selfenergy useful in many calculations (such as estimating strength of replica bands in FeSe on STO paper)

The Hamiltonian for a generic el-ph interaction is given by

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{q}} \left(\Omega b^\dagger_{\mathbf{q}} b_{\mathbf{q}} + \frac{1}{2} \right) + \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} g(\mathbf{k},\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(b_{\mathbf{q}} + b^\dagger_{-\mathbf{q}} \right) \tag{1}$$

The lowest order contribution to the phonon self-energy in Matsubara frequency is

$$\Pi(i\nu_n, \mathbf{q}) = \frac{2}{N\beta} \sum_{m,\mathbf{k}} |g(\mathbf{k},\mathbf{q})|^2 \, G(i\omega_m, \mathbf{k}) G(i\omega_m + i\nu_n, \mathbf{k}+\mathbf{q}) \tag{2}$$

Applying the spectral representation for $G(i\omega_m, \mathbf{k})$ gives

$$\Pi(i\nu_n, \mathbf{q}) = \frac{2}{N\beta} \sum_{m,\mathbf{k}} \int dz dz' \, |g(\mathbf{k},\mathbf{q})|^2 \, \frac{S(z,\mathbf{k})}{(i\omega_m - z)} \frac{S(z',\mathbf{k}+\mathbf{q})}{(i\omega_m + i\nu_n - z')} \tag{3}$$

To evaluate the Matsubara frequency sum, consider the contour integral

$$\begin{aligned}
0 &= \oint dz'' \int dz dz' \frac{S(z,\mathbf{k})}{(z'' - z)} \frac{S(z',\mathbf{k}+\mathbf{q})}{(z'' + i\nu_n - z')} n_F(z'') \\
&= -\frac{2\pi i}{\beta} \sum_m \frac{S(z,\mathbf{k}) S(z',\mathbf{k}+\mathbf{q})}{(i\omega_m - z)(i\omega_m + i\nu_n - z')} \\
&+ 2\pi i \int dz dz' S(z,\mathbf{k}) S(z',\mathbf{k}+\mathbf{q}) \left[\frac{n_F(z)}{z + i\nu_n - z'} + \frac{n_F(-i\nu_n + z')}{-i\nu_n + z' - z} \right] \\
&= -\frac{2\pi i}{\beta} \sum_m \frac{S(z,\mathbf{k}) S(z',\mathbf{k}+\mathbf{q})}{(i\omega_m - z)(i\omega_m + i\nu_n - z')} \\
&+ 2\pi i \int dz dz' S(z,\mathbf{k}) S(z',\mathbf{k}+\mathbf{q}) \frac{n_F(z) - n_F(z' - i\nu_n)}{i\nu_n + z - z'}
\end{aligned} \tag{4}$$

Where the the first term on the right hand side is multiplied by a factor of $\frac{-1}{\beta}$ because of the residue of n_F.

Note that $n_F(z' - i\nu_n) = [e^{\beta z'} e^{-\beta i \nu_n} + 1]^{-1} = n_F(z')$ so

$$\frac{1}{\beta} \sum_m \frac{S(z,\mathbf{k}) S(z',\mathbf{k}+\mathbf{q})}{(i\omega_m - z)(i\omega_m + i\nu_n - z')} = \int dz dz' \frac{S(z,\mathbf{k}) S(z',\mathbf{k}+\mathbf{q}) \left[n_F(z) - n_F(z') \right]}{i\nu_n + z - z'} \tag{5}$$

Therefore

$$\Pi(i\nu_n, \mathbf{q}) = \frac{2}{N} \sum_{m,\mathbf{k}} \int dz dz' \, |g(\mathbf{k},\mathbf{q})|^2 \, \frac{S(z,\mathbf{k}) S(z',\mathbf{k}+\mathbf{q}) \left[n_F(z) - n_F(z') \right]}{i\nu_n + z - z'} \tag{6}$$

Then analytically continuing $\omega \to \omega + i\delta$ and using $S(z,\mathbf{k}) = -\frac{1}{\pi} \mathrm{Im} G^R(z,\mathbf{k})$ gives

$$\Pi(\omega + i\delta, \mathbf{q}) = -\frac{2}{N\pi} \sum_{m,\mathbf{k}} \int dz dz' \, |g(\mathbf{k},\mathbf{q})|^2 \, \frac{S(z',\mathbf{k}+\mathbf{q}) \mathrm{Im} G^R(z,\mathbf{k}) \left[n_F(z) - n_F(z') \right]}{\omega + z - z' + i\delta} \tag{7}$$

The next goal is to evaluate the integral over z. We break up the integrand into real and imaginary parts using the fact that

$$\begin{aligned}\frac{1}{\omega+z-z'+i\delta} &= \frac{1}{2}\left(\frac{1}{\omega_+}+\frac{1}{\omega_-}\right)+i\frac{1}{2i}\left(\frac{1}{\omega_+}-\frac{1}{\omega_-}\right) \\ &= \frac{1}{2}\left(\frac{1}{\omega_+}+\frac{1}{\omega_-}\right)-i\frac{i}{2}\left(\frac{1}{\omega_+}-\frac{1}{\omega_-}\right)\end{aligned} \tag{8}$$

where $w_+ = \omega+z-z'+i\delta$ and $\omega_- = \omega+z-z'-i\delta$.

Note that

$$\begin{aligned}\frac{\mathrm{Im}G^R(z,\mathbf{k})}{\omega+z-z'+i\delta} &= \frac{\mathrm{Im}G^R(z,\mathbf{k})}{2}\left(\frac{1}{\omega_+}+\frac{1}{\omega_-}\right)-i\frac{\mathrm{Im}G^R(z,\mathbf{k})i}{2}\left(\frac{1}{\omega_+}-\frac{1}{\omega_-}\right) \\ &= \mathrm{Im}\left[\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+}+\frac{1}{\omega_-}\right)\right]-i\mathrm{Im}\left[\frac{G^R(z,\mathbf{q})i}{2}\left(\frac{1}{\omega_+}-\frac{1}{\omega_-}\right)\right] \\ &= \mathrm{Im}\left[\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+}+\frac{1}{\omega_-}\right)\right]-i\mathrm{Re}\left[\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+}-\frac{1}{\omega_-}\right)\right]\end{aligned} \tag{9}$$

Let us consider only the parts of the integral over z in equation 7 and break it up into real and imaginary parts as

$$\begin{aligned}\mathrm{I} \equiv& \int dzdz'\frac{S(z',\mathbf{k}+\mathbf{q})\mathrm{Im}G^R(z,\mathbf{k})\left[n_F(z)-n_F(z')\right]}{\omega+z-z'+i\delta} \\ =& \,\mathrm{Im}\left\{\int dz\left[n_F(z)-n_F(z')\right]\frac{G^R(z,\mathbf{k})}{2}\left(\frac{1}{\omega_+}+\frac{1}{\omega_-}\right)\right\}- \\ &i\mathrm{Re}\left\{\int dz\left[n_F(z)-n_F(z')\right]\frac{G^R(z,\mathbf{k})}{2}\left(\frac{1}{\omega_+}-\frac{1}{\omega_-}\right)\right\}\end{aligned} \tag{10}$$

Now consider the following contour integral in the upper-half plane

$$\begin{aligned}\int dz\left[n_F(z)-n_F(z')\right]\frac{G^R(z,\mathbf{k})}{2}\left(\frac{1}{\omega_+}\pm\frac{1}{\omega_-}\right) =& \pm 2\pi i\left[n_F(z'-\omega+i\delta)-n_F(z')\right]\frac{G^R(z'-\omega+i\delta,\mathbf{k})}{2} \\ &-\frac{2\pi i}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{k})}{2}\left(\frac{1}{\omega+i\omega_m-z'+i\delta}\pm\frac{1}{\omega+i\omega_m-z'-i\delta}\right)\end{aligned} \tag{11}$$

Note about signs: the first term on the right hand side gets the sign of $1/\omega_-$. Also note that $1/\omega_+$ does not contribute to integral over the upper half plane. And the second term gets a factor of -1 from the residue of n_F.

Next combine the real and imaginary parts given that $\mathrm{Im}(F)-i\mathrm{Re}(F)=-iF$ and $\mathrm{Im}(F)+i\mathrm{Re}(F)=iF^*$.

$$\begin{aligned}I =& -i\left\{-\frac{\pi i}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z'}\right\} \\ &+i\left\{\pi i\left[n_F(z'-\omega)-n_F(z')\right]G^R(z'-\omega,\mathbf{k})-\frac{\pi i}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z'}\right\}^* \\ =& -\frac{\pi}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z'}+i\left\{-\pi i\left[n_F(z'-\omega)-n_F(z')\right]G^{R*}(z'-\omega,\mathbf{k})+\frac{\pi i}{\beta}\sum_{m=0}^{\infty}\frac{G^*(i\omega_m,\mathbf{k})}{\omega-i\omega_m-z'}\right\} \\ =& +\pi\left[n_F(z'-\omega)-n_F(z')\right]G^{R*}(z'-\omega,\mathbf{k})-\frac{\pi}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z'}-\frac{\pi}{\beta}\sum_{m=0}^{\infty}\frac{G(-i\omega_m,\mathbf{k})}{\omega-i\omega_m-z'} \\ =& +\pi\left[n_F(z'-\omega)-n_F(z')\right]G^{R*}(z'-\omega,\mathbf{k})-\frac{\pi}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z'}-\frac{\pi}{\beta}\sum_{m=-\infty}^{-1}\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z'} \\ =& +\pi\left[n_F(z'-\omega)-n_F(z')\right]G^{A}(z'-\omega,\mathbf{k})-\frac{\pi}{\beta}\sum_{m}\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z'}\end{aligned} \tag{12}$$

where we neglected the $i\delta$ of the argument to n_F and also used the fact that $G^*(i\omega_m,\mathbf{q})=G(-i\omega_m,\mathbf{q})$ and $G^{R*}(z,\mathbf{k})=G^A(z,\mathbf{k})$.

Finally plugging this result into equation 7 gives

$$\Pi(\omega+i\delta,\mathbf{q}) = -\frac{2}{N\pi}\sum_{\mathbf{k}}\int dz'\,|g(\mathbf{k},\mathbf{q})|^2\,S(z',\mathbf{k}+\mathbf{q})\left\{\pi\left[n_F(z'-\omega)-n_F(z')\right]G^A(z'-\omega,\mathbf{k}) - \frac{\pi}{\beta}\sum_m \frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z'}\right\} \tag{13}$$

$$\begin{aligned}\Pi(\omega+i\delta,\mathbf{q}) &= \frac{2}{N\beta}\int dz\sum_{m,\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,S(z,\mathbf{k}+\mathbf{q})\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z}\\ &\quad-\frac{2}{N}\sum_{\mathbf{k}}\int dz\,|g(\mathbf{k},\mathbf{q})|^2\,S(z,\mathbf{k}+\mathbf{q})G^A(z-\omega,\mathbf{k})\left[n_F(z-\omega)-n_F(z)\right]\end{aligned} \tag{14}$$

$$\boxed{\Pi(\omega+i\delta,\mathbf{q}) = \frac{2}{N}\sum_{\mathbf{k}}\int dz\,|g(\mathbf{k},\mathbf{q})|^2\,S(z,\mathbf{k}+\mathbf{q})\left[\frac{1}{\beta}\sum_{m,\mathbf{k}}\frac{G(i\omega_m,\mathbf{k})}{\omega+i\omega_m-z} - G^A(z-\omega,\mathbf{k})\left[n_F(z-\omega)-n_F(z)\right]\right]} \tag{15}$$

which can be rewritten as

$$\begin{aligned}\Pi(\omega+i\delta,\mathbf{q}) &= \frac{2}{N\beta}\sum_{m,\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,G^R(\omega+i\omega_m,\mathbf{k}+\mathbf{q})G(i\omega_m,\mathbf{k})\\ &\quad+\frac{2}{N\pi}\sum_{\mathbf{k}}\int dz\,|g(\mathbf{k},\mathbf{q})|^2\,\mathrm{Im}G^R(z,\mathbf{k}+\mathbf{q})G^A(z-\omega,\mathbf{k})\left[n_F(z-\omega)-n_F(z)\right]\end{aligned} \tag{16}$$

Consistency check: let's check this expression by using the non-interacting Green's function $G(i\omega_m,\mathbf{k}) = (i\omega_m-\epsilon_{\mathbf{k}})^{-1}$ and $G^R(\omega+i\delta,\mathbf{k}) = (\omega-\epsilon_{\mathbf{k}}+i\delta)^{-1}$.

Using $-\frac{1}{\pi}G^R(z,\mathbf{k}) = -\frac{1}{\pi}\mathrm{Im}\left(\frac{1}{z-\epsilon_{\mathbf{k}}+i\delta}\right) = -\frac{1}{\pi}\left(\frac{-\delta}{(z-\epsilon_{\mathbf{k}})^2+\delta^2}\right) = \delta(z-\epsilon_{\mathbf{k}})$

$$\begin{aligned}\Pi^0(\omega+i\delta,\mathbf{q}) &= \frac{2}{N\beta}\sum_{m,\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{1}{(\omega+i\delta+i\omega_m-\epsilon_{\mathbf{k}+\mathbf{q}})(i\omega_m-\epsilon_{\mathbf{k}})}\\ &\quad-\frac{2}{N}\sum_{\mathbf{k}}\int dz\,|g(\mathbf{k},\mathbf{q})|^2\,\delta(z-\epsilon_{\mathbf{k}+\mathbf{q}})\frac{1}{z-\omega-\epsilon_{\mathbf{k}}-i\delta}\left[n_F(z-\omega)-n_F(z)\right]\\ &= \frac{2}{N\beta}\sum_{m,\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{1}{(\omega+i\delta+i\omega_m-\epsilon_{\mathbf{k}+\mathbf{q}})(i\omega_m-\epsilon_{\mathbf{k}})}\\ &\quad-\frac{2}{N}\sum_{\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{1}{\epsilon_{\mathbf{k}+\mathbf{q}}-\omega-\epsilon_{\mathbf{k}}-i\delta}\left[n_F(\epsilon_{\mathbf{k}+\mathbf{q}}-\omega)-n_F(\epsilon_{\mathbf{k}+\mathbf{q}})\right]\\ &= \frac{2}{N\beta}\sum_{\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{1}{(\omega+i\delta+i\omega_m-\epsilon_{\mathbf{k}+\mathbf{q}})(i\omega_m-\epsilon_{\mathbf{k}})}\\ &\quad-\frac{2}{N}\sum_{\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{1}{\epsilon_{\mathbf{k}+\mathbf{q}}-\omega-\epsilon_{\mathbf{k}}-i\delta}\left[n_F(\epsilon_{\mathbf{k}+\mathbf{q}}-\omega)-n_F(\epsilon_{\mathbf{k}+\mathbf{q}})\right]\end{aligned} \tag{17}$$

To perform the frequency sum, consider

$$\begin{aligned}0 &= \oint dz\frac{n_F(z)}{(z+\omega+i\delta-\epsilon_{\mathbf{k}+\mathbf{q}})(z-\epsilon_{\mathbf{k}})}\\ &= \frac{-2\pi i}{\beta}\sum_m\frac{1}{(i\omega_m+\omega+i\delta-\epsilon_{\mathbf{k}+\mathbf{q}})(i\omega_m-\epsilon_{\mathbf{k}})}+2\pi i\frac{n_F(\epsilon_{\mathbf{k}+\mathbf{q}}-w)}{\epsilon_{\mathbf{k}-\mathbf{q}}-\omega-i\delta-\epsilon_{\mathbf{k}}}+2\pi i\frac{n_F(\epsilon_{\mathbf{k}})}{\epsilon_{\mathbf{k}}+\omega+i\delta-\epsilon_{\mathbf{k}+\mathbf{q}}}\end{aligned} \tag{18}$$

Which shows that

$$\frac{1}{\beta}\sum_m\frac{1}{(i\omega_m+\omega+i\delta-\epsilon_{\mathbf{k}+\mathbf{q}})(i\omega_m-\epsilon_{\mathbf{k}})} = \frac{n_F(\epsilon_{\mathbf{k}})-n_F(\epsilon_{\mathbf{k}+\mathbf{q}}-w)}{\epsilon_{\mathbf{k}}+\omega+i\delta-\epsilon_{\mathbf{k}+\mathbf{q}}} \tag{19}$$

Which then gives:

$$\begin{aligned}\Pi^0(\omega+i\delta,\mathbf{q}) &= \frac{2}{N}\sum_{\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{n_F(\epsilon_{\mathbf{k}})-n_F(\epsilon_{\mathbf{k}+\mathbf{q}}-w)}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}}+\omega+i\delta}\\ &\quad-\frac{2}{N}\sum_{\mathbf{k}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{n_F(\epsilon_{\mathbf{k}+\mathbf{q}}-\omega)-n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}-\omega-i\delta}\end{aligned} \tag{20}$$

$$\Pi^0(\omega + i\delta, \mathbf{q}) = \frac{2}{N}\sum_{\mathbf{k}} |g(\mathbf{k},\mathbf{q})|^2 \left[\frac{n_F(\epsilon_{\mathbf{k}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}} + \omega + i\delta} + \frac{n_F(\epsilon_{\mathbf{k+q}})}{\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}} - \omega - i\delta}\right] \tag{21}$$

$$\Pi^0(\omega + i\delta, \mathbf{q}) = \frac{2}{N}\sum_{\mathbf{k}} |g(\mathbf{k},\mathbf{q})|^2 \frac{n_F(\epsilon_{\mathbf{k}}) - n_F(\epsilon_{\mathbf{k+q}})}{\omega + i\delta + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}}} \tag{22}$$

which is the correct expression!