8.512 Theory of Solids II
Spring 2009

# Lecture 3: Properties of the Response Function

In this lecture we will discuss some general properties of the response functions $\chi$, and some useful relations that they satisfy.

## 3.1 General Properties of $\chi(\vec{q},\omega)$

Recall that

$$\chi(\vec{q},\omega) = \frac{\delta n(\vec{q},\omega)}{U(\vec{q},\omega)} \tag{3.1}$$

with $n(\vec{r},t) \in \mathbb{R}$ and $U(\vec{r},t) \in \mathbb{R}$. Under Fourier transform, this implies

$$n(-\vec{q},-\omega) = n^*(\vec{q},\omega) \tag{3.2}$$

$$U(-\vec{q},-\omega) = U^*(\vec{q},\omega) \tag{3.3}$$

As a result,

$$\chi(\vec{q},\omega) = \chi^*(-\vec{q},-\omega) \tag{3.4}$$

$$\chi''(-\vec{q},-\omega) = -\chi''(\vec{q},\omega) \tag{3.5}$$

where $\chi''$ is the imaginary part of the response function $\chi(\vec{q},\omega)$.

Consider the extension of $\omega$ to the complex plane. We can then rewrite the expression for $\chi(\vec{q},\omega)$ as

$$\chi(\vec{q},\omega) = \lim_{\eta\to 0+} - \sum_n |\langle n|\hat{\rho}^\dagger_{\vec{q}}|\phi_0\rangle|^2 \left\{ \frac{1}{\omega-(E_n-E_0)+i\eta} - \frac{1}{\omega+(E_n-E_0)+i\eta} \right\} \tag{3.6}$$

Without the $+i\eta$ term in the energy denominator, there would be singularities (poles) on the real axis whenever $\omega$ is equal to the spacing between the ground state and some excited state. The presence of $+i\eta$ pushes these poles just into the lower 1/2-plane, ensuring that $\chi(\vec{q},\omega)$ is analytic in the entire upper-1/2 $\omega$-plane including the real axis.

Analyticity of $\chi(\vec{q},\omega)$ in the upper-1/2 plane is needed to build *causality* into the theory. Consider the response function in time, $\chi(t)$:

$$\chi(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\chi(\omega)\,e^{-i\omega t} \tag{3.7}$$

To evaluate this integral, we perform a contour integral in the complex $\omega$ plane. For $t < 0$, closing the contour in the *upper 1/2 plane* ensures that $|e^{-i\omega t}| \to 0$ on the curved portion of the contour. Since we have ensured that $\chi(\omega)$ is analytic in the upper half plane, Cauchy's residue theorem guarantees that the integral over the entire contour is 0. As a result, the piece we need, i.e. the integral from $-\infty$ to $\infty$ along the real axis, must also be 0. Thus $\chi(t) = 0$ for $t < 0$, which means that the system cannot respond to a perturbation until *after* the perturbation has occurred.

What about the $t > 0$ case? In this case, the contour must be closed in the lower 1/2 plane to prevent the exponential from blowing up. However, the $i\eta$ in the energy denominator has pushed the singularities into this region of the complex $\omega$ plane. Thus the value of the contour integral will be nonzero, and the system will respond to perturbations for $t > 0$.

## 3.2 Kramers-Kronig

Consider the integral

$$\oint d\omega' \frac{\chi(\vec{q},\omega')}{\omega-\omega'} = 0 \tag{3.8}$$

As we have just shown in the previous section, our definition of $\chi(\vec{q},\omega)$ ensures that $\chi(\vec{q},\omega)$ is analytic in the upper-1/2 complex $\omega$ plane. Although the integrand here has a pole on the real axis due to the $\omega - \omega'$ in the denominator, by making a hump over this pole we can ensure that the value of the contour integral itself vanishes by Cauchy's residue theorem.

Assuming that $\chi(\vec{q},\omega) \to 0$ as $|\omega| \to \infty$,

$$0 = \int_{-\infty}^{\infty} d\omega' \chi(\vec{q},\omega')\, \mathrm{Pr}\left[\frac{1}{\omega-\omega'}\right] + i\pi\chi(\vec{q},\omega) \tag{3.9}$$

where the additional term $i\pi\chi(\vec{q},\omega)$ is one half of the contribution from the pole at $\omega' = \omega$ that we picked up by making a hump over the pole. Thus for fixed $\vec{q}$,

$$\chi'(\vec{q},\omega) = -\frac{1}{\pi}\,\mathrm{Pr}\left[\int_{-\infty}^{\infty} d\omega' \frac{\chi''(\vec{q},\omega)}{\omega-\omega'}\right] \tag{3.10}$$

$$\chi''(\vec{q},\omega) = -\frac{1}{\pi}\,\mathrm{Pr}\left[\int_{-\infty}^{\infty} d\omega' \frac{\chi'(\vec{q},\omega)}{\omega-\omega'}\right] \tag{3.11}$$

or equivalently

$$\chi(\vec{q},\omega) = \lim_{\eta\to 0^+} -\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi(\vec{q},\omega}{\omega-\omega'+i\eta} \tag{3.12}$$

The important message from all of this is that the entire response function $\chi(\vec{q},\omega)$ can be reconstructed from its imaginary (or real) part *alone*.