Marsiglio Derivation

Ben

March 4, 2019

Abstract

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

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

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

$$\Sigma(i\omega_n, \mathbf{k}) = -\frac{1}{N\beta} \sum_{m,\mathbf{q}} |g(\mathbf{k},\mathbf{q})|^2 G(i\omega_m, \mathbf{k}-\mathbf{q}) D(i\omega_n - i\omega_m, \mathbf{q}) \tag{2}$$

question: is $|g(\mathbf{k},\mathbf{q})|^2 = |g(\mathbf{k},\mathbf{k}-\mathbf{q})|^2$? If so, then after the relabeling $\mathbf{q} \to \mathbf{k}-\mathbf{q}$, $\Sigma(i\omega_n, \mathbf{k})$ becomes

$$\Sigma(i\omega_n, \mathbf{k}) = -\frac{1}{N\beta} \sum_{m,\mathbf{q}} |g(\mathbf{k},\mathbf{q})|^2 G(i\omega_m, \mathbf{q}) D(i\omega_n - i\omega_m, \mathbf{k}-\mathbf{q}) \tag{3}$$

which is the starting point in Marsiglio's paper.

Applying the spectral representation for G and D:

$$\Sigma(i\omega_n, \mathbf{k}) = -\frac{1}{N\beta} \sum_{m,\mathbf{q}} \int dz dz' \, |g(\mathbf{k},\mathbf{q})|^2 \frac{S(z,q) B(z', \mathbf{k}-\mathbf{q})}{(i\omega_m - z)(i\omega_n - i\omega_m - z')} \tag{4}$$

Now we consider the following contour integral in order to evaluate the Matsubara frequency sum in equation 4:

$$\begin{aligned} 0 = \oint dz'' \int dz dz' \frac{S(z,\mathbf{q}) B(z', \mathbf{k}-\mathbf{q})}{(z''-z)(i\omega_n - z'' - z')} n_F(z'') \\ = \frac{-2\pi i}{\beta} \sum_m \int dz dz' \frac{S(z,q) B(z', \mathbf{k}-\mathbf{q})}{(i\omega_m - z)(i\omega_n - i\omega_m - z')} \\ + 2\pi i \int dz dz' S(z,\mathbf{q}) B(z', \mathbf{k}-\mathbf{q}) \left[\frac{n_F(z)}{i\omega_n - z - z'} - \frac{n_F(i\omega_n - z')}{i\omega_n - z - z'} \right] \end{aligned} \tag{5}$$

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 and the last fraction in the brackets has a minus sign because the denominator $i\omega_n - z'' - z$ has a minus sign in front of z''.

The contour integral is zero, so we obtain:

$$\frac{-1}{\beta} \sum_m \int dz dz' \frac{S(z,q) B(z', \mathbf{k}-\mathbf{q})}{(i\omega_m - z)(i\omega_n - i\omega_m - z')} = - \int dz dz' \frac{S(z,\mathbf{q}) B(z', \mathbf{k}-\mathbf{q})}{i\omega_n - z - z'} \left[n_F(z) - n_F(i\omega_n - z') \right] \tag{6}$$

We evaluate

$$n_F(i\omega_n - z') = \left(e^{\beta i\omega_n} e^{-\beta z'} + 1 \right)^{-1} = e^{\beta z'} \left(e^{\beta z'} - 1 \right)^{-1} = \left(1 + \frac{1}{n_B(z')} \right) n_B(z') = 1 + n_B(z') \tag{7}$$

So we have:

$$\frac{-1}{\beta}\sum_m \int dzdz' \frac{S(z,q)B(z',\mathbf{k}-\mathbf{q})}{(i\omega_m - z)(i\omega_n - i\omega_m - z')} = \int dzdz' \frac{S(z,\mathbf{q})B(z',\mathbf{k}-\mathbf{q})}{i\omega_n - z - z'}\left[1+n_B(z') - n_F(z)\right] \tag{8}$$

Plugging back into equation 4 and analytically continuing $i\omega_n \to \omega + i\delta$, we obtain

$$\Sigma(\omega+i\delta,\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{q}}\int dzdz'\, |g(\mathbf{k},\mathbf{q})|^2\,\frac{S(z,q)B(z',\mathbf{k}-\mathbf{q})}{\omega - z - z' + i\delta}\left[1+n_B(z')-n_F(z)\right] \tag{9}$$

Now use $S(z,\mathbf{q}) = -\frac{1}{\pi}\text{Im}G^R(z,\mathbf{q})$ so that

$$\Sigma(\omega+i\delta,\mathbf{k}) = -\frac{1}{N\pi}\sum_{\mathbf{q}}\int dzdz'\, |g(\mathbf{k},\mathbf{q})|^2\,\frac{\text{Im}G^R(z,\mathbf{q})B(z',\mathbf{k}-\mathbf{q})}{\omega - z - z' + i\delta}\left[1+n_B(z')-n_F(z)\right] \tag{10}$$

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

$$\begin{aligned}\frac{1}{\omega - z - z' + i\delta} &= \frac{1}{2}\left(\frac{1}{\omega_+} + \frac{1}{\omega_-}\right) + i\frac{1}{2i}\left(\frac{1}{\omega_+} - \frac{1}{\omega_-}\right)\\ &= \frac{1}{2}\left(\frac{1}{\omega_+} + \frac{1}{\omega_-}\right) - i\frac{i}{2}\left(\frac{1}{\omega_+} - \frac{1}{\omega_-}\right)\end{aligned} \tag{11}$$

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

Note that

$$\begin{aligned}\frac{\text{Im}G^R(z,\mathbf{q})}{\omega - z - z' + i\delta} &= \frac{\text{Im}G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+} + \frac{1}{\omega_-}\right) - i\frac{\text{Im}G^R(z,\mathbf{q})i}{2}\left(\frac{1}{\omega_+} - \frac{1}{\omega_-}\right)\\ &= \text{Im}\left[\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+} + \frac{1}{\omega_-}\right)\right] - i\text{Im}\left[\frac{G^R(z,\mathbf{q})i}{2}\left(\frac{1}{\omega_+} - \frac{1}{\omega_-}\right)\right]\\ &= \text{Im}\left[\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+} + \frac{1}{\omega_-}\right)\right] - i\text{Re}\left[\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+} - \frac{1}{\omega_-}\right)\right]\end{aligned} \tag{12}$$

Let us consider only the parts of the integral over z in equation 10 break it up into real an imaginary parts as

$$\begin{aligned}\text{I} &\equiv \int dz \frac{\text{Im}G^R(z,\mathbf{q})}{\omega - z - z' + i\delta}\left[1+n_B(z')-n_F(z)\right]\\ &= \text{Im}\left\{\int dz\left[1+n_B(z')-n_F(z)\right]\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+} + \frac{1}{\omega_-}\right)\right\} - \\ &i\text{Re}\left\{\int dz\left[1+n_B(z')-n_F(z)\right]\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+} - \frac{1}{\omega_-}\right)\right\}\end{aligned} \tag{13}$$

Now consider the contour integral in the upper-half plane for the imaginary part

$$\begin{aligned}\int dz\left[1+n_B(z')-n_F(z)\right]\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+} + \frac{1}{\omega_-}\right) =& -2\pi i\left[1+n_B(z')-n_F(\omega - z' + i\delta)\right]\\ &+ \frac{2\pi i}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{q})}{2}\left(\frac{1}{\omega - i\omega_m - z' + i\delta} + \frac{1}{\omega - i\omega_m - z' - i\delta}\right)\end{aligned} \tag{14}$$

Note about signs: the first term on the right hand side gets minus sign due to $-z$ in denominator of $1/\omega_+$. Also note that $1/\omega_-$ does not contribute to integral over the upper half plane. And the second term gets two factors of -1 which cancel (one from the residue of n_F and another from the sign in front of n_F).

Therefore,

$$\begin{aligned}\int dz\left[1+n_B(z')-n_F(z)\right]\frac{G^R(z,\mathbf{q})}{2}\left(\frac{1}{\omega_+} \pm \frac{1}{\omega_-}\right) &= -2\pi i\left[1+n_B(z')-n_F(\omega - z' + i\delta)\right]\frac{G^R(\omega - z' + i\delta,\mathbf{q})}{2}\\ &+ \frac{2\pi i}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{q})}{2}\left(\frac{1}{\omega - i\omega_m - z' + i\delta} \pm \frac{1}{\omega - i\omega_m - z' - i\delta}\right)\end{aligned} \tag{15}$$

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

$$
\begin{aligned}
I &= -i\left\{-\pi i\left[1+n_B(z')-n_F(\omega-z')\right]G^R(\omega-z'+i\delta,\mathbf{q}) + \frac{2\pi i}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{q})}{2(\omega-i\omega_m-z')}\right\} \\
&+ i\left\{+\frac{2\pi i}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{q})}{2(\omega-i\omega_m-z')}\right\}^* \\
&= -\pi\left[1+n_B(z')-n_F(\omega-z')\right]G^R(\omega-z'+i\delta,\mathbf{q}) + \frac{2\pi}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{q})}{2(\omega-i\omega_m-z')} + \frac{2\pi}{\beta}\sum_{m=0}^{\infty}\frac{G^*(i\omega_m,\mathbf{q})}{2(\omega+i\omega_m-z')} \\
&= -\pi\left[1+n_B(z')-n_F(\omega-z')\right]G^R(\omega-z'+i\delta,\mathbf{q}) + \frac{\pi}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{q})}{\omega-i\omega_m-z'} + \frac{\pi}{\beta}\sum_{m=0}^{\infty}\frac{G(-i\omega_m,\mathbf{q})}{\omega+i\omega_m-z'} \\
&= -\pi\left[1+n_B(z')-n_F(\omega-z')\right]G^R(\omega-z'+i\delta,\mathbf{q}) + \frac{\pi}{\beta}\sum_{m=0}^{\infty}\frac{G(i\omega_m,\mathbf{q})}{\omega-i\omega_m-z'} + \frac{\pi}{\beta}\sum_{m=-1}^{-\infty}\frac{G(i\omega_m,\mathbf{q})}{\omega-i\omega_m-z'} \\
&= -\pi\left[1+n_B(z')-n_F(\omega-z')\right]G^R(\omega-z'+i\delta,\mathbf{q}) + \frac{\pi}{\beta}\sum_{m}\frac{G(i\omega_m,\mathbf{q})}{\omega-i\omega_m-z'}
\end{aligned}
\tag{16}
$$

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

Finally, plugging this result into equation 10 gives

$$
\Sigma(\omega+i\delta,\mathbf{k}) = -\frac{1}{N\pi}\sum_{\mathbf{q}}\int dz'\,|g(\mathbf{k},\mathbf{q})|^2 B(z',\mathbf{k}-\mathbf{q})\left\{-\pi\left[1+n_B(z')-n_F(\omega-z'+i\delta)\right]G^R(\omega-z'+i\delta,\mathbf{q}) + \frac{\pi}{\beta}\sum_m\frac{G(i\omega_m,\mathbf{q})}{\omega-i\omega_m-z'+i\delta}\right\}
\tag{17}
$$

$$
\begin{aligned}
\Sigma(\omega+i\delta,\mathbf{k}) = &-\frac{1}{N\beta}\sum_{m,\mathbf{q}}\int dz'\,|g(\mathbf{k},\mathbf{q})|^2 B(z',\mathbf{k}-\mathbf{q})\frac{G(i\omega_m,\mathbf{q})}{\omega-i\omega_m-z'} \\
&+\frac{1}{N}\sum_{\mathbf{q}}\int dz'\,|g(\mathbf{k},\mathbf{q})|^2 B(z',\mathbf{k}-\mathbf{q})\left[1+n_B(z')-n_F(\omega-z')\right]G^R(\omega-z'+i\delta,\mathbf{q})
\end{aligned}
\tag{18}
$$

$$
\boxed{\Sigma(\omega,\mathbf{k}) = -\frac{1}{N}\sum_{\mathbf{q}}\int dz\,|g(\mathbf{k},\mathbf{q})|^2 B(z,\mathbf{k}-\mathbf{q})\left[\frac{1}{\beta}\sum_m\frac{G(i\omega_m,\mathbf{q})}{\omega-i\omega_m-z} - G^R(\omega-z,\mathbf{q})\left[1+n_B(z)-n_F(\omega-z)\right]\right]}
\tag{19}
$$

which can also be rewritten as

$$
\boxed{
\begin{aligned}
\Sigma(\omega+i\delta,\mathbf{k}) = &-\frac{1}{N\beta}\sum_{m,\mathbf{q}}|g(\mathbf{k},\mathbf{q})|^2 D(\omega-i\omega_m,\mathbf{k}-\mathbf{q})G(i\omega_m,\mathbf{q}) \\
&-\frac{1}{\pi N}\sum_{\mathbf{q}}\int dz'\,|g(\mathbf{k},\mathbf{q})|^2\,\mathrm{Im}D(z',\mathbf{k}-\mathbf{q})\left[1+n_B(z')-n_F(\omega-z')\right]G^R(\omega-z'+i\delta,\mathbf{q})
\end{aligned}}
\tag{20}
$$

In the case of a bare phonon propagator,

$$
\begin{aligned}
D(i\nu_n,\mathbf{q}) &= \frac{1}{i\nu_n-\Omega_{\mathbf{q}}} - \frac{1}{i\nu_n+\Omega_{\mathbf{q}}} \\
D(\omega+i\delta,\mathbf{q}) &= \frac{1}{\omega-\Omega_{\mathbf{q}}+i\delta} - \frac{1}{\omega+\Omega_{\mathbf{q}}+i\delta} = \frac{2\Omega_{\mathbf{q}}}{(\omega+i\delta)^2-\Omega_{\mathbf{q}}^2} \\
-\frac{1}{\pi}\mathrm{Im}D(\omega+i\delta,\mathbf{q}) &= \frac{-1}{\pi}\left\{\frac{-\delta}{(\omega-\Omega_{\mathbf{q}})^2+\delta^2} + \frac{\delta}{(\omega+\Omega_{\mathbf{q}})^2+\delta^2}\right\} \\
-\frac{1}{\pi}\mathrm{Im}D(\omega+i\delta,\mathbf{q}) &= \delta(\omega-\Omega_{\mathbf{q}}) - \delta(\omega+\Omega_{\mathbf{q}})
\end{aligned}
\tag{21}
$$

where the δ in the last line is the Dirac delta function.

In the case of a bare phonon propagator, equation 20 becomes

$$\begin{aligned}
\Sigma(\omega+i\delta,\mathbf{k}) =& -\frac{1}{N\beta}\sum_{m,\mathbf{q}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{2\Omega_{\mathbf{k}-\mathbf{q}}}{(\omega-i\omega_m)^2-\Omega_{\mathbf{k}-\mathbf{q}}^2}G^R(i\omega_m,\mathbf{q}) \\
&+\frac{1}{N}\sum_{\mathbf{q}}|g(\mathbf{k},\mathbf{q})|^2\left[1+n_B(\Omega_{\mathbf{k}-\mathbf{q}})-n_F(\omega-\Omega_{\mathbf{k}-\mathbf{q}})\right]G^R(\omega-\Omega_{\mathbf{k}-\mathbf{q}}+i\delta,\mathbf{q}) \\
&-\frac{1}{N}\sum_{\mathbf{q}}|g(\mathbf{k},\mathbf{q})|^2\left[1+n_B(-\Omega_{\mathbf{k}-\mathbf{q}})-n_F(\omega+\Omega_{\mathbf{k}-\mathbf{q}})\right]G^R(\omega+\Omega_{\mathbf{k}-\mathbf{q}}+i\delta,\mathbf{q})
\end{aligned} \tag{22}$$

$$\boxed{\begin{aligned}
\Sigma(\omega+i\delta,\mathbf{k}) =& -\frac{1}{N\beta}\sum_{m,\mathbf{q}}|g(\mathbf{k},\mathbf{q})|^2\,\frac{2\Omega_{\mathbf{k}-\mathbf{q}}}{(\omega-i\omega_m)^2-\Omega_{\mathbf{k}-\mathbf{q}}^2}G^R(i\omega_m,\mathbf{q}) \\
&+\frac{1}{N}\sum_{\mathbf{q}}|g(\mathbf{k},\mathbf{q})|^2\left[1+n_B(\Omega_{\mathbf{k}-\mathbf{q}})-n_F(\omega-\Omega_{\mathbf{k}-\mathbf{q}})\right]G^R(\omega-\Omega_{\mathbf{k}-\mathbf{q}}+i\delta,\mathbf{q}) \\
&+\frac{1}{N}\sum_{\mathbf{q}}|g(\mathbf{k},\mathbf{q})|^2\left[n_B(\Omega_{\mathbf{k}-\mathbf{q}})+n_F(\omega+\Omega_{\mathbf{k}-\mathbf{q}})\right]G^R(\omega+\Omega_{\mathbf{k}-\mathbf{q}}+i\delta,\mathbf{q})
\end{aligned}} \tag{23}$$