Physics 219
Summary of linear response theory

I. INTRODUCTION

We apply a small perturbation of strength $f(t)$ which is switched on gradually ("adiabatically") from $t = -\infty$, *i.e.* the amplitude of the perturbation grows as $e^{\epsilon t}$ for $\epsilon \to 0^+$. We assume that the perturbation couples to some operator of the system B, so the additional Hamiltonian due to the perturbation is

$$\Delta\mathcal{H} = -e^{\epsilon t} f(t) B \,. \tag{1}$$

For example, $f(t)$ might be a time dependent magnetic field and B the total magnetization of the system. We wish to compute the response of some operator of the system, A say, to the perturbation. (In many cases A will be the same as B but this is not always the case.) We shall just consider the *linear response* *i.e.* the response to first order in the perturbation. We will show in class, see also Refs. [1–3], that

$$\boxed{\overline{A(t)} = \int_{-\infty}^{t} \chi_{AB}(t-t') e^{\epsilon t'} f(t')\, dt' \,,} \tag{2}$$

where

$$\chi_{AB}(t-t') = \begin{cases} \boxed{\dfrac{i}{\hbar}\, \langle [A(t), B(t')] \rangle} & (t > 0), \\ 0 & (t < 0). \end{cases} \tag{3}$$

Since we define $\chi_{AB}(t) = 0$ for $t < 0$ we can replace the upper limit in Eq. (2) by ∞. The fact that there is no contribution in Eq. (2) for $t' > t$ reflects "causality", *i.e.* the perturbation at time t' cannot effect the system at an *earlier* time t. We denote (equilibrium) averages in the absence of the pertubation by angular brackets $\langle \cdots \rangle$, and averages in the presence of the perturbation by an overbar $\overline{\cdots}$. It will also be convenient to define a function $\phi_{AB}(t)$ to be given by

$$\phi_{AB}(t) = \frac{i}{\hbar}\, \langle [A(t), B(t')] \rangle, \tag{4}$$

for *all* time.

Frequently the perturbation is at a frequency ω, *i.e.* $f(t) = f_\omega e^{-i\omega t}$, in which case the system responds at the same frequency (at least to first order in the perturbation) and we have

$$\boxed{\overline{A_\omega} = \chi_{AB}(\omega + i\epsilon) f_\omega,} \tag{5}$$

where the complex Fourier transform is defined by

$$\boxed{\chi_{AB}(z) = \int_{0}^{\infty} \chi_{AB}(t) e^{izt}\, dt \,,} \qquad (\mathrm{Im}(z) > 0)\,, \tag{6}$$

in which the condition on $\mathrm{Im}(z)$ is needed to ensure convergence of the integral at ∞. We define real and imaginary parts of the physical (*i.e.* $z = \omega + i\epsilon$) response function by $\chi'(\omega)$ and $\chi''(\omega)$ respectively, *i.e.*

$$\boxed{\chi_{AB}(\omega + i\epsilon) = \chi'_{AB}(\omega) + i\chi''_{AB}(\omega)\,.} \tag{7}$$

If A and B are Hermitian (which they will be) then one can show that $\chi_{AB}(t)$ (and hence also $\phi_{AB}(t)$) is real. Furthermore, if A and B have the same signature under time reversal (discussed in class), which will usually be the case, then $\phi_{AB}(t)$ is an odd function of time. From now on we will assume that A and B are Hermitian and have the same signature under time reversal. Except where necessary, we will also omit the subscript AB on the linear response functions.

It is convenient to define a real frequency Fourier transform of $\phi(t)$ in the usual way,

$$\phi(\omega) = \int_{-\infty}^{\infty} \phi(t) e^{i\omega t}\, dt. \tag{8}$$

Comparing Eq. (8) with Eq. (6), and noting that $\phi(t)$ and $\chi(t)$ are the same for $t > 0$ while $\chi(-t) = 0, \phi(-t) = -\phi(t)$ for $t < 0$ we have

$$\phi(\omega) = 2i\chi''(\omega). \tag{9}$$

Fourier transforming back to time, and using Eq. (4) we see that

$$\boxed{\chi''(t) = \frac{1}{2\hbar}\, \langle [A(t), B(t')] \rangle.} \tag{10}$$

II. ANALYTIC PROPERTIES OF THE LINEAR RESPONSE FUNCTION

It is convenient to also define a linear response function $\chi(z)$ also for z in the lower half plane. It then turns out that $\chi(z)$ is an *analytic* function of z everywhere in the complex plane, except along the real axis. This can be seen from the *spectral representation*

$$\boxed{\chi(z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{J(\omega')\, d\omega'}{\omega' - z}\,,} \tag{11}$$

where $J(\omega)$ is called the spectral function and is usually real. Noting that

$$\frac{1}{\omega' - \omega - i\epsilon} = \mathcal{P}\frac{1}{\omega' - \omega} + i\pi\delta(\omega' - \omega)\,, \tag{12}$$

where $\mathcal{P}$ denotes the principal part, we see from Eq. (11) that usually

$$J(\omega) = 2\chi''(\omega), \quad (= -i\phi(\omega))\,, \tag{13}$$

so the spectral function is just (twice) the imaginary part of the response function. The last equality in Eq. (13) comes from Eq. (9). The same argument shows that usually

$$\chi(\omega - i\epsilon) = \chi'(\omega) - i\chi''(\omega)\,, \tag{14}$$

so $\chi(z)$ has a branchcut along the real axis everywhere where $\chi''(\omega)$ is non-zero, and the size of the discontinuity is $2i\chi''(\omega)$.

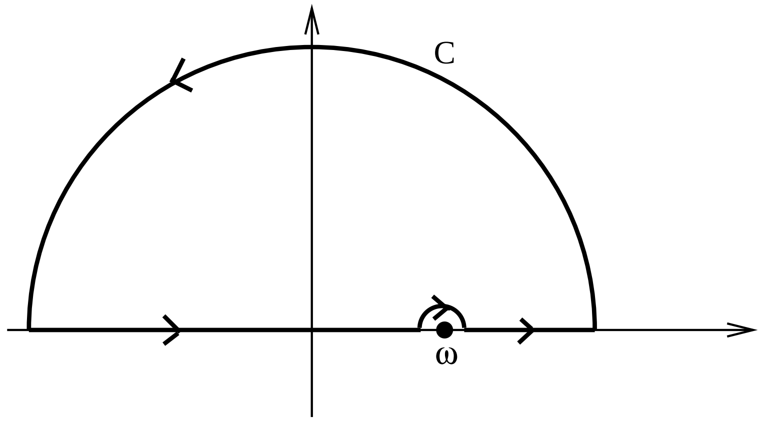

FIG. 1: Contour in the complex frequency (z) plane used to derive the Kramers-Kronig relations. The radius of the outer semicircle tends to infinity. The radius of the small semicircle about $z = \omega$ tends to zero.

III. KRAMERS-KRÖNIG RELATIONS

In the previous section we showed that the linear response function $\chi(z)$ is an analytic function of complex frequency z in the upper-half plane because of causality. We now use this property to derive important relationships between the real and imaginary parts of $\chi(\omega + i\eta) = \chi'(\omega) + i\chi''(\omega)$, due to Kramers and Kronig.

We evaluate

$$\oint_C \frac{\chi(z)}{z-\omega}\, dz\,, \tag{15}$$

over the contour shown in Fig. (1).

Because $\chi(z)$ is analytic inside the region of integration and the pole at $z = \omega$ is also excluded, the integral is 0. The contribution from the "semicircle at infinity" vanishes if $\chi(z) \to 0$ for $z \to \infty$.[4] The integral along the real axis is a principal value integral, and the contribution from the semicircle is $-i\pi$ times the residue at $z = \omega$, *i.e.* $-i\pi\chi(\omega + i\eta) = -i\pi[\chi'(\omega) + i\chi''(\omega)]$. Hence we have

$$\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi'(\omega') + i\chi''(\omega')}{\omega' - \omega}\, d\omega' - i\pi\left[\chi'(\omega) + i\chi''(\omega)\right] = 0\,. \tag{16}$$

Equation real and imaginary parts gives the desired Kramers-Kronig relations:

$$\boxed{\chi'(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega}\, d\omega'\,,} \tag{17}$$

$$\boxed{\chi''(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi'(\omega')}{\omega' - \omega}\, d\omega'\,.} \tag{18}$$

IV. FLUCTUATION DISSIPATION THEOREM

Let us denote the correlation function between $A(t)$ and $B(t')$ by $S_{AB}(t-t')$, *i.e.*

$$S_{AB}(t - t') = \langle A(t)B(t')\rangle. \tag{19}$$

On physical grounds it is clear that S_{AB} only depends on the time difference $t - t'$ and it is easy to show this using the cyclic invariance of the trace. From Eq. (4) we see that the linear response functions are related to the correlation functions by

$$\phi_{AB}(t) = \frac{i}{\hbar} \left[S_{AB}(t) - S_{BA}(-t) \right]. \tag{20}$$

Fourier transforming and using Eq. (9) gives

$$\chi''_{AB}(\omega) = \frac{1}{2\hbar} \left[S_{AB}(\omega) - S_{BA}(\omega) \right]. \tag{21}$$

The two correlation functions on the RHS of Eq. (21) are actually closely related. To see this let us write our the expression for $S_{AB}(t)$ in terms of eigenstates of the system,

$$S_{AB}(t) = \frac{1}{Z} \sum_n e^{-\beta E_n} \sum_m \langle n|A|m\rangle\langle m|B|n\rangle \exp[i(E_n - E_m)t/\hbar], \tag{22}$$

so

$$S_{AB}(\omega) = \frac{2\pi\hbar}{Z} \sum_n e^{-\beta E_n} \sum_m \langle n|A|m\rangle\langle m|B|n\rangle \delta(E_n - E_m + \hbar\omega). \tag{23}$$

Similarly

$$S_{BA}(-\omega) = \frac{2\pi\hbar}{Z} \sum_n e^{-\beta E_n} \sum_m \langle n|B|m\rangle\langle m|A|n\rangle \delta(E_n - E_m - \hbar\omega). \tag{24}$$

Interchanging n with m in the last expression gives

$$S_{BA}(-\omega) = \frac{2\pi\hbar}{Z} \sum_{n,m} e^{-\beta(E_n - E_m)} e^{-\beta E_n} \langle m|B|n\rangle\langle n|A|m\rangle \delta(E_n - E_m + \hbar\omega) \tag{25}$$

$$= e^{-\beta\hbar\omega} S_{AB}(\omega). \tag{26}$$

Substituting into Eq. (21) gives

$$\boxed{\chi''_{AB}(\omega) = \frac{1}{2\hbar} \left(1 - e^{-\beta\hbar\omega}\right) S_{AB}(\omega) \quad \text{(FDT)},} \tag{27}$$

which is known as the fluctuation-dissipation theorem. (The word “dissipation” is used because χ'' is the dissaptive part of the response function, *i.e.* the rate of energy dissipation is proportional to χ''.)

Note that the classical limit corresponds to $|\beta\hbar\omega| \ll 1$, in which case the fluctuation dissipation theorem becomes

$$\phi_{AB}(\omega) = i\beta\omega S_{AB}(\omega), \tag{28}$$

where we used Eq. (9). Fourier transforming back to time, and remembering that $\phi(t) = \chi(t)$ for $t > 0$ we have

$$\boxed{k_B T \chi_{AB}(t) = -\frac{\partial S_{AB}(t)}{\partial t}, \quad \text{(classical FDT)},} \tag{29}$$

where we used the fact that the Fourier transform of $\partial S(t)/\partial t$ is $-i\omega S(\omega)$. If we integrate Eq. (29) from $t = 0$ to ∞ we get

$$k_B T \chi_{AB}(\omega = 0) = S_{AB}(t = 0) - S_{AB}(t = \infty) \,. \tag{30}$$

For $t \to \infty$. the system will have lost the memory of its initial state and so we expect $\lim_{t\to\infty}\langle A(t)B(0)\rangle = \langle A\rangle\langle B\rangle$. Hence Eq. (30) becomes

$$\boxed{k_B T \chi_{AB}(\omega = 0) = \langle AB\rangle - \langle A\rangle\langle B\rangle,} \tag{31}$$

which is a special case of the classical FDT (met already in class) which is easily derived from equilibrium classical statistical mechanics.

V. CONCLUSION

In many body theory, the approach taken is to calculate the linear response function (often called a "Green's function" and defined with an overall minus sign) and then obtain the correlation functions from the fluctuation-dissipation theorem.

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[1] M. Plischke and B. Bergesen *Equilibrium Statistical Mechanics*

[2] W. Marshall and S. W. Lovesey "*Theory of Thermal Neutron Scattering*", Appendix B, Oxford University Press.

[3] Zubarev, Sov. Phys. Uspekhi, **3**, 320 (1960)

[4] If $\chi(z) \to$ const. for $z \to \infty$ then $\chi(z)$ is replaced by $\chi(z) - \chi(\infty)$ in the integrand in Eq. (15) and in the subsequent results.